Comparison of linear and non-linear monotonicity-based shape reconstruction using exact matrix characterizations

Detecting inhomogeneities in the electrical conductivity is a special case of the inverse problem in electrical impedance tomography, that leads to fast direct reconstruction methods. One such method can, under reasonable assumptions, exactly characterize the inhomogeneities based on monotonicity properties of either the Neumann-to-Dirichlet map (non-linear) or its Fréchet derivative (linear). We give a comparison of the non-linear and linear approach in the presence of measurement noise, and show numerically that the two methods give essentially the same reconstruction in the unit disk domain. For a fair comparison, exact matrix characterizations are used when probing the monotonicity relations to avoid errors from numerical solution to PDEs and numerical integration. Using a special factorization of the Neumann-to-Dirichlet map also makes the non-linear method as fast as the linear method in the unit disk geometry.
Computing segmentations directly from x-ray projection data via parametric deformable curves: Paper

We describe an efficient algorithm that computes a segmented reconstruction directly from x-ray projection data. Our algorithm uses a parametric curve to define the segmentation. Unlike similar approaches which are based on level-sets, our method avoids a pixel or voxel grid; hence the number of unknowns is reduced to the set of points that define the curve, and attenuation coefficients of the segments. Our current implementation uses a simple closed curve and is capable of separating one object from the background. However, our basic algorithm can be applied to an arbitrary topology and multiple objects corresponding to different attenuation coefficients in the reconstruction. Through systematic tests we demonstrate a high robustness to the noise, and an excellent performance under a small number of projections.
Near-wellbore modeling of a horizontal well with Computational Fluid Dynamics

The oil production by horizontal wells is a complex phenomenon that involves flow through the porous reservoir, completion interface and the well itself. Conventional reservoir simulators can hardly resolve the flow through the completion into the wellbore. On the contrary, Computational Fluid Dynamics (CFD) is capable of modeling the complex interaction between the creeping reservoir flow and turbulent well flow for single phases, while capturing both the completion geometry and formation damage. A series of single phase steady-state simulations are undertaken, using such fully coupled three dimensional numerical models, to predict the inflow to the well. The present study considers the applicability of CFD for near-wellbore modeling through benchmark cases with available analytical solutions. Moreover, single phase steady-state numerical investigations are performed on a specific perforated horizontal well producing from the Siri field, offshore Denmark. The performance of the well is investigated with an emphasis on the inflow profile and the productivity index for different formation damage scenarios. A considerable redistribution of the inflow profile were found when the filtrate invasion extended beyond the tip of the perforations.

General information

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Organisations: Department of Mechanical Engineering, Scientific Computing, Fluid Mechanics, Coastal and Maritime Engineering, Department of Chemistry, CERE – Center for Energy Resources Engineering, Technical University of Denmark, Lloyd’s Register Consulting
Authors: Szanyi, M. L. (Ekstern), Hemmingsen, C. S. (Intern), Yan, W. (Intern), Walther, J. H. (Intern), Glimberg, S. L. (Ekstern)
Pages: 119-128
Overnight glucose control in people with type 1 diabetes

This paper presents an individualized model predictive control (MPC) algorithm for overnight blood glucose stabilization in people with type 1 diabetes (T1D). The MPC formulation uses an asymmetric objective function that penalizes low glucose levels more heavily. We compute the model parameters in the MPC in a systematic way based on a priori available patient information. The model used by the MPC algorithm for filtering and prediction is an autoregressive integrated moving average with exogenous input (ARIMAX) model implemented as a linear state space model in innovation form. The control algorithm uses frequent glucose measurements from a continuous glucose monitor (CGM) and its decisions are implemented by a continuous subcutaneous insulin infusion (CSII) pump. We provide guidelines for tuning the control algorithm and computing the Kalman gain in the linear state space model in innovation form. We test the controller on a cohort of 100 randomly generated virtual patients with a representative inter-subject variability. We use the same control algorithm for a feasibility overnight study using 5 real patients. In this study, we compare the performance of this control algorithm with the patient’s usual pump setting. We discuss the results of the numerical simulations and the in vivo clinical study from a control engineering perspective. The results demonstrate that the proposed control strategy increases the time spent in euglycemia.

General information

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  ISI indexed (2013): ISI indexed yes
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Evaluation of pharmacokinetic model designs for subcutaneous infusion of insulin aspart

Effective mathematical modelling of continuous subcutaneous infusion pharmacokinetics should aid understanding and control in insulin therapy. Thorough analysis of candidate model performance is important for selecting the appropriate models. Eight candidate models for insulin pharmacokinetics included a range of modelled behaviours, parameters and complexity. The models were compared using clinical data from subjects with type 1 diabetes with continuous subcutaneous insulin infusion. Performance of the models was compared through several analyses: $R^2$ for goodness of fit; the Akaike Information Criterion; a bootstrap analysis for practical identifiability; a simulation exercise for predictability. The simplest model fit poorly to the data ($R^2 = 0.53$), had the highest Akaike score, and worst prediction. Goodness of fit improved with increasing model complexity ($R^2 = 0.85-0.92$) but Akaike scores were similar for these models. Complexity increased practical non-identifiability, where small changes in the dataset caused large variation (CV > 10%) in identified parameters in the most complex models. Best prediction was achieved in a relatively simple model. Some model complexity was necessary to achieve good data fit but further complexity introduced practical non-identifiability and worsened prediction capability. The best model used two linear subcutaneous compartments, an interstitial and plasma compartment, and two identified variables for interstitial clearance and subcutaneous transfer rate. This model had optimal performance trade-off with reasonable fit ($R^2 = 0.85$) and parameterisation, and best prediction and practical identifiability (CV < 2%).
Continuous subcutaneous insulin infusion, Goodness of fit, Parameter identification, Pharmacokinetic modelling, Practical identifiability, Type 1 diabetes

Cauchy Noise Removal by Nonconvex ADMM with Convergence Guarantees

Image restoration is one of the essential tasks in image processing. In order to restore images from blurs and noise while also preserving their edges, one often applies total variation (TV) minimization. Cauchy noise, which frequently appears in engineering applications, is a kind of impulsive and non-Gaussian noise. Removing Cauchy noise can be achieved by solving a nonconvex TV minimization problem, which is difficult due to its nonconvexity and nonsmoothness. In this paper, we adapt recent results in the literature and develop a specific alternating direction method of multiplier to solve this problem. Theoretically, we establish the convergence of our method to a stationary point. Experimental results demonstrate that the proposed method is competitive with other methods in visual and quantitative measures. In particular, our method achieves higher PSNRs for 0.5 dB on average.
A Convex Reconstruction Model for X-ray Tomographic Imaging with Uncertain Flat-fields

Classical methods for X-ray computed tomography are based on the assumption that the X-ray source intensity is known, but in practice, the intensity is measured and hence uncertain. Under normal operating conditions, when the exposure time is sufficiently high, this kind of uncertainty typically has a negligible effect on the reconstruction quality. However, in time- or dose-limited applications such as dynamic CT, this uncertainty may cause severe and systematic artifacts known as ring artifacts. By carefully modeling the measurement process and by taking uncertainties into account, we derive a new convex model that leads to improved reconstructions despite poor quality measurements. We demonstrate the effectiveness of the methodology based on simulated and real data sets.
Adaptive control in an artificial pancreas for people with type 1 diabetes

In this paper, we discuss overnight blood glucose stabilization in patients with type 1 diabetes using a Model Predictive Controller (MPC). We compute the model parameters in the MPC using a simple and systematic method based on a priori available patient information. We describe and compare 3 different model structures. The first model structure is an autoregressive integrated moving average with exogenous input (ARIMAX) structure. The second model structure is an autoregressive moving average with exogenous input (ARMAX) model, i.e. a model without an integrator. The third model structure is an adaptive ARMAX model in which we use a recursive extended least squares (RELS) method to estimate parameters of the stochastic part. In addition, we describe some safety layers in the control algorithm that improve the controller robustness and reduce the risk of hypoglycemia. We test and compare our control strategies using a virtual clinic of 100 randomly generated patients with a representative inter-subject variability. This virtual clinic is based on the Hovorka model. We consider the case where only half of the meal bolus is administered at mealtime, and the case where the insulin sensitivity increases during the night. The numerical results suggest that the use of an integrator leads to higher occurrence of hypoglycemia than for the controllers without the integrator. Compared to other control strategies, the adaptive MPC reduces both the time spent in hypoglycemia and the time spent in hyperglycemia.
The purpose of this study is to develop an adaptive unscented Kalman filter (UKF) by tuning the measurement noise covariance. We use the maximum likelihood estimation (MLE) and the covariance matching (CM) method to estimate the noise covariance. The multi-step prediction errors generated by the UKF are used for covariance estimation by MLE and CM. Then we apply the two covariance estimation methods on an example application. In the example, we identify the covariance of the measurement noise for a continuous glucose monitoring (CGM) sensor. The sensor measures the subcutaneous glucose concentration for a type 1 diabetes patient. The root-mean square (RMS) error and the computation time are used to compare the performance of the two covariance estimation methods. The results indicate that as the prediction horizon expands, the RMS error for the MLE declines, while the error remains relatively large for the CM method. For larger prediction horizons, the MLE provides an estimate of the noise covariance that is less biased than the estimate by the CM method. The CM method is computationally less expensive though.

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Model predictive control, Adaptive control, Artificial pancreas, Type 1 diabetes, Closed-loop glucose control

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Adaptive Unscented Kalman Filter using Maximum Likelihood Estimation

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Number of pages: 6
A deep learning approach to adherence detection for type 2 diabetics

Diabetes has become one of the biggest health problems in the world. In this context, adherence to insulin treatment is essential in order to avoid life-threatening complications. In this pilot study, a novel adherence detection algorithm using Deep Learning (DL) approaches was developed for type 2 diabetes (T2D) patients, based on simulated Continuous Glucose Monitoring (CGM) signals. A large and diverse amount of CGM signals were simulated for T2D patients using a T2D adapted version of the Medtronic Virtual Patient (MVP) model for T1D. By using these signals, different classification algorithms were compared using a comprehensive grid search. We contrast a standard logistic regression baseline to Multi-Layer Perceptrons (MLPs) and Convolutional Neural Networks (CNNs). The best classification performance with an average accuracy of 77.5% was achieved with CNN. Hence, this indicates the potential of DL, when considering adherence detection systems for T2D patients.
Adiabatic continuous stirred tank reactor

The present report documents the adiabatic CSTR experimental setup after it was refurbished in September 2017. The goal of the refurbishment was firstly to enable computer control of the experiment using the Open Process Control Unified Architecture (OPC-UA) standard, and secondly to improve the experiment for use in course 28845 Chemical Reaction Engineering Laboratory.

Initially the experimental setup is described in terms of programmable logic controller (PLC) hardware, laboratory apparatus and software. This is followed by a description of how to connect to the PLC via OPC-UA.

The appendix contains an experimental guide for use in course 28845, step-by-step instructions on how to control the setup with a computer, sample code and datasheets.

A high-performance Riccati based solver for tree-structured quadratic programs

Robust multi-stage Model Predictive Control (MPC) is an increasingly popular approach to handle model uncertainties due to the simplicity of its problem formulation and other attractive properties. However, the exponential growth of the problem dimensions with respect to the robust horizon renders the online solution of such problems challenging and the development of tailored solvers crucial. In this paper, an interior point method is presented that can solve Quadratic Programs (QPs) arising in multi-stage MPC efficiently by means of a tree-structured Riccati recursion and a high-performance linear algebra library. A performance comparison with code-generated and general purpose sparse QP solvers shows that the computation times can be significantly reduced for all problem sizes that are practically relevant in embedded MPC applications. The presented implementation is freely available as part of the open-source software HPMPC.
We present a MATLAB software package with efficient, robust, and flexible implementations of algebraic iterative reconstruction (AIR) methods for computing regularized solutions to discretizations of inverse problems. These methods are of particular interest in computed tomography and similar problems where they easily adapt to the particular geometry of the problem. All our methods are equipped with stopping rules as well as heuristics for computing a good relaxation parameter, and we also provide several test problems from tomography. The package is intended for users who want to experiment with algebraic iterative methods and their convergence properties. The present software is a much expanded and improved version of the package AIR Tools from 2012, based on a new modular design. In addition to improved performance and memory use, we provide more flexible iterative methods, a column-action method, new test problems, new demo functions, and perhaps most importantly the ability to use function handles instead of (sparse) matrices, allowing larger problems to be handled.

**General information**

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Authors: Hansen, P. C. (Intern), Jørgensen, J. S. (Ekstern)
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A least squares approach for efficient and reliable short-term versus long-term optimization

The uncertainties related to long-term forecasts of oil prices impose significant financial risk on ventures of oil production. To minimize risk, oil companies are inclined to maximize profit over short-term horizons ranging from months to a few years. In contrast, conventional production optimization maximizes long-term profits over horizons that span more than a decade. To address this challenge, the oil literature has introduced short-term versus long-term optimization. Ideally, this problem is solved by a posteriori multi-objective optimization methods that generate an approximation to the Pareto front of optimal short-term and long-term trade-offs. However, such methods rely on a large number of reservoir simulations and scale poorly with the number of objectives subject to optimization. Consequently, the large-scale nature of production optimization severely limits applications to real-life scenarios. More practical alternatives include ad hoc hierarchical switching schemes. As a drawback, such methods lack robustness due to unclear convergence properties and do not naturally generalize to cases of more than two objectives. Also, as this paper shows, the hierarchical formulation may skew the balance between the objectives, leaving an unfulfilled potential to increase profits. To promote efficient and reliable short-term versus long-term optimization, this paper introduces a natural way to characterize desirable Pareto points and proposes a novel least squares (LS) method. Unlike hierarchical approaches, the method is guaranteed to converge to a Pareto optimal point. Also, the LS method is designed to properly balance multiple objectives, independently of Pareto front’s shape. As such, the method poses a practical alternative to a posteriori methods in situations where the
frontier is intractable to generate.

**General information**

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Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Informatics and Mathematical Modeling, Copenhagen Center for Health Technology
Authors: Christiansen, L. H. (Intern), Capolei, A. (Intern), Jørgensen, J. B. (Intern)
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- Web of Science (2012): Indexed yes
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- Scopus rating (2011): SJR 0.691 SNIP 1.01 CiteScore 1.92
- ISI indexed (2011): ISI indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 0.741 SNIP 1.266
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.122 SNIP 1.787
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- Scopus rating (2008): SJR 0.664 SNIP 1.548
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- Scopus rating (2005): SJR 0.807 SNIP 1.376
- Scopus rating (2004): SJR 1.689 SNIP 1.182
- Scopus rating (2003): SJR 0.598 SNIP 1.08
- Scopus rating (2002): SJR 0.466 SNIP 0.886
- Scopus rating (2001): SJR 0.822 SNIP 0.995
- Scopus rating (2000): SJR 0.463 SNIP 0.781
- Scopus rating (1999): SJR 0.478 SNIP 0.499
An Adaptive Nonlinear Basal-Bolus Calculator for Patients With Type 1 Diabetes

Background: Bolus calculators help patients with type 1 diabetes to mitigate the effect of meals on their blood glucose by administering a large amount of insulin at mealtime. Intraindividual changes in patients physiology and nonlinearity in insulin-glucose dynamics pose a challenge to the accuracy of such calculators.

Method: We propose a method based on a continuous-discrete unscented Kalman filter to continuously track the postprandial glucose dynamics and the insulin sensitivity. We augment the Medtronic Virtual Patient (MVP) model to simulate noise-corrupted data from a continuous glucose monitor (CGM). The basal rate is determined by calculating the steady state of the model and is adjusted once a day before breakfast. The bolus size is determined by optimizing the postprandial glucose values based on an estimate of the insulin sensitivity and states, as well as the announced meal size. Following meal announcements, the meal compartment and the meal time constant are estimated, otherwise insulin sensitivity is estimated.

Results: We compare the performance of a conventional linear bolus calculator with the proposed bolus calculator. The proposed basal-bolus calculator significantly improves the time spent in glucose target ($P < .01$) compared to the conventional bolus calculator.

Conclusion: An adaptive nonlinear basal-bolus calculator can efficiently compensate for physiological changes. Further clinical studies will be needed to validate the results.
An algorithm for gradient-based dynamic optimization of UV flash processes

This paper presents a novel single-shooting algorithm for gradient-based solution of optimal control problems with vapor-liquid equilibrium constraints. Such optimal control problems are important in several engineering applications, for instance in control of distillation columns, in certain two-phase flow problems, and in operation of oil reservoirs. The single-shooting algorithm uses an adjoint method for the computation of gradients. Furthermore, the algorithm uses either a simultaneous or a nested approach for the numerical solution of the dynamic vapor-liquid equilibrium model equations. Two numerical examples illustrate that the simultaneous approach is faster than the nested approach and that the efficiency of the underlying thermodynamic computations is important for the overall performance of the single-shooting algorithm. We compare the performance of different optimization software as well as the performance of different compilers in a Linux operating system. The tests indicate that real-time nonlinear model predictive control of UV flash processes is computationally feasible.

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Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Ritschel, T. K. S. (Intern), Capolei, A. (Intern), Gaspar, J. (Intern), Jørgensen, J. B. (Intern)
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Web of Science (2014): Indexed yes
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An efficient and rigorous thermodynamic library and optimal-control of a cryogenic air separation unit

Cryogenic air separation (CAS) is the leading technology for large scale production of pure N2, O2 and Ar. This process is very electric-energy intensive; thus it is a likely candidate for load balancing of power stations in a smart grid. This type of intermittent operation of CAS, requires a non-linear model based control to achieve optimal techno-economic performance. Accordingly, this work presents a computationally efficient and novel approach for solving a tray-by-tray equilibrium model and its implementation for open-loop optimal-control of a cryogenic distillation column. Here, the optimisation objective is to reduce the cost of compression in a volatile electricity market while meeting the production requirements, i.e. product flow rate and purity. This model is implemented in Matlab and uses the ThermoLib rigorous thermodynamic library. The present work represents a first step towards plant-wide dynamic modelling and smart control of a cryogenic distillation plant.

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering
Authors: Gaspar, J. (Intern), Ritschel, T. K. S. (Intern), Jørgensen, J. B. (Intern)
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An experimentally validated simulation model for a four-stage spray dryer

In this paper, we develop a dynamic model of an industrial type medium size four-stage spray dryer. The purpose of the model is to enable simulations of the spray dryer at different operating points, such that the model facilitates development and comparison of control strategies. The dryer is divided into four consecutive stages: a primary spray drying stage, two heated fluid bed stages, and a cooling fluid bed stage. Each of these stages in the model is assumed ideally mixed and the dynamics are described by mass- and energy balances. These balance equations are coupled with constitutive equations such as a thermodynamic model, the water evaporation rate, the heat transfer rates, and an equation for the stickiness of the powder (glass transition temperature). Laboratory data is used to model the equilibrium moisture content and the glass transition temperature of the powder. The resulting mathematical model is an index-1 differential algebraic equation (DAE) model with 12 states, 9 inputs, 8 disturbances, and 30 parameters. The parameters in the model are identified from well-excited experimental data obtained from the industrial type spray dryer. The simulated outputs of the model are validated using independent well-excited experimental data from the same spray dryer. The simulated temperatures, humidities, and residual moistures in the spray dryer compare well to the validation data. The model also provides the profit of operation, the production rate, the energy consumption, and the energy efficiency. In addition, it computes stickiness of the powder in different stages of the spray dryer. These facilities make the model well suited as a simulation model for comparison of the process economics associated to different control strategies.
A Novel Approach for Risk Minimization in Life-Cycle Oil Production Optimization

The oil research community has invested much effort into computer aided optimization to enhance oil recovery. While simulation studies have demonstrated the potential of model-based technology to improve industrial standards, the largely unknown geology of subsurface reservoirs limits applications to commercial oil fields. In particular, uncertain model descriptions lead to risks of profit loss. To address the challenges of geological uncertainty, this paper proposes offset risk minimization. As opposed to existing methodologies of the oil literature, the offset approach minimizes risk of profit loss relative to industrial standards. A numerical case study compares the offset approach to a representative selection of current state-of-the-art methodologies. The results show that the offset approach offers the overall lowest risk of profit loss relative to industrial best practices. This suggests that it may be more relevant to consider offset risk minimization than conventional ensemble-based methods for the purpose of life-cycle production optimization.

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A Riccati-Based Interior Point Method for Efficient Model Predictive Control of SISO Systems

This paper presents an algorithm for Model Predictive Control of SISO systems. Based on a quadratic objective in addition to (hard) input constraints it features soft upper as well as lower constraints on the output and an input rate-of-change penalty term. It keeps the deterministic and stochastic model parts separate. The controller is designed based on the deterministic model, while the Kalman filter results from the stochastic part. The controller is implemented as a primal-dual interior point (IP) method using Riccati recursion and the computational savings possible for SISO systems. In particular the computational complexity scales linearly with the control horizon. No warm-start strategies are considered. Numerical examples are included illustrating applications to Artificial Pancreas technology. We provide typical execution times for a single iteration of the IP algorithm and the number of iterations required for convergence in different situations.

General information
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Scopus rating (2006): SJR 0.101 SNIP 0.005
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Artifacts and Visible Singularities in Limited Data X-Ray Tomography

We describe a principle to determine which features of an object will be easy to reconstruct from limited X-ray CT data and which will be difficult. The principle depends on the geometry of the data set, and it applies to any limited data set. We also describe a characterization of Frikel and the author explaining artifacts that can be added to limited angle reconstructions, and we provide an easy-to-implement method to decrease them. These ideas are justified using microlocal analysis, deep mathematics that involves Fourier theory. Reconstructions from simulated and real limited data are given to illustrate our ideas.

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Quinto, T. (Intern)
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Scopus rating (2015): SJR 0.178 SNIP 0.788 CiteScore 0.59
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.156 SNIP 0.868 CiteScore 1.09
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.194 SNIP 0.617 CiteScore 0.59
ISI indexed (2013): ISI indexed no
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Scopus rating (2012): SJR 0.165 SNIP 0.486 CiteScore 0.79
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.111 SNIP 0.425 CiteScore 0.47
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.426 SNIP 1.298
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.372 SNIP 1.142
BFI (2008): BFI-level 1
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Scopus rating (2007): SJR 0.207 SNIP 1.023
Scopus rating (2006): SJR 0.162 SNIP 0.378

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A Thermodynamic Library for Simulation and Optimization of Dynamic Processes

Process system tools, such as simulation and optimization of dynamic systems, are widely used in the process industries for development of operational strategies and control for process systems. These tools rely on thermodynamic models and many thermodynamic models have been developed for different compounds and mixtures. However, rigorous thermodynamic models are generally computationally intensive and not available as open-source libraries for process simulation and optimization. In this paper, we describe the application of a novel open-source rigorous thermodynamic library, ThermoLib, which is designed for dynamic simulation and optimization of vapor-liquid processes. ThermoLib is implemented in Matlab and C and uses cubic equations of state to compute vapor and liquid phase thermodynamic properties. The novelty of ThermoLib is that it provides analytical first and second order derivatives. These derivatives are needed for efficient dynamic simulation and optimization. The analytical derivatives improve the computational performance by a factor between 12 and 35 as compared to finite difference approximations. We present two examples that use ThermoLib routines in their implementations: (1) simulation of a vapor-compression cycle, and (2) optimal control of an isoenergetic-isochoric flash separation process. The ThermoLib software used in this paper is distributed as open-source software at www.psetools.org.

General information
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Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Ritschel, T. K. S. (Intern), Gaspar, J. (Intern), Jørgensen, J. B. (Intern)
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Scopus rating (2012): SJR 0.247 SNIP 0.278
Scopus rating (2011): SJR 0.257 SNIP 0.312
Scopus rating (2010): SJR 0.196 SNIP 0.26
Scopus rating (2009): SJR 0.215 SNIP 0.296
Scopus rating (2008): SJR 0.125 SNIP 0.105
Scopus rating (2007): SJR 0.126 SNIP 0.065
Scopus rating (2006): SJR 0.101 SNIP 0.005
Scopus rating (2005): SJR 0.21 SNIP 0.467
Scopus rating (2004): SJR 0.268 SNIP 0.432
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Bounds on the stably recoverable information for the Helmholtz equation in $\mathbb{R}^2$

General information
C code generation applied to nonlinear model predictive control for an artificial pancreas

This paper presents a method to generate C code from MATLAB code applied to a nonlinear model predictive control (NMPC) algorithm. The C code generation uses the MATLAB Coder Toolbox. It can drastically reduce the time required for development compared to a manual porting of code from MATLAB to C, while ensuring a reliable and fairly optimized code. We present an application of code generation to the numerical solution of nonlinear optimal control problems (OCP). The OCP uses a sequential quadratic programming algorithm with multiple shooting and sensitivity computation. We consider the problem of glucose regulation for people with type 1 diabetes as a case study. The average computation time when using generated C code is 0.21 s (MATLAB: 1.5 s), and the maximum computation time when using generated C code is 0.97 s (MATLAB: 5.7 s). Compared to the MATLAB implementation, generated C code can run in average more than 7 times faster.

Comparison of three control strategies for optimization of spray dryer operation

Spray drying is the preferred process to reduce the water content of many chemicals, pharmaceuticals, and foodstuffs. A significant amount of energy is used in spray drying to remove water and produce a free flowing powder product. In this paper, we present and compare the performance of three controllers for operation of a four-stage spray dryer. The three controllers are a proportional-integral (PI) controller that is used in industrial practice for spray dryer operation, a linear model predictive controller with real-time optimization (MPC with RTO, MPC-RTO), and an economically optimizing nonlinear model predictive controller (E-NMPC). The MPC with RTO is based on the same linear state space model in the MPC and the RTO layer. The E-NMPC consists of a single optimization layer that uses a nonlinear system of ordinary differential equations for its predictions. The PI control strategy has a fixed target that is independent of the disturbances, while the MPC-RTO and the E-NMPC adapt the operating point to the disturbances. The goal of spray dryer operation is to optimize the profit of operation in the presence of feed composition and ambient air humidity variations; i.e. to maximize the production rate, while minimizing the energy consumption, keeping the residual moisture content of the powder below a maximum limit, and avoiding that the powder sticks to the chamber walls. We use an industrially recorded disturbance scenario in order to produce realistic simulations and conclusions. The key performance indicators such as the profit of operation, the product flow rate, the specific energy
consumption, the energy efficiency, and the residual moisture content of the produced powder are computed and compared for the three controllers. In this simulation study, we find that the economic performance of the MPC with RTO as well as the E-NMPC is considerably improved compared to the PI control strategy used in industrial practice. The MPC with RTO improves the profit of operation by 8.61%, and the E-NMPC improve.

General information
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Organisations: Scientific Computing, Department of Applied Mathematics and Computer Science, Dynamical Systems, Department of Electrical Engineering, Automation and Control, GEA Process Engineering A/S
Authors: Petersen, L. N. (Intern), Poulsen, N. K. (Intern), Niemann, H. H. (Intern), Utzen, C. (Ekstern), Jørgensen, J. B. (Intern)
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Scopus rating (2015): SJR 1.338 SNIP 2.028 CiteScore 3.35
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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.521 SNIP 2.735 CiteScore 3.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.507 SNIP 2.607 CiteScore 3.47
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
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ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.316 SNIP 2.59 CiteScore 2.9
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.305 SNIP 2.203
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.282 SNIP 2.772
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 1.458 SNIP 2.698
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.425 SNIP 2.086
Scopus rating (2006): SJR 1.739 SNIP 2.369
Scopus rating (2005): SJR 1.016 SNIP 2.362
Scopus rating (2004): SJR 1.019 SNIP 1.824
Scopus rating (2003): SJR 1.617 SNIP 2.247
Computation of Phase Equilibrium and Phase Envelopes

In this technical report, we describe the computation of phase equilibrium and phase envelopes based on expressions for the fugacity coefficients. We derive those expressions from the residual Gibbs energy. We consider 1) ideal gases and liquids modeled with correlations from the DIPPR database and 2) nonideal gases and liquids modeled with cubic equations of state. Next, we derive the equilibrium conditions for an isothermal-isobaric (constant temperature, constant pressure) vapor-liquid equilibrium process (PT flash), and we present a method for the computation of phase envelopes. We formulate the involved equations in terms of the fugacity coefficients. We present expressions for the first-order derivatives. Such derivatives are necessary in computationally efficient gradient-based methods for solving the vapor-liquid equilibrium equations and for computing phase envelopes. Finally, we describe a Matlab program that computes the phase envelope of a mixture. We present the source code and discuss practical details of the implementation.

Cross-Validation of a Glucose-Insulin-Glucagon Pharmacodynamics Model for Simulation using Data from Patients with Type 1 Diabetes

Background:
Currently, no consensus exists on a model describing endogenous glucose production (EGP) as a function of glucagon concentrations. Reliable simulations to determine the glucagon dose preventing or treating hypoglycemia or to tune a dual-hormone artificial pancreas control algorithm need a validated glucoregulatory model including the effect of glucagon.

Methods:
Eight type 1 diabetes (T1D) patients each received a subcutaneous (SC) bolus of insulin on four study days to induce mild hypoglycemia followed by a SC bolus of saline or 100, 200, or 300 µg of glucagon. Blood samples were analyzed for concentrations of glucagon, insulin, and glucose. We fitted pharmacokinetic (PK) models to insulin and glucagon data using maximum likelihood and maximum a posteriori estimation methods. Similarly, we fitted a pharmacodynamic (PD) model to glucose data. The PD model included multiplicative effects of insulin and glucagon on EGP. Bias and precision of PD model test fits were assessed by mean predictive error (MPE) and mean absolute predictive error (MAPE).

Results:
Assuming constant variables in a subject across nonoutlier visits and using thresholds of ±15% MPE and 20% MAPE, we accepted at least one and at most three PD model test fits in each of the seven subjects. Thus, we successfully validated the PD model by leave-one-out cross-validation in seven out of eight T1D patients.

Conclusions:
The PD model accurately simulates glucose excursions based on plasma insulin and glucagon concentrations. The reported PK/PD model including equations and fitted parameters allows for in silico experiments that may help improve diabetes treatment involving glucagon for prevention of hypoglycemia.

**General information**

**State:** Published  
**Organisations:** Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Copenhagen Center for Health Technology, Center for Energy Resources Engineering, Copenhagen University Hospital, Zealand Pharma A/S  
**Authors:** Wendt, S. L. (Intern), Ranjan, A. (Forskerdatabase), Møller, J. K. (Intern), Schmidt, S. (Ekstern), Boye Knudsen, C. (Ekstern), Holst, J. J. (Ekstern), Madsbad, S. (Ekstern), Madsbad, S. (Ekstern), Madsen, H. (Intern), Nørgaard, K. (Ekstern), Jørgensen, J. B. (Intern)  
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- Scopus rating (2014): SJR 0.871 SNIP 0.971 CiteScore 1.84  
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- ISI indexed (2013): ISI indexed no  
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- Scopus rating (2012): SJR 0.69 SNIP 0.972 CiteScore 1.33  
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- BFI (2011): BFI-level 1  
- Scopus rating (2011): SJR 0.687 SNIP 0.916 CiteScore 0.6  
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- Scopus rating (2010): SJR 0.452 SNIP 0.683  
- BFI (2009): BFI-level 1  
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**Original language:** English  
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**Data Descriptor: A multiscale imaging and modelling dataset of the human inner ear**

Understanding the human inner ear anatomy and its internal structures is paramount to advance hearing implant technology. While the emergence of imaging devices allowed researchers to improve understanding of intracochlear
Design, economics and parameter uncertainty in dynamic operation of post-combustion CO₂ capture using piperazine (PZ) and MEA

Post-combustion capture is a promising solution to mitigate the anthropogenic CO₂ emission rate and reduce global warming. However, to make it economically attractive, the techno-economic performance of this process needs to be improved. This includes steady-state but also dynamic operation of the plant. Flexibility is particularly crucial from an economic and operational point of view since plants must balance the power production and the electricity demand on a daily basis.

This work shows the impact of design decisions and uncertainties on the dynamic operation and economics of a CO₂ capture plant using piperazine (PZ), compared to the benchmark MEA solvent. This is exemplified through dynamic model calculations. The results show that the capacity of the buffer tank is a key parameter for the flexibility of the plant. A small tank corresponds to lower capital cost but it leads to increased operation cost and also to flexibility/controllability issues. Both, the PZ and MEA plants present inverse response for small tanks. These plants are challenging to control.
Directional Total Generalized Variation Regularization for Impulse Noise Removal

A recently suggested regularization method, which combines directional information with total generalized variation (TGV), has been shown to be successful for restoring Gaussian noise corrupted images. We extend the use of this regularizer to impulse noise removal and demonstrate that using this regularizer for directional images is highly advantageous. In order to estimate directions in impulse noise corrupted images, which is much more challenging compared to Gaussian noise corrupted images, we introduce a new Fourier transform-based method. Numerical experiments show that this method is more robust with respect to noise and also more efficient than other direction estimation methods.
Distinguishability Revisited: Depth Dependent Bounds on Reconstruction Quality in Electrical Impedance Tomography: Depth dependent bounds on reconstruction quality in electrical impedance tomography

The reconstruction problem in electrical impedance tomography is highly ill-posed, and it is often observed numerically that reconstructions have poor resolution far away from the measurement boundary but better resolution near the measurement boundary. The observation can be quantified by the concept of distinguishability of inclusions. This paper provides mathematically rigorous results supporting the intuition. Indeed, for a model problem lower and upper bounds on the distinguishability of an inclusion are derived in terms of the boundary data. These bounds depend explicitly on the distance of the inclusion to the boundary, i.e. the depth of the inclusion. The results are obtained for disk inclusions in a homogeneous background in the unit disk. The theoretical bounds are verified numerically using a novel, exact characterization of the forward map as a tridiagonal matrix.

General information
State: Published
Organisations: Scientific Computing, Applied functional analysis, Department of Applied Mathematics and Computer Science
Authors: Garde, H. (Intern), Knudsen, K. (Intern)
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BFI (2017): BFI-level 2
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Scopus rating (2016): SJR 1.046 SNIP 1.311 CiteScore 1.76
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.945 SNIP 1.222 CiteScore 1.63
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.09 SNIP 1.271 CiteScore 1.58
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.972 SNIP 1.151 CiteScore 1.61
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.028 SNIP 1.251 CiteScore 1.69
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.798 SNIP 1.193 CiteScore 1.49
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.8 SNIP 1.078
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.191 SNIP 1.539
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.101 SNIP 1.215
Scopus rating (2007): SJR 0.975 SNIP 1.262
In this paper, we propose a distributed algorithm for solving coupled problems with chordal sparsity or an inherent tree structure which relies on primal–dual interior-point methods. We achieve this by distributing the computations at each iteration, using message-passing. In comparison to existing distributed algorithms for solving such problems, this algorithm requires far fewer iterations to converge to a solution with high accuracy. Furthermore, it is possible to compute an upper-bound for the number of required iterations which, unlike existing methods, only depends on the coupling structure in the problem. We illustrate the performance of our proposed method using a set of numerical examples.
UV ash processes, also referred to as isoenergetic-isochoric ash processes, occur for dynamic simulation and optimization of vapor-liquid equilibrium processes. Dynamic optimization and nonlinear model predictive control of distillation columns, certain two-phase ow problems, as well as oil reservoirs with signiﬁcant compositional and thermal eﬀects may be conducted as dynamic optimization of UV ash processes. The dynamic optimization problem involving a UV ash problem is formulated as a bilevel optimization problem. This problem is solved using a gradient based single-shooting method. The gradients are computed using the adjoint method and diﬀerent oﬀ-the-shelf optimization software (fmincon, IPOPT, KNITRO, NPSOL) are used for the numerical optimization. Computational results are reported for a ash process involving benzene, toluene and diphenyl. The computational experiments demonstrate that the optimization solver, the compiler, and high-performance linear algebra software are all important for eﬃcient dynamic optimization of UV ash processes.
Economic MPC based on LPV model for thermostatically controlled loads

Rapid increase of the renewable energy share in electricity production requires optimization and flexibility of the power consumption side. Thermostatically controlled loads (TCLs) have a large potential for regulation service provision. Economic model predictive control (MPC) is an advanced control method which can be used to synchronize the power consumption with undispachable renewable electricity production. Thermal behavior of TCLs can be described by linear models based on energy balance of the system. In some cases, parameters of the model may be time-varying. In this work, we present a modified economic MPC based on linear parameter-varying model. In particular, we provide an exact transformation from a standard economic MPC formulation to a linear program. We assume that the variables influencing the model parameters are known (predictable) for the prediction horizon of the controller. As a case study, we present control system that minimizes operational cost of swimming pool heating system, where parameters of the model depend on the weather forecast. Simulation results demonstrate that the proposed method is able to deal with this kind of systems.

General information
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Organisations: Department of Applied Mathematics and Computer Science, Dynamical Systems, Scientific Computing, Technical University of Liberec, Novosibirsk State Technical University
Authors: Zemtsov, N. (Ekstern), Hlava, J. (Ekstern), Frantsuzova, G. (Ekstern), Madsen, H. (Intern), Junker, R. G. (Intern), Jørgensen, J. B. (Intern)
Number of pages: 5
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Economic Optimizing Control for Single-Cell Protein Production in a U-Loop Reactor

The production of single-cell protein (SCP) in a U-loop reactor by a methanotroph is a cost efficient sustainable alternative to protein from fish meal obtained by over-fishing the oceans. SCP serves as animal feed. In this paper, we present a mathematical model that describes the dynamics of SCP production in a U-loop reactor. We use this model to compute an optimal start-up trajectory by solution of an economic optimizing optimal control problem. The optimal start-up trajectory is an unstable attractor. The practical implementation of this optimal start-up trajectory can be conducted by a proportional controller for the substrate concentration in the top tank of the U-loop reactor.

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, Centre for oil and gas – DTU, Technical University of Denmark
Authors: Drejer, A. (Ekstern), Ritschel, T. K. S. (Intern), Jørgensen, S. B. (Intern), Jørgensen, J. B. (Intern)
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Fault and meal detection by redundant continuous glucose monitors and the unscented Kalman filter
The purpose of this study is to develop a method for detecting and compensating the anomalies of continuous glucose monitoring (CGM) sensors as well as detecting unannounced meals. Both features, sensor fault detection/correction and meal detection, are necessary to have a reliable artificial pancreas. The aim is to investigate the best detection results achievable with the proposed detection configuration in a perfect situation, and to have the results as a benchmark against which the imperfect scenarios of the proposed fault detection can be compared. The perfect situation that we set up here is in terms of a patient simulation model, where the model in the detector is the same as the patient simulation model used for evaluation of the detector. The detection module consists of two CGM sensors, two fault detectors, a fault isolator, and an adaptive unscented Kalman filter (UKF). Two types of sensor faults, i.e., drift and pressure induced sensor attenuation (PISA), are simulated by a Gaussian random walk model. Each of the fault detectors has a local UKF that receives the signal from the associated sensor, detects faults, and finally tunes the adaptive UKF. A fault isolator that accepts data from the two fault detectors differentiates between a sensor fault and an unannounced meal appearing as an anomaly in the CGM data. If the fault isolator indicates a sensor fault, a method based on the covariance matching technique tunes the covariance of the measurement noise associated with the faulty sensor. The main UKF uses the tuned noise covariances and fuses the CGM data from the two sensors. The drift detection sensitivity and specificity are 80.9% and 92.6%, respectively. The sensitivity and specificity of PISA detection are 78.1% and 82.7%, respectively. The fault detectors can detect 100 out of 100 simulated drifts and 485 out of 500 simulated PISA events. Compared to a nonadaptive UKF, the adaptive UKF reduces the deviation of the CGM measurements from their paired blood glucose concentrations from 72.0% to 12.5% when CGM is corrupted by drift, and from 10.7% to 6.8% when CGM is corrupted by PISA. The fault isolator can detect 199 out of 200 unannounced meals. The average change in the glucose concentrations between the meals and the detection time points is 46.3 mg/dL.
Finite volume method room acoustic simulations integrated into the architectural design process

In many cases, room acoustics are neglected during the early stage of building design. This can result in serious acoustical problems that could have been easily avoided and can be difficult or expensive to remedy at later stages. Ideally, the room acoustic design should interact with the architectural design from the earliest design stage, as a part of a holistic design process. A new procedure to integrate room acoustics into architectural design is being developed in a Ph.D. project, with the aim of promoting this early stage holistic design process. This project aims to develop a new hybrid simulation tool combining wave-based and geometrical acoustics methods. One of the important aspects is the flexibility to represent realistic geometric shapes, for which the finite volume method (FVM) is chosen for the wave-based part of the tool. As a starting point, the computational efficiency of high-order two-dimensional FVM for defining an efficient wave-based simulation tool is investigated. Preliminary two-dimensional FVM simulation results are presented, which illuminate the suitability for handling complex geometries compared to other wave based simulation methods.

General information
State: Published
Authors: Pind Jörgensson, F. K. (Intern), Jeong, C. (Intern), Engsig-Karup, A. P. (Intern), Strømann-Andersen, J. (Ekstern)
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 1.83 SJR 0.749 SNIP 1.27
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.802 SNIP 1.437 CiteScore 1.77
Web of Science (2015): Indexed yes
Hardware Tailored Linear Algebra for Implicit Integrators in Embedded NMPC.

Nonlinear Model Predictive Control (NMPC) requires the efficient treatment of the dynamic model in the form of a system of continuous-time differential equations. Newton-type optimization relies on a numerical simulation method in addition to the propagation of first or higher order derivatives. In the case of stiff or implicitly defined dynamics, implicit integration schemes are typically preferred. This paper proposes a tailored implementation of the necessary linear algebra routines (LU factorization and triangular solutions), in order to allow for a considerable computational speedup of such integrators.
In particular, the open-source BLASFEO framework is presented as a library of efficient linear algebra routines for small to medium-scale embedded optimization applications. Its performance is illustrated on the nonlinear optimal control example of a chain of masses. The proposed library allows for considerable speedups and it is found to be overall competitive with both a code-generated solver and a high-performance BLAS implementation.

General information
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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, University of Freiburg
Authors: Frison, G. (Intern), Quirynen, R. (Ekstern), Zanelli, A. (Ekstern), Diehl, M. (Ekstern), Jørgensen, J. B. (Intern)
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Helbredstjek af dansk sundhedsteknologi: Sektorudviklingsrapport
Sådan kan samarbejde mellem industrien, universiteterne og sundhedsvæsenet skabe gode løsninger til forebyggelse, diagnostik, patientbehandling og rehabilitering

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Image fusion and denoising using fractional-order gradient information

Image fusion and denoising are significant in image processing because of the availability of multi-sensor and the presence of the noise. The first-order and second-order gradient information have been effectively applied to deal with fusing the noiseless source images. In this paper, due to the advantage of the fraction-order derivative, we first integrate the fractional order gradients of noisy source images as the target fraction-order feature, and make it fit with the fractional-order gradient of the fused image. Then we introduce the total variation (TV) regularization for removing the noise. By adding the data fitting term between the fused image and a preprocessed image, a new convex variational model is proposed for fusing the noisy source images. Furthermore, an alternating direction method of multiplier (ADMM) is developed for solving the proposed variational model. Numerical experiments show that the proposed method outperforms the conventional total variation in methods for simultaneously fusing and denoising.

Image reconstruction under non-Gaussian noise

During acquisition and transmission, images are often blurred and corrupted by noise. One of the fundamental tasks of image processing is to reconstruct the clean image from a degraded version. The process of recovering the original image from the data is an example of inverse problem. Due to the ill-posedness of the problem, the simple inversion of the degradation model does not give any good reconstructions. Therefore, to deal with the ill-posedness it is necessary to use some prior information on the solution or the model and the Bayesian approach.

Additive Gaussian noise has been extensively studied since it produces simple and tractable mathematical models. However, in the real applications, the noise is much more complicated and it cannot be well simulated by additive Gaussian noise, for instance, it may be signal dependent, very impulsive, multiplicative, mixed, etc. This PhD thesis intends to solve some of the many open questions for image restoration under non-Gaussian noise. The two main kinds of noise studied in this PhD project are the impulse noise and the Cauchy noise.

Impulse noise is due to for instance the malfunctioning pixel elements in the camera sensors, errors in analogue-to-digital conversion, faulty memory locations in hardware. Cauchy noise is characterized by a very impulsive behaviour and it is mainly used to simulate atmospheric and underwater acoustic noise, in radar and sonar applications, biomedical images and synthetic aperture radar images. For both noise models we introduce new variational models to recover the clean and sharp images from degraded images. Both methods are verified by using some simulated test problems. The experiments clearly show that the new methods outperform the former ones.

Furthermore, we have carried out a theoretical study on the two most known estimates: maximum a posteriori (MAP) estimate and conditional mean (CM) estimate for non-Gaussian noise. With only the
convexity assumption on the data delity term, we introduce some cost functions for which the CM and MAP estimates are proper Bayes estimators and we also prove that the CM estimate outperforms the MAP estimate, when the error depends on Bregman distances.

This PhD project can have many applications in the modern society, in fact the reconstruction of high quality images with less noise and more details enhances the image processing operations, such as edge detection, segmentation, etc.

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Authors: Sciacchitano, F. (Intern), Dong, Y. (Intern), Hansen, P. C. (Intern)
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**Implementation of advanced process control on the four tank pilot plant**
The four tank process laboratory experiment is used as a relevant case to unfold problems that arise when implementing advanced process control such as model predictive control. The controller, which is executed on a computer, and the process equipment communicate using OPC to exchange process measurements and actuator set points. The process equipment is described along with the setup of the PLC and the OPC server in order to be able to access process variables on a dimensional scale. A process emulator in which a process simulator is embedded in an OPC interface has been developed in Python. Using the detailed information of sensor and actuator calibration as well as PLC functionality, the emulator appears identical to the actual process and may be used to perform virtual tests of controllers prior to commissioning. Examples of how to interact with OPC servers are presented for both Matlab and Python. An MPC has been designed based on a linearized model of the process and tested using the emulator. This controller was then implemented on a realization of the process at the Technical University of Denmark, demonstrating MPC experimentally.

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Organisations: Centre for IT-Intelligent Energy Systems in Cities, Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Chemical and Biochemical Engineering, CAPEC-PROCESS
Authors: Schroll-Fleischer, E. (Intern), Huusom, J. K. (Intern), Jørgensen, J. B. (Intern)
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Iterative Reconstruction Methods for Inverse Problems in Tomography with Hybrid Data

General information
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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Sherina, E. (Intern), Knudsen, K. (Intern)
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LBAS: Lanczos Bidiagonalization with Subspace Augmentation for Discrete Inverse Problems
The regularizing properties of Lanczos bidiagonalization are powerful when the underlying Krylov subspace captures the dominating components of the solution. In some applications the regularized solution can be further improved by augmenting the Krylov subspace with a low-dimensional subspace that represents specific prior information. Inspired by earlier work on GMRES we demonstrate how to carry these ideas over to the Lanczos bidiagonalization algorithm

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Linear discrete-time state space realization of a modified quadruple tank system with state estimation using Kalman filter
In this paper, we used the modified quadruple tank system that represents a multi-input-multi-output (MIMO) system as an example to present the realization of a linear discrete-time state space model and to obtain the state estimation using Kalman filter in a methodical mannered. First, an existing dynamics of the system of stochastic differential equations is linearized to produce the deterministic-stochastic linear transfer function. Then the linear transfer function is discretized to produce a linear discrete-time state space model that has a deterministic and a stochastic component. The filtered part of the Kalman filter is used to estimates the current state, based on the model and the measurements. The static and dynamic Kalman filter is compared and all results is demonstrated through simulations.

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Model for Simulating Fasting Glucose in Type 2 Diabetes and the Effect of Adherence to Treatment.

The primary goal of this paper is to predict fasting glucose levels in type 2 diabetes (T2D) in long-acting insulin treatment.

The paper presents a model for simulating insulin-glucose dynamics in T2D patients. The model combines a physiological model of type 1 diabetes (T1D) and an endogenous insulin production model in T2D. We include a review of sources of...
variance in fasting glucose values in long-acting insulin treatment, with respect to dose guidance algorithms. We use the
model to simulate fasting glucose levels in T2D long-acting insulin treatment and compare the results with clinical trial
results where a dose guidance algorithm was used. We investigate sources of variance and through simulations evaluate
the contribution of adherence to variance and dose guidance quality. The results suggest that the model for simulation of
T2D patients is sufficient for simulating fasting glucose levels during titration in a clinical trial. Adherence to insulin
injections plays an important role considering variance in fasting glucose. For adherence levels 100%, 70% and 50%, the
coefficient of variation of simulated fasting glucose levels were similar to observed variances in insulin treatment. The
dose guidance algorithm suggested too large doses in 0.0%, 5.3% and 24.4% of cases, respectively. Adherence to
treatment is an important source of variance in long-acting insulin titration.

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Modeling Pharmacokinetics and Pharmacodynamics of Glucagon for Simulation of the Glucoregulatory System in Patients
with Type 1 Diabetes.
The goal of this thesis was to develop a pharmacokinetics/pharmacodynamics (PK/PD) model for glucagon. The proposed
PD model included multiplication of the stimulating glucagon effect and inhibiting insulin effect on the endogenous glucose
production (EGP). Moreover, the concentration-response relationship of glucagon and EGP was characterized by a non-
linear function, where the response saturated for high concentrations of glucagon. The novel EGP model extended
Hovorka's glucoregulatory model to include the effect of glucagon. The PK/PD model described both regular glucagon and
a novel glucagon analogue in healthy dogs. The extended glucoregulatory model translated to the human species and
described glucose-insulin-glucagon dynamics in healthy subjects and patients with type 1 diabetes (T1D). The extended
glucoregulatory model was successfully validated by leave-one-out cross-validation in seven T1D patients which justified
its use for simulations. The final model parameters were estimated from three to four datasets from each patient. The
validated extended glucoregulatory model was used for in silico studies. The model replicated a clinical study of the effect
of glucagon at varying insulin levels. The simulations also suggested new glucagon doses to be tested in a similar in vivo
study to provide new insight to the relationship between insulin, glucagon, and EGP. Finally, the model was used to conduct a large original simulation study investigating an insulin dependent glucagon dosing regimen for treatment of insulin-induced mild hypoglycemia.

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**Modeling surface imperfections in thin films and nanostructured surfaces**

Accurate scatterometry and ellipsometry characterization of non-perfect thin films and nanostructured surfaces are challenging. Imperfections like surface roughness make the associated modelling and inverse problem solution difficult due to the lack of knowledge about the imperfection on the surface. Combining measurement data from several instruments increases the knowledge of non-perfect surfaces. In this paper we investigate how to incorporate this knowledge of surface imperfection into inverse methods used in scatterometry and ellipsometry using the Rigorous Coupled Wave Analysis. Three classes of imperfections are examined. The imperfections are introduced as periodic structures with a super cell periods ten times larger than the simple grating period. Two classes of imperfections concern the grating and one class concern the substrate. It is shown that imperfections of a few nanometers can severely change the reflective response on silicon gratings. Inverse scatterometry analyses of gratings with imperfection using simulated data with white noise have been performed. The results show that scatterometry is a robust technology that is able to characterize grating imperfections provided that the imperfection class is known.

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Multilevel techniques for Reservoir Simulation

The subject of this thesis is the development, application and study of novel multilevel methods for the acceleration and improvement of reservoir simulation techniques. The motivation for addressing this topic is a need for more accurate predictions of porous media flow and the ability to carry out these computations in a timely manner. This will lead to better decision making in the production of oil and gas. The goal is attained in various ways throughout the thesis work. Specifically, three fields of multilevel methods have been addressed in this work, namely

• Nonlinear multigrid (the Full Approximation Scheme)
• Variational (Galerkin) upscaling
• Linear solvers and preconditioners

First, a nonlinear multigrid scheme in the form of the Full Approximation Scheme (FAS) is implemented and studied for a 3D three-phase compressible rock/fluids immiscible reservoir simulator with a coupled well model. In a fair way, it is compared to the state-of-the-art solution scheme used in industry and research simulators. It is found that FAS improves time-to-solution by having a larger basin of attraction, faster initial convergence, data locality and a lower memory footprint. The study is extended to include a hybrid strategy, where FAS is combined with Newton’s method to construct a multilevel nonlinear preconditioner. This method demonstrates high efficiency and robustness.

Second, an improved IMPES formulated reservoir simulator is implemented using a novel variational upscaling approach based on element-based Algebraic Multigrid (AMGe). In particular, an advanced AMGe technique with guaranteed approximation properties is used to construct a coarse multilevel hierarchy of Raviart-Thomas and L2 spaces for the Galerkin coarsening of a mixed formulation of the reservoir simulation equations. By experimentation it is found that the AMGe based upscaling technique provided very accurate results while reducing the computational time proportionally to the reduction in degrees of freedom. Furthermore, it is demonstrated that the AMGe coarse spaces (interpolation operators) can be used for both variational upscaling and the construction of linear solvers. In particular, it is found to be beneficial (or even necessary) to apply an AMGe based multigrid solver to solve the upscaled problems. It is found that the AMGe upscaling changes the spectral properties of the matrix, which renders well-known state-of-the-art solvers for this type of system useless.

Third, FAS is combined with AMGe with guaranteed approximation properties to obtain a nonlinear multigrid solver for unstructured meshes. The FAS-AMGe solver is applied to a simplistic but numerically challenging mixed (velocity-/pressure) model for porous media flow. In a fair way, FAS-AMGe is compared to Newton’s method and Picard iterations. It is found that FAS-AMGe is faster for the cases considered.

Finally, a number of multigrid linear solvers and preconditioners are implemented for various linear systems. In particular AMGe are used in the construction of multigrid preconditioners. These are compared to two state-of-the-art block diagonal preconditioners based on 1) a Schur complement with an Algebraic Multigrid (AMG) solver and 2) an augmented Lagrangian formulation using the Auxiliary Space AMG solver.

In addition to the research mentioned above, a sequential in-house COmpositional reservoir SImulator (COSI) with many features is parallelized in a distributed setting (MPI) using the PETSc framework. A parallel preconditioner based on the Constrained Pressure Residual method, Algebraic Multigrid and Restricted Additive Overlapping Schwarz with Incomplete LU solves on each subdomain is implemented. It is found that switching the traditionally used method, namely parallel ILU, with Restricted Additive Overlapping Schwarz results in a significant increase in parallel scalability while still maintaining similar robustness and efficiency.
Multiple shooting applied to robust reservoir control optimization including output constraints on coherent risk measures

The production life of oil reservoirs starts under significant uncertainty regarding the actual economical return of the recovery process due to the lack of oil field data. Consequently, investors and operators make management decisions based on a limited and uncertain description of the reservoir. In this work, we propose a new formulation for robust optimization of reservoir well controls. It is inspired by the multiple shooting (MS) method which permits a broad range of parallelization opportunities and output constraint handling. This formulation exploits coherent risk measures, a concept traditionally used in finance, to bound the risk on constraint violation. We propose a reduced sequential quadratic programming (rSQP) algorithm to solve the underlying optimization problem. This algorithm exploits the structure of the coherent risk measures, thus a large set of constraints are solved within sub-problems. Moreover, a variable elimination procedure allows solving the optimization problem in a reduced space and an iterative active-set method helps to handle a large set of inequality constraints. Finally, we demonstrate the application of constraints to bound the risk of water production peaks rather than worst-case satisfaction.
Numerical Multilevel Upscaling for Incompressible Flow in Reservoir Simulation: An Element-based Algebraic Multigrid (AMGe) Approach

We study the application of a finite element numerical upscaling technique to the incompressible two-phase porous media total velocity formulation. Specifically, an element agglomeration based Algebraic Multigrid (AMGe) technique with improved approximation proper ties [37] is used, for the first time, to generate upscaled and accurate coarse systems for the reservoir simulation equations. The upscaling technique is applied to both the mixed system for velocity and pressure and to the hyperbolic transport equations providing fully upscaled systems. By introducing additional degrees of freedom associated with non-planar interfaces between agglomerates, the coarse velocity space has guaranteed approximation properties. The employed AMGe technique provides coarse spaces with desirable local mass conservation and stability properties analogous to the original pair of Raviart-Thomas and piecewise discontinuous polynomial spaces, resulting in strong mass conservation for the upscaled systems. Due to the guaranteed approximation properties and the generic nature of the AMGe method, recursive multilevel upscaling is automatically obtained. Furthermore, this technique works for both structured and unstructured meshes. Multiscale Mixed Finite Elements exhibit accuracy for general unstructured meshes but do not in general lead to nested hierarchy of spaces. Multiscale multilevel mimetic finite differences generate nested spaces but lack the adaptivity of the flux representation on coarser levels that the proposed AMGe approach offers. Thus, the proposed approach can be seen as a rigorous bridge that merges the best properties of these two existing methods. The accuracy and stability of the studied multilevel AMGe upscaling technique is demonstrated on two challenging test cases.
Offset Risk Minimization for Open-loop Optimal Control of Oil Reservoirs

Simulation studies of oil field water flooding have demonstrated a significant potential of optimal control technology to improve industrial practices. However, real-life applications are challenged by unknown geological factors that make reservoir models highly uncertain. To minimize the associated financial risks, the oil literature has used ensemble-based methods to manipulate the net present value (NPV) distribution by optimizing sample estimated risk measures. In general, such methods successfully reduce overall risk. However, as this paper demonstrates, ensemble-based control strategies
may result in individual profit outcomes that perform worse than real-life dominating strategies. This poses significant
financial risks to oil companies whose main concern is to avoid unacceptable low profits. To remedy this, this paper
proposes offset risk minimization. Unlike existing methodology, the offset method uses the NPV offset distribution to
minimize risk relative to a competing reference strategy. Open-loop simulations of a 3D two-phase synthetic reservoir
demonstrate the potential of offset risk minimization to significantly improve the worst case profit offset relative to real-life
best practices. The results suggest that it may be more relevant to consider the NPV offset distribution than the NPV
distribution when minimizing risk in production optimization.

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Polynomial Collocation for Handling an Inaccurately Known Measurement Configuration in Electrical Impedance
Tomography
The objective of electrical impedance tomography is to reconstruct the internal conductivity of a physical body based on
measurements of current and potential at a finite number of electrodes attached to its boundary. Although the conductivity
is the quantity of main interest in impedance tomography, a real-world measurement configuration includes other unknown
parameters as well: The information on the contact resistances, electrode positions, and body shape is almost always
incomplete. In this work, the dependence of the electrode measurements on all aforementioned model properties is
parametrized via polynomial collocation. The availability of such a parametrization enables efficient simultaneous
reconstruction of the conductivity and other unknowns by a Newton-type output least squares algorithm, which is
demonstrated by two-dimensional numerical experiments based on both noisy simulated data and experimental data from
two water tanks.

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Random walks with statistical shape prior for cochlea and inner ear segmentation in micro-CT images

A cochlear implant is an electronic device which can restore sound to completely or partially deaf patients. For surgical planning, a patient-specific model of the inner ear must be built using high-resolution images accurately segmented. We propose a new framework for segmentation of micro-CT cochlear images using random walks, where a region term estimated by a Gaussian mixture model is combined with a shape prior initially obtained by a statistical shape model (SSM). The region term can then take advantage of the high contrast between the background and foreground, while the shape prior guides the segmentation to the exterior of the cochlea and to less contrasted regions inside the cochlea. The prior is obtained via a non-rigid registration regularized by a statistical shape model. The SSM constrains the inner parts of the cochlea and ensures valid output shapes of the inner ear.

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Authors: Ruiz Pujadas, E. (Ekstern), Piella, G. (Ekstern), Kjer, H. M. (Intern), González Ballester, M. A. (Ekstern)
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Reduction of variable-truncation artifacts from beam occlusion during in situ x-ray tomography: Paper

Many in situ x-ray tomography studies require experimental rigs which may partially occlude the beam and cause parts of the projection data to be missing. In a study of fluid flow in porous chalk using a percolation cell with four metal bars, drastic streak artifacts arise in the filtered backprojection (FBP) reconstruction at certain orientations. Projections with non-trivial variable truncation caused by the metal bars are the source of these variable-truncation artifacts. To understand the artifacts, a mathematical model of variable-truncation data as a function of metal bar radius and distance to sample is derived and verified numerically and with experimental data. The model accurately describes the arising variable-truncation artifacts across simulated variations of the experimental setup. Three variable-truncation artifact-reduction methods are proposed, all aimed at addressing sinogram discontinuities that are shown to be the source of the streaks. The ‘reduction to limited angle’ (RLA) method simply keeps only non-truncated projections; the ‘detector-directed smoothing’ (DDS) method smooths the discontinuities; while the ‘reflexive boundary condition’ (RBC) method enforces a zero derivative at the discontinuities. Experimental results using both simulated and real data show that the proposed methods effectively reduce variable-truncation artifacts. The RBC method is found to provide the best artifact reduction and preservation of image features using both visual and quantitative assessment. The analysis and artifact-reduction methods are designed in context of FBP reconstruction motivated by computational efficiency practical for large, real synchrotron data. While a specific variable-truncation case is considered, the proposed methods can be applied to general data cut-offs arising in different in situ x-ray tomography experiments.
Relationship between Optimum Mini-doses of Glucagon and Insulin Levels when Treating Mild Hypoglycaemia in Patients with Type 1 Diabetes - A Simulation Study

Hypoglycaemia remains the main limiting factor in type 1 diabetes management. We developed an insulin-dependent glucagon dosing regimen for treatment of mild hypoglycaemia based on simulations. A validated glucose-insulin-glucagon model was used to describe seven virtual patients with insulin pump-treated type 1 diabetes. In each simulation, one of ten different and individualized subcutaneous insulin boluses was administered to decrease plasma glucose (PG) from 7.0 to ≤3.9 mmol/l. Insulin levels were estimated as ratio of actual to baseline serum insulin concentration (se/ba-insulin), insulin on board (IOB) or percentage of IOB to total daily insulin dose (IOB/TDD). Insulin bolus sizes were chosen to provide predefined insulin levels when PG reached 3.9 mmol/l, where one of 17 subcutaneous glucagon boluses was administered. Optimum glucagon bolus to treat mild hypoglycaemia at varying insulin levels was the lowest dose that in most patients caused PG peak between 5.0 and 10.0 mmol/l and sustained PG ≥ 3.9 mmol/l for 2 hr after the bolus. PG response to
glucagon declined with increasing insulin levels. The glucagon dose to optimally treat mild hypoglycaemia depended exponentially on insulin levels, regardless of how insulin was estimated. A 125-μg glucagon dose was needed to optimally treat mild hypoglycaemia when insulin levels were equal to baseline levels. In contrast, glucagon doses >500 μg were needed when se/ba-insulin >2.5, IOB >2.0 U or IOB/TDD >6%. Although the proposed model-based glucagon regimen needs confirmation in clinical trials, this is the first attempt to develop an insulin-dependent glucagon dosing regimen for treatment of insulin-induced mild hypoglycaemia in patients with type 1 diabetes.

**General information**

State: Published
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**Segmentation-Driven Tomographic Reconstruction.**
The tomographic reconstruction problem is concerned with creating a model of the interior of an object from some measured data, typically projections of the object. After reconstructing an object it is often desired to segment it, either
automatically or manually. For computed tomography (CT), the classical reconstruction methods suffer from their inability to handle limited and/or corrupted data. Form any analysis tasks computationally demanding segmentation methods are used to automatically segment an object, after using a simple reconstruction method as a first step. In the literature, methods that completely combine reconstruction and segmentation have been suggested, but these are often non-convex and have very high computational demand. We propose to move the computational effort from the segmentation process to the reconstruction process, and instead design reconstruction methods such that the segmentation subsequently can be carried out by use of a simple segmentation method, for instance just a thresholding method. We tested the advantages of going from a two-stage reconstruction method to a one stage segmentation-driven reconstruction method for the phase contrast tomography reconstruction problem. The tests showed a clear improvement for realistic materials simulations and that the one-stage method was clearly more robust toward noise. The noise-robustness result could be a step toward making this method more applicable for lab-scale experiments. We have introduced a segmentation-driven reconstruction method which incorporates information about the main texture direction in an object. We proved that this method has mathematically desirable properties such as being convex and lower semicontinuous. We have also demonstrated the practical applicability of the method.

within image denoising, image deblurring and CT reconstruction. In order to use the proposed method we also proposed efficient and robust methods for estimating the main direction in either corrupted images or from limited and corrupted CT projection data. For directional object we also proposed two different reconstruction methods that separates the directional parts in the object from the non-directional parts. These method could for example be used for objects consisting of fibres and cracks. The results can be categorized as either completely combined reconstruction and segmentation of the object, or as highly supporting for the following segmentation process. Computed tomography is used within medical diagnosis, food science, materials science, production inspection, quality assessment, etc. Segmentation-driven reconstruction methods can help improve both manual and automated segmentation processes that are used to analyze an object after the scanning. The results in this thesis are both of theoretical interest within regularization theory and directly applicable for image denoising, image deblurring and surely within tomographic reconstruction.
SparseBeads data: benchmarking sparsity-regularized computed tomography

Sparse regularization (SR) such as total variation (TV) minimization allows accurate image reconstruction in x-ray computed tomography (CT) from fewer projections than analytical methods. Exactly how few projections suffice and how this number may depend on the image remain poorly understood. Compressive sensing connects the critical number of projections to the image sparsity, but does not cover CT, however empirical results suggest a similar connection. The present work establishes for real CT data a connection between gradient sparsity and the sufficient number of projections for accurate TV-regularized reconstruction. A collection of 48 x-ray CT datasets called SparseBeads was designed for benchmarking SR reconstruction algorithms. Beadpacks comprising glass beads of five different sizes as well as mixtures were scanned in a micro-CT scanner to provide structured datasets with variable image sparsity levels, number of projections and noise levels to allow the systematic assessment of parameters affecting performance of SR reconstruction algorithms. Using the SparseBeads data, TV-regularized reconstruction quality was assessed as a function of numbers of projections and gradient sparsity. The critical number of projections for satisfactory TV-regularized reconstruction increased almost linearly with the gradient sparsity. This establishes a quantitative guideline from which one may predict how few projections to acquire based on expected sample sparsity level as an aid in planning of dose- or time-critical experiments. The results are expected to hold for samples of similar characteristics, i.e. consisting of few, distinct phases with relatively simple structure. Such cases are plentiful in porous media, composite materials, foams, as well as non-destructive testing and metrology. For samples of other characteristics the proposed methodology may be used to investigate similar relations.
Stochastic derivation and solution of simplified radiative transfer using the Fokker-Planck equation

General information
State: Published
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Publication date: 2017
Event:
Main Research Area: Technical/natural sciences
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The Adjoint Method for Gradient-based Dynamic Optimization of UV Flash Processes
This paper presents a novel single-shooting algorithm for gradient-based solution of optimal control problems with vapor-liquid equilibrium constraints. Dynamic optimization of UV flash processes is relevant in nonlinear model predictive control of distillation columns, certain two-phase flow problems, and oil reservoir production with significant compositional and thermal effects. Gradients are computed with the adjoint method and we use various optimization software (fmincon, IPOPT, KNITRO, and NPSOL) for the numerical optimization. We present computational results for a non-ideal five-component flash process which demonstrate the importance of the optimization solver, the compiler, and the linear algebra software for the efficiency of dynamic optimization of UV flash processes.

Tomographic image reconstruction using training images
We describe and examine an algorithm for tomographic image reconstruction where prior knowledge about the solution is available in the form of training images. We first construct a non-negative dictionary based on prototype elements from the training images; this problem is formulated within the framework of sparse learning as a regularized non-negative matrix factorization. Incorporating the dictionary as a prior in a convex reconstruction problem, we then find an approximate solution with a sparse representation in the dictionary. The dictionary is applied to non-overlapping patches of the image, which reduces the computational complexity compared to previous formulations. Computational experiments clarify the choice and interplay of the model parameters and the regularization parameters, and we show that in few-projection low-dose settings our algorithm is competitive with total variation regularization and tends to include more texture and more correct edges.
Tomographic Reconstruction Methods for Decomposing Directional Components

X-ray computed tomography technique has many different practical applications. In this paper, we propose two new reconstruction methods that can decompose objects at the same time. By incorporating direction information, the proposed methods can decompose objects into various directional components. Furthermore, we propose a method to obtain the direction information in the objects directly from the measured sinogram data. We demonstrate the proposed methods on simulated and real samples to show their practical applicability. The numerical results show the differences between the two methods and effectiveness as dealing with fibre-crack decomposition problem.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Kongskov, R. D. (Intern), Dong, Y. (Intern)
Total Variation Based Parameter-Free Model for Impulse Noise Removal

We propose a new two-phase method for reconstruction of blurred images corrupted by impulse noise. In the first phase, we use a noise detector to identify the pixels that are contaminated by noise, and then, in the second phase, we reconstruct the noisy pixels by solving an equality constrained total variation minimization problem that preserves the exact values of the noise-free pixels. For images that are only corrupted by impulse noise (i.e., not blurred) we apply the semismooth Newton's method to a reduced problem, and if the images are also blurred, we solve the equality constrained reconstruction problem using a first-order primal-dual algorithm. The proposed model improves the computational efficiency (in the denoising case) and has the advantage of being regularization parameter-free. Our numerical results suggest that the method is competitive in terms of its restoration capabilities with respect to the other two-phase methods.

Towards characterizing and reducing artifacts caused by varying projection truncation

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Sciacchitano, F. (Intern), Dong, Y. (Intern), Andersen, M. S. (Intern)
Number of pages: 43
Unified quantum theory of elastic and inelastic atomic scattering from a physisorbed monolayer solid

A unified quantum theory of the elastic and inelastic scattering of low energy He atoms by a physisorbed monolayer solid in the one-phonon approximation is given. It uses a time-dependent wave packet with phonon creation and annihilation components and has a self-consistent feedback between the wave functions for elastic and inelastic scattered atoms. An attenuation of diffraction scattering by inelastic processes thus is inherent in the theory. The atomic motion and monolayer vibrations in the harmonic approximation are treated quantum mechanically and unitarity is preserved. The evaluation of specific one-phonon events includes contributions from diffuse inelastic scattering in other phonon modes. Effects of thermally excited phonons are included using a mean field approximation. The theory is applied to an incommensurate Xe/Pt(111) monolayer (incident energy $E_i = 4$-16 meV), a commensurate Xe/graphite monolayer ($E_i$ similar or equal to 64 meV), and an incommensurate Xe/Cu(001) monolayer ($E_i$ similar or equal to 8 meV). The monolayers are very corrugated targets and there are transient closed diffraction and inelastic channels in the calculations. In many cases, the energy gain events have strengths comparable to the energy loss events.
User-friendly simultaneous tomographic reconstruction and segmentation with class priors

Simultaneous Reconstruction and Segmentation (SRS) strategies for computed tomography (CT) present a way to combine the two tasks, which in many applications traditionally are performed as two successive and separate steps. A combined model has a potentially positive effect by allowing the two tasks to influence one another, at the expense of a more complicated algorithm. The combined model increases in complexity due to additional parameters and settings requiring tuning, thus complicating the practical usability. This paper takes it outset in a recently published variational algorithm for SRS. We propose a simplification that reduces the number of required parameters, and we perform numerical experiments investigating the effect and the conditions under which this approach is feasible.

General information
State: Published
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Validation of a Simulation Model Describing the Glucose-Insulin-Glucagon Pharmacodynamics in Patients with Type 1 Diabetes

Currently, no consensus exists on a model describing endogenous glucose production (EGP) as a function of glucagon concentrations. Reliable simulations to determine the glucagon dose preventing or treating hypoglycemia or to tune a dual-hormone artificial pancreas control algorithm need a validated glucoregulatory model including the effect of glucagon.

A Hierarchical Algorithm for Integrated Scheduling and Control With Applications to Power Systems

The contribution of this paper is a hierarchical algorithm for integrated scheduling and control via model predictive control of hybrid systems. The controlled system is a linear system composed of continuous control, state, and output variables. Binary variables occur as scheduling decisions in the optimal control problem (OCP). The scheduling decisions are made on a slow time scale compared with the system dynamics. This gives rise to a temporal separation of the scheduling and control variables in the OCP. Accordingly, the proposed hierarchical algorithm consists of two optimization levels. The upper level (scheduling level) solves a mixed-integer linear program (MILP) with a low frequency. The lower level (control level) solves an LP with a high frequency. The main advantage of the proposed approach is that it requires online solution of an LP rather than an MILP. Simulations based on a power portfolio case study show that the hierarchical algorithm reduces the computation to solve the OCP by several orders of magnitude. The improvement in computation time is achieved without a significant increase in the overall cost of operation.
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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.958 SNIP 3.042 CiteScore 4.34
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Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 1.62 SNIP 3.037 CiteScore 3.7
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.698 SNIP 3.013 CiteScore 3.26
ISI indexed (2011): ISI indexed yes
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Scopus rating (2009): SJR 1.737 SNIP 2.84
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Algorithms and Methods for High-Performance Model Predictive Control

The goal of this thesis is to investigate algorithms and methods to reduce the solution time of solvers for Model Predictive Control (MPC). The thesis is accompanied with an open-source toolbox for High-Performance implementation of solvers for MPC (HPMPC), that contains the source code of all routines employed in the numerical tests. The main focus of this thesis is on linear MPC problems.

In this thesis, both the algorithms and their implementation are equally important. About the implementation, a novel implementation strategy for the dense linear algebra routines in embedded optimization is proposed, aiming at improving the computational performance in case of small matrices. About the algorithms, they are built on top of the proposed linear algebra, and they are tailored to exploit the high-level structure of the MPC problems, with special care on reducing the computational complexity.

General information
State: Published
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An analytic mapping property of the Dirichlet-to-Neumann operator in Helmholtz boundary problems

The analytic version of microlocal analysis shows that if the boundary and the Dirichlet datum of a Helmholtz boundary value problem are real-analytic, then so is the corresponding Neumann datum. However, the domain of analytic continuation of the Neumann datum is, in general, unknown. We shall here relate, in terms of explicit estimates, the domains of analytic continuation of Dirichlet and Neumann boundary data for Helmholtz problems in two or more independent variables, and in neighbourhoods of planar pieces of the boundary. For this purpose, we shall characterise a special subspace of the standard pseudodifferential operators with real-analytic symbols, to which the Dirichlet-to-Neumann operator belongs. The result can be applied in the estimation of the domain of analytic continuation of solutions across planar pieces of the boundary.

General information
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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Neutrons and X-rays for Materials Physics
Authors: Karamehmedovic, M. (Intern)
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Main Research Area: Technical/natural sciences

An Efficient Implementation of Partial Condensing for Nonlinear Model Predictive Control

Partial (or block) condensing is a recently proposed technique to reformulate a Model Predictive Control (MPC) problem into a form more suitable for structure-exploiting Quadratic Programming (QP) solvers. It trades off horizon length for input vector size, and this degree of freedom can be employed to find the best problem size for the QP solver at hand. This paper proposes a Hessian condensing algorithm particularly well suited for partial condensing, where a state component is
An Efficient UD-Based Algorithm for the Computation of Maximum Likelihood Sensitivity of Continuous-Discrete Systems

This paper addresses maximum likelihood parameter estimation of continuous-time nonlinear systems with discrete-time measurements. We derive an efficient algorithm for the computation of the log-likelihood function and its gradient, which can be used in gradient-based optimization algorithms. This algorithm uses UD decomposition of symmetric matrices and the array algorithm for covariance update and gradient computation. We test our algorithm on the Lotka-Volterra equations. Compared to the maximum likelihood estimation based on finite difference gradient computation, we get a significant speedup without compromising the numerical accuracy.

An Ensemble Nonlinear Model Predictive Control Algorithm in an Artificial Pancreas for People with Type 1 Diabetes

This paper presents a novel ensemble nonlinear model predictive control (NMPC) algorithm for glucose regulation in type 1 diabetes. In this approach, we consider a number of scenarios describing different uncertainties, for instance meals or metabolic variations. We simulate a population of 9 patients with different physiological parameters and a time-varying insulin sensitivity using the Medtronic Virtual Patient (MVP) model. We augment the MVP model with stochastic diffusion terms, time-varying insulin sensitivity and noise-corrupted CGM measurements. We consider meal challenges where the uncertainty in meal size is ±50%. Numerical results show that the ensemble NMPC reduces the risk of hypoglycemia compared to standard NMPC in the case where the meal size is overestimated or correctly estimated at the expense of a slightly increased number of hyperglycemia. Therefore, ensemble MPC-based algorithms can improve the safety of the AP compared to the classical MPC-based algorithms.
An open-source thermodynamic software library

This is a technical report which accompanies the article "An open-source thermodynamic software library" which describes an efficient Matlab and C implementation for evaluation of thermodynamic properties. In this technical report we present the model equations, that are also presented in the paper, together with a full set of first and second order derivatives with respect to temperature and pressure, and in cases where applicable, also with respect to mole numbers. The library is based on parameters and correlations from the DIPPR database and the Peng-Robinson and the Soave-Redlich-Kwong equations of state.

General information
State: Published
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Application of Economic MPC to Frequency Control in a Single-Area

This paper presents a novel model predictive control scheme for frequency control in a single-area power system. The proposed controller provides set-point corrections to the system power generators, based on the solution to an optimal control problem. The optimal control problem directly incorporates the cost of operation into its objective function. A trade-off parameter is used to balance set-point tracking and cost minimization. Simulations based on a Faroe Islands case study show that the proposed approach reduces cost of operation by almost an order of magnitude, compared to both set-point based model predictive control as well as conventional frequency-based PI-control.

General information
State: Published
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Application of the Continuous-Discrete Extended Kalman Filter for Fault Detection in Continuous Glucose Monitors for Type 1 Diabetes

The purpose of this study is the online detection of faults and anomalies of a continuous glucose monitor (CGM). We simulated a type 1 diabetes patient using the Medtronic virtual patient model. The model is a system of stochastic differential equations and includes insulin pharmacokinetics, insulin-glucose interaction, and carbohydrate absorption. We simulated and detected two types of CGM faults, i.e., spike and drift. A fault was defined as a CGM value in any of the zones C, D, and E of the Clarke error grid analysis classification. Spike was modelled by a binomial distribution, and drift was modelled by a Gaussian random walk. We used a continuous-discrete extended Kalman filter for the fault detection, based on the statistical tests of the filter innovation and the 90-min prediction residuals of the sensor measurements. The spike detection had a sensitivity of 93% and a specificity of 100%. Also, the drift detection had a sensitivity of 80% and a specificity of 85%. Furthermore, with 100% sensitivity the proposed method was able to detect if the drift overestimates or underestimates the interstitial glucose concentration.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Copenhagen University Hospital
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A robust WENO scheme for nonlinear waves in a moving reference frame

For robust nonlinear wave simulation in a moving reference frame, we recast the free surface problem in Hamilton-Jacobi form and propose a Weighted Essentially Non-Oscillatory (WENO) scheme to automatically handle the upwinding of the convective term. A new automatic procedure for deriving the linear WENO weights based on a Taylor series expansion is introduced. A simplified smoothness indicator is proposed and is shown to perform well. The scheme is combined with high-order explicit Runge-Kutta time integration and a dissipative Lax-Friedrichs-type flux to solve for nonlinear wave propagation in a moving frame of reference. The WENO scheme is robust and less dissipative than the equivalent order upwind-biased finite difference scheme for all ratios of frame of reference to wave propagation speed tested. This provides the basis for solving general nonlinear wave-structure interaction problems at forward speed.

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
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Pages: 482-488
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A Spectral Geometrical Model for Compton Scatter Tomography Based on the SSS Approximation

The forward model of single scatter in the Positron Emission Tomography for a detector system possessing an excellent spectral resolution under idealized geometrical assumptions is investigated. This model has the form of integral equations describing a flux of photons emanating from the same annihilation event and undergoing a single scattering at a certain angle. The equations for single scatter calculation are derived using the Single Scatter Simulation approximation. We show that the three-dimensional slice-by-slice filtered backprojection algorithm is applicable for scatter data inversion provided some assumptions on the attenuation map are justified.
A stabilised nodal spectral element method for fully nonlinear water waves

We present an arbitrary-order spectral element method for general-purpose simulation of non-overturning water waves, described by fully nonlinear potential theory. The method can be viewed as a high-order extension of the classical finite element method proposed by Cai et al. (1998) [5], although the numerical implementation differs greatly. Features of the proposed spectral element method include: nodal Lagrange basis functions, a general quadrature-free approach and gradient recovery using global L2 projections. The quartic nonlinear terms present in the Zakharov form of the free surface conditions can cause severe aliasing problems and consequently numerical instability for marginally resolved or very steep waves. We show how the scheme can be stabilised through a combination of over-integration of the Galerkin projections and a mild spectral filtering on a per element basis. This effectively removes any aliasing driven instabilities while retaining the high-order accuracy of the numerical scheme. The additional computational cost of the over-integration is found insignificant compared to the cost of solving the Laplace problem. The model is applied to several benchmark cases in two dimensions. The results confirm the high order accuracy of the model (exponential convergence), and demonstrate the potential for accuracy and speedup. The results of numerical experiments are in excellent agreement with both analytical and experimental results for strongly nonlinear and irregular dispersive wave propagation. The benefit of using a high-order – possibly adapted – spatial discretisation for accurate water wave propagation over long times and distances is particularly attractive for marine hydrodynamics applications.
A tensor-based dictionary learning approach to tomographic image reconstruction

We consider tomographic reconstruction using priors in the form of a dictionary learned from training images. The reconstruction has two stages: first we construct a tensor dictionary prior from our training data, and then we pose the reconstruction problem in terms of recovering the expansion coefficients in that dictionary. Our approach differs from past approaches in that (a) we use a third-order tensor representation for our images and (b) we recast the reconstruction problem using the tensor formulation. The dictionary learning problem is presented as a non-negative tensor factorization problem with sparsity constraints. The reconstruction problem is formulated in a convex optimization framework by looking for a solution with a sparse representation in the tensor dictionary. Numerical results show that our tensor formulation leads to very sparse representations of both the training images and the reconstructions due to the ability of representing repeated features compactly in the dictionary.

General information
State: Published
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Number of pages: 30
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Main Research Area: Technical/natural sciences
A two-stage model of rough-interface scattering for embedded nano-structures

We decompose scattering by nanostructures on rough substrates into two surface transfer functions: one heuristic, computed for the bare substrate from experimental BRDF data, and the other sparse and constructed for nanostructures.
on smooth surfaces. We explore numerically the performance and the commutativity of this approach.

**Automatic Model Generation Framework for Computational Simulation of Cochlear Implantation**

Recent developments in computational modeling of cochlear implantation are promising to study in silico the performance of the implant before surgery. However, creating a complete computational model of the patient's anatomy while including an external device geometry remains challenging. To address such a challenge, we propose an automatic framework for the generation of patient-specific meshes for finite element modeling of the implanted cochlea. First, a statistical shape model is constructed from high-resolution anatomical μCT images. Then, by fitting the statistical model to a patient's CT image, an accurate model of the patient-specific cochlea anatomy is obtained. An algorithm based on the parallel transport frame is employed to perform the virtual insertion of the cochlear implant. Our automatic framework also incorporates the surrounding bone and nerve fibers and assigns constitutive parameters to all components of the finite element model. This model can then be used to study in silico the effects of the electrical stimulation of the cochlear implant. Results are shown on a total of 25 models of patients. In all cases, a final mesh suitable for finite element simulations was obtained, in an average time of 94 s. The framework has proven to be fast and robust, and is promising for a detailed prognosis of the cochlear implantation surgery.
Bregman Cost for Non-Gaussian Noise

One of the tasks of the Bayesian inverse problem is to find a good estimate based on the posterior probability density. The most common point estimators are the conditional mean (CM) and maximum a posteriori (MAP) estimates, which correspond to the mean and the mode of the posterior, respectively. From a theoretical point of view it has been argued that the MAP estimate is only in an asymptotic sense a Bayes estimator for the uniform cost function, while the CM estimate is a Bayes estimator for the means squared cost function. Recently, it has been proven that the MAP estimate is a proper Bayes estimator for the Bregman cost if the image is corrupted by Gaussian noise. In this work we extend this result to other noise models with log-concave likelihood density, by introducing two related Bregman cost functions for which the CM and the MAP estimates are proper Bayes estimators. Moreover, we also prove that the CM estimate outperforms the MAP estimate, when the error is measured in a certain Bregman distance, a result previously unknown also in the case of additive Gaussian noise.

General information
State: Published
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Cauchy Noise Removal by Nonconvex ADMM with Convergence Guarantees

Image restoration is one of the most important and essential issues in image processing. Cauchy noise in engineering application has the non-Gaussian and impulsive property. In order to preserve edges and details of images, the total variation (TV) based variational model has been studied for restoring images degraded by blur and Cauchy noise. Due to the nonconvexity and nonsmoothness, there exist computational and theoretical challenges. In this paper, adapting recent results, we develop an alternating direction method of multiplier (ADMM) in spite of the challenges. The convergence to a stationary point is guaranteed theoretically under certain conditions. Experimental results demonstrate that the proposed method is competitive with other methods in terms of visual and quantitative measures. Especially, by comparing to the PSNR values, our method can improve about 0.5dB on average.

Cochlear implant electrode localization in post-operative CT using a spherical measure

When implanting cochlear implants the positions of electrodes have a large impact on the quality of the restored hearing. Due to metal artifacts it is difficult to estimate the precise location in post-operative scans. In this paper we present a method for automatically locating and determining the ordering of electrode contacts on implanted electrode arrays from post-operative CT images. Our method applies a specialized filter chain to the images based on a threshold and spherical measure, and selects contact positions at local maxima in the filtered image. Two datasets of 13 temporal bone specimens scanned in CBCT are used to validate the method, which successfully locates the electrode array in every image.
Cochlea Segmentation using Iterated Random Walks with Shape Prior

Cochlear implants can restore hearing to deaf or partially deaf patients. In order to plan the intervention, a model from high resolution μCT images is to be built from accurate cochlea segmentations and then, adapted to a patient-specific model. Thus, a precise segmentation is required to build such a model. We propose a new framework for segmentation of μCT cochlear images using random walks where a region term is combined with a distance shape prior weighted by a confidence map to adjust its influence according to the strength of the image contour. Then, the region term can take advantage of the high contrast between the background and foreground and the distance prior guides the segmentation to the exterior of the cochlea as well as to less contrasted regions inside the cochlea. Finally, a refinement is performed preserving the topology using a topological method and an error control map to prevent boundary leakage. We tested the proposed approach with 10 datasets and compared it with the latest techniques with random walks and priors. The experiments suggest that this method gives promising results for cochlea segmentation.

General information
State: Published
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Comparison of Three Nonlinear Filters for Fault Detection in Continuous Glucose Monitors

The purpose of this study is to compare the performance of three nonlinear filters in online drift detection of continuous glucose monitors. The nonlinear filters are the extended Kalman filter (EKF), the unscented Kalman filter (UKF), and the particle filter (PF). They are all based on a nonlinear model of the glucose-insulin dynamics in people with type 1 diabetes. Drift is modelled by a Gaussian random walk and is detected based on the statistical tests of the 90-min prediction residuals of the filters. The unscented Kalman filter had the highest average F score of 85.9%, and the smallest average detection delay of 84.1%, with the average detection sensitivity of 82.6%, and average specificity of 91.0%.

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Copenhagen University Hospital
Pages: 3507-3510
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Contrast Invariant SNR
We design an image quality measure independent of local contrast changes, which constitute simple models of illumination changes. Given two images, the algorithm provides the image closest to the first one with the component tree of the second. This problem can be cast as a specific convex program called isotonic regression. We provide a few analytic properties of the solutions to this problem. We also design a tailored first order optimization procedure together with a full complexity analysis. The proposed method turns out to be practically more efficient and reliable than the best existing algorithms based on interior point methods. The algorithm has potential applications in change detection, color image processing or image fusion. A Matlab implementation is available at http://www.math.univ-toulouse.fr/_weiss/PageCodes.html.

Controllability and flexibility analysis of CO2 post-combustion capture using piperazine and MEA
In this study, we developed a decentralized control scheme and investigate the performance of the piperazine (PZ) and monoethanolamine (MEA) CO2 capture process for industrially-relevant operation scenarios. The base for the design of the control schemes is Relative Gain Array (RGA) analysis combined with open-loop dynamic sensitivity analysis.

This study suggests that controllers with smaller time integrals and larger gains are required to maintain the PZ plant within reasonable short closed-loop settling times when compared to MEA. It also shows that the offset from the designated set-points in the presence of disturbances in the flue gas flow and heat duty is larger using PZ compared to MEA. The settling time for the PZ plant is generally larger than for MEA. However, the PZ plant rejects the disturbances faster and with less variability in the load of the power plant. Furthermore, this study indicates that the proposed PI-based control structure can handle large changes in the load provided that the manipulated variables, i.e. lean solvent flow or reboiler duty, do not reach their saturation limit. Additionally, we observed that shortage in the steam supply (reboiler duty) may represent a critical operational bottleneck, especially when PZ is being used. The MEA plant controllers drive the system towards drying out/flooding while the CO2 capture rate performance of the PZ plant reduces drastically in the presence of constraints in the availability of steam. These findings suggest the need for advanced control structures, e.g. MPC, which can explicitly account for constraints in the process variables.
Convergence analysis for column-action methods in image reconstruction

Column-oriented versions of algebraic iterative methods are interesting alternatives to their row-version counterparts: they converge to a least squares solution, and they provide a basis for saving computational work by skipping small updates. In this paper we consider the case of noise-free data. We present a convergence analysis of the column algorithms, we discuss two techniques (loping and flagging) for reducing the work, and we establish some convergence results for methods that utilize these techniques. The performance of the algorithms is illustrated with numerical examples from computed tomography.

General information
Convergence and regularization for monotonicity-based shape reconstruction in electrical impedance tomography

The inverse problem of electrical impedance tomography is severely ill-posed, meaning that, only limited information about the conductivity can in practice be recovered from boundary measurements of electric current and voltage. Recently it was shown that a simple monotonicity property of the related Neumann-to-Dirichlet map can be used to characterize shapes of inhomogeneities in a known background conductivity. In this paper we formulate a monotonicity-based shape reconstruction scheme that applies to approximative measurement models, and regularizes against noise and modelling error. We demonstrate that for admissible choices of regularization parameters the inhomogeneities are detected, and under reasonable assumptions, asymptotically exactly characterized. Moreover, we rigorously associate this result with the complete electrode model, and describe how a computationally cheap monotonicity-based reconstruction algorithm can be implemented. Numerical reconstructions from both simulated and real-life measurement data are presented.

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DeRisk - Accurate prediction of ULS wave loads. Outlook and first results

Loads from extreme waves can be dimensioning for the substructures of offshore wind turbines. The DeRisk project (2015-2019) aims at an improved load evaluation procedure for extreme waves through application of advanced wave models, laboratory tests of load effects, development of hydrodynamic load models, aero-elastic response calculations and statistical analysis. This first paper from the project outlines the content and philosophy behind DeRisk. Next, the first results from laboratory tests with irregular waves are presented, including results for 2D and 3D focused wave groups. The results of focused wave group tests and a 6-hour (full scale duration) test are reproduced numerically by re-application of the wave paddle signal in a fully nonlinear potential flow wave model. A good match for the free surface elevation and associated exceedance probability curve is obtained. Finally, the utilization of DeRisk’s results in practical design is discussed. (C) 2016 Published by Elsevier Ltd.
Development of a numerical modelling tool for combined near field and far field wave transformations using a coupling of potential flow solvers

Wave energy converters (WECs) need to be deployed in large numbers in an array layout in order to have a significant power production. Each WEC has an impact on the incoming wave field, diffracting, reflecting and radiating waves. Simulating the wave transformations within and around a WEC farm is complex; it is difficult to simulate both near field and far field effects with a single numerical model, with relatively fast computing times. Within this research a numerical tool is developed to model near-field and far-field wave transformations caused by WECs. The tool is based on the coupling of a wave-structure interaction solver and a wave propagation model, both based on the potential flow theory. This paper discusses the coupling method and illustrates the functionality with a proof-of-concept. Additionally, a projection of the evolution of the numerical tool is given. It can be concluded that the coupling of the two solvers is an efficient and promising numerical tool to perform simulations on near – and far field wave elevations and kinematics nearby WEC farms.

Distributed Model Predictive Control for Smart Energy Systems

Integration of a large number of flexible consumers in a smart grid requires a scalable power balancing strategy. We formulate the control problem as an optimization problem to be solved repeatedly by the aggregator in a model predictive control framework. To solve the large-scale control problem in real-time requires decomposition methods. We propose a decomposition method based on Douglas–Rachford splitting to solve this large-scale control problem. The method decomposes the problem into smaller subproblems that can be solved in parallel, e.g., locally by each unit connected to an aggregator. The total power consumption is controlled through a negotiation procedure between all cooperating units and an aggregator that coordinates the overall objective. For large-scale systems, this method is faster than solving the original problem and can be distributed to include an arbitrary number of units. We show how different aggregator
Dynamic Operation and Simulation of Post-Combustion CO2 Capture

Thermal power need to operate, on a daily basis, with frequent and fast load changes to balance the large variations of intermittent energy sources, such as wind and solar energy. To make the integration of carbon capture to power plants economically and technically feasible, the carbon capture process has to be able to follow these fast and large load changes without decreasing the overall performance of the carbon capture plant. Therefore, dynamic models for simulation, optimization and control system design are essential. In this work, we compare the transient behavior of the model against dynamic pilot data for CO2 absorption and desorption for step-changes in the flue gas flow rate. In addition we investigate the dynamic behavior of a full-scale post-combustion capture plant using monoethanolamine (MEA) and piperazine (PZ). This analysis demonstrates the good agreement between the developed model (dCAPCO2) and the pilot measurements at both, transient and steady-state conditions. It outlines how the time needed to reach a new steady-state varies with respect to amine type and concentration. The simulation study reveals that it is essential to control the lean
solvent flow to avoid sudden changes in the CO2 removal rate and to avoid increased heat demand of solvent regeneration. In addition, it shows how storage tanks (liquid hold-up of the system) can be designed to accommodate significant upstream changes in the power plant management. This flexibility is especially needed for operation in future mixed green energy market. [All rights reserved Elsevier].
the performance of this plant under critical operation. In this work, we evaluate the transient response of an absorber and a desorber for step changes of key process parameters, e.g. flue gas flow and composition, lean and rich CO₂ loading, etc. We show the results for the baseline 30 wt% MEA and the low energy piperazine (PZ) solutions. This analysis reveals that the absorber reaches steady-state faster using MEA compared to PZ. This is related to the shift of the mass transfer zone due to changes in temperature. The transient operation in the regeneration unit is somewhat similar while using both solvents: an initial fast decrease of the lean loading is followed by a slow transient period as the system approaches steady-state conditions. We show the presence of inverse response in the stripper column when the rich loading decreases or the feed's temperature reduces using PZ solvent. Thus, we demonstrate that the dynamics of the MEA system cannot be extrapolated to other solvents.

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General information
State: Published
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Economic Model Predictive Control for Spray Drying Plants
The main challenge in cost optimal operation of a spray dryer, is to maximize the production rate while minimizing the energy consumption, keeping the residual moisture content of the powder below a maximum limit and avoiding that the powder sticks to the chamber walls. The conventional PI control strategy is simple, but known to be insufficient at providing optimal operation in the presence of variations in the feed and the ambient air humidity. This motivates our investigation of Model Predictive Control (MPC) strategies.

In this thesis, we consider the development and application of new models and MPC strategies to optimize the operation of four-stage spray dryers. The models are first-principle dynamic models with parameters identified from dryer specific experiments and powder properties identified from laboratory tests. A simulation model is used for detailed closed-loop simulations and a complexity reduced control model is used for state estimation and prediction in the controllers. These models facilitate development and comparison of control strategies. We develop two MPC strategies; a linear tracking MPC with a Real-Time Optimization layer (MPC with RTO) and an Economic Nonlinear MPC (E-MPC). We tailor these for the spray drying process to optimize the cost of operation by adjustments to the inputs of the dryer according to the present disturbances and process constraints. Simulations show that MPC strategies improve the profit of operation by up to 9.69%, the production of powder by up to 9.6%, the residual moisture content by up to 0.114 p.p. and the energy efficiency by up to 6.06% while the produced powder is within the given quality specifications and sticky powder on the walls of the chamber is avoided. Thus, we are able to improve the cost of operation significantly compared to the conventional PI control strategy.

The proposed MPC strategies are based on a feedback control algorithm that explicitly handles constrained control inputs and uses a model to predict and optimize the future behavior of the dryer. The solution of the control problem results in a sequence of inputs for a finite horizon, out of which only the first input is applied to the dryer. This procedure is repeated at each sample instant and is solved numerically in real-time. The MPC with RTO tracks a target that optimizes the cost of operation at steady-state. The E-MPC optimizes the cost of operation directly by having this objective directly in the controller. The need for the RTO layer is then eliminated.

We demonstrate the application of the proposed MPC with RTO to control an industrial GEA MSDTM-1250 spray dryer,
which produces approximately 7500 kg/hr of enriched milk powder. Compared to the conventional PI controller, our first results shows that the MPC improves the profit of operation by approximately 228,000 €/year, the product rate by 322 kg/hr, the residual moisture content by 0.166 p.p. and the energy efficiency by 1% at comparable ambient air humidity conditions. The demonstrated MPC with RTO is fully integrated in the daily operation of the spray dryer today.

Our primary objectives in the thesis are: 1) Spray dryer modeling of a smallscale four-stage spray dryer. The purpose of the models are to enable simulations of the spray drying process at different operating points, such that the models facilitate development and comparison of control strategies; 2) Development of MPC strategies that automatically adjust the dryer to variations in the feed and the ambient air humidity, such that the energy consumption is minimized, the residual moisture content in the powder is controlled within the specifications and sticky powder is avoided from building up on the dryer walls; 3) Demonstrate the industrial application of an MPC strategy to a full-scale industrial four-stage spray dryer.

The main scientific contributions can be summarized to:

- Modeling of a four-stage spray dryer. We develop new first-principles engineering models for simulation of a four-stage spray dryer. These models enables simulations of the spray dryer at different operating points with high accuracy.
- Development and simulation of control strategies. We develop two control strategies, the MPC with RTO and the E-MPC strategy. The performance of the controllers is studied and evaluated by simulation.
- Industrial application of MPC to a spray dryer. We demonstrate that our proposed MPC with RTO is applicable to an industrial GEA MSDTM-1250 spray dryer, that produces enriched milk powder.

General information
State: Published
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Economic MPC for a linear stochastic system of energy units
This paper summarizes comprehensively the work in four recent PhD theses from the Technical University of Denmark related to Economic MPC of future power systems. Future power systems will consist of a large number of decentralized power producers and a large number of controllable power consumers in addition to stochastic power producers such as wind turbines and solar power plants. Control of such large scale systems requires new control algorithms. In this paper, we formulate the control of such a system as an Economic Model Predictive Control (MPC) problem. When the power producers and controllable power consumers have linear dynamics, the Economic MPC may be expressed as a linear program. We provide linear models for a number of energy units in an energy system, formulate an Economic MPC for coordination of such a system. We indicate how advances in computational MPC makes the solutions of such large-scale models feasible in real-time. The system presented may serve as a benchmark for simulation and control of smart energy systems and we indicate how advances in computational MPC.

General information
State: Published
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Effect of sparsity and exposure on total variation regularized X-ray tomography from few projections

We address effects of exposure and image gradient sparsity for total variation-regularized reconstruction: is it better to collect many low-quality or few high-quality projections, and can gradient sparsity predict how many projections are necessary? Preliminary results suggest collecting many low-quality projections is favorable, and that a link may exist between gradient sparsity level and successful reconstruction.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, University of Manchester
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Efficient uncertainty quantification of a fully nonlinear and dispersive water wave model with random inputs

A major challenge in next-generation industrial applications is to improve numerical analysis by quantifying uncertainties in predictions. In this work we present a formulation of a fully nonlinear and dispersive potential flow water wave model with random inputs for the probabilistic description of the evolution of waves. The model is analyzed using random sampling techniques and nonintrusive methods based on generalized polynomial chaos (PC). These methods allow us to accurately and efficiently estimate the probability distribution of the solution and require only the computation of the solution at different points in the parameter space, allowing for the reuse of existing simulation software. The choice of the applied methods is driven by the number of uncertain input parameters and by the fact that finding the solution of the considered model is computationally intensive. We revisit experimental benchmarks often used for validation of deterministic water wave models. Based on numerical experiments and assumed uncertainties in boundary data, our analysis reveals that some of the known discrepancies from deterministic simulation in comparison with experimental measurements could be partially explained by the variability in the model input. Finally, we present a synthetic experiment studying the variance-based sensitivity of the wave load on an offshore structure to a number of input uncertainties. In the numerical examples presented the PC methods exhibit fast convergence, suggesting that the problem is amenable to analysis using such methods.

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Organisations: Scientific Computing, Department of Applied Mathematics and Computer Science, Chalmers University of Technology
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Enzymes in CO2 Capture
The enzyme Carbonic Anhydrase (CA) can accelerate the absorption rate of CO2 into aqueous solutions by several-fold. It exist in almost all living organisms and catalyses different important processes like CO2 transport, respiration and the acid-base balances. A new technology in the field of carbon capture is the application of enzymes for acceleration of...
typically slow ternary amines or inorganic carbonates. There is a hidden potential to revive currently infeasible amines which have an interesting low energy consumption for regeneration but too slow kinetics for viable CO2 capture. The aim of this work is to discuss the measurements of kinetic properties for CA promoted CO2 capture solvent systems. The development of a rate-based model for enzymes will be discussed showing the principles of implementation and the results on using a well-known ternary amine for CO2 capture. Conclusions will be drawn revealing basic unexpected process conditions which are beneficial to enzyme promoted amines like water presence, temperatures, and similar basic variables.

General information
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High-definition velocity-space tomography of fast-ion dynamics
Velocity-space tomography of the fast-ion distribution function in a fusion plasma is usually a photon-starved tomography method due to limited optical access and signal-to-noise ratio of fast-ion Dα (FIDA) spectroscopy as well as the strive for high-resolution images. In high-definition tomography, prior information makes up for this lack of data. We restrict the target velocity space through the measured absence of FIDA light, impose phase-space densities to be non-negative, and encode the known geometry of neutral beam injection (NBI) sources. We further use a numerical simulation as prior information to reconstruct where in velocity space the measurements and the simulation disagree. This alternative approach is demonstrated for four-view as well as for two-view FIDA measurements. The high-definition tomography tools allow us to study fast ions in sawtooothing plasmas and the formation of NBI peaks at full, half and one-third energy by time-resolved tomographic movies.

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Industrial application of model predictive control to a milk powder spray drying plant

In this paper, we present our first results from an industrial application of model predictive control (MPC) with real-time steady-state target optimization (RTO) for control of an industrial spray dryer that produces enriched milk powder. The MPC algorithm is based on a continuous-time transfer function model identified from data and states estimated by a time-varying Kalman filter. The RTO layer utilizes the same linear model and a nonlinear economic objective function for calculation of the economically optimized targets. We demonstrate, by industrial application of the MPC, that this method
provides significantly better control of the residual moisture content, increases the throughput and decreases the energy consumption compared to conventional PI-control. The MPC operates the spray dryer closer to the residual moisture constraint of the powder product. Thus, the same amount of feed produces more powder product by increasing the average water content. The value of this is 186,000 €/year. In addition, the energy savings account to 6,900 €/year.

**General information**
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Organisations: Department of Applied Mathematics and Computer Science, Dynamical Systems, Department of Electrical Engineering, Automation and Control, Scientific Computing, GEA Process Engineering A/S
Authors: Petersen, L. N. (Intern), Poulsen, N. K. (Intern), Niemann, H. H. (Intern), Utzen, C. (Ekstern), Jørgensen, J. B. (Intern)
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

**Inexact proximal Newton methods for self-concordant functions**
We analyze the proximal Newton method for minimizing a sum of a self-concordant function and a convex function with an inexpensive proximal operator. We present new results on the global and local convergence of the method when inexact search directions are used. The method is illustrated with an application to L1-regularized covariance selection, in which prior constraints on the sparsity pattern of the inverse covariance matrix are imposed. In the numerical experiments the proximal Newton steps are computed by an accelerated proximal gradient method, and multifrontal algorithms for positive definite matrices with chordal sparsity patterns are used to evaluate gradients and matrix-vector products with the Hessian of the smooth component of the objective.

**General information**
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, University of California
Authors: Li, J. (Ekstern), Andersen, M. S. (Intern), Vandenberghe, L. (Ekstern)
Pages: 19–41
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Main Research Area: Technical/natural sciences

**Publication information**
Journal: Mathematical Methods of Operations Research
Volume: 85
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ISSN (Print): 1432-2994
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.542 SNIP 0.866 CiteScore 0.87
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.38 SNIP 0.661 CiteScore 0.62
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.652 SNIP 1.236 CiteScore 1.02
Large-scale Optimization of Contoured Beam Reflectors and Reflectarrays

Designing a contoured beam reflector or performing a direct optimization of a reflectarray requires a mathematical optimization procedure to determine the optimum design of the antenna. A popular approach, used in the market-leading TICRA software POS, can result in computation times on the order of days, due to the optimization algorithm. The present paper discusses recent improvements, allowing reductions in optimization time by two orders of magnitude or more on several application examples.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Software Engineering, TICRA
Authors: Borries, O. (Ekstern), Serensen, S. B. (Ekstern), Jørgensen, E. (Ekstern), Zhou, M. (Ekstern), Andersen, M. S. (Intern), Sokoler, L. E. (Intern)
Pages: 1617-1618
Publication date: 2016

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Title of host publication: Proceedings of the 2016 IEEE Antennas and Propagation Society International Symposium (APSURSI)
Publisher: IEEE
ISBN (Print): 978-1-5090-2886-3
Main Research Area: Technical/natural sciences
Electronic versions: pospaper.pdf
Limited Data Problems for the Generalized Radon Transform in $\mathbb{R}^n$

We consider the generalized Radon transform (defined in terms of smooth weight functions) on hyperplanes in $\mathbb{R}^n$. We analyze general filtered backprojection type reconstruction methods for limited data with filters given by general pseudodifferential operators. We provide microlocal characterizations of visible and added singularities in $\mathbb{R}^n$ and define modified versions of reconstruction operators that do not generate added artifacts. We calculate the symbol of our general reconstruction operators as pseudodifferential operators and provide conditions for the filters under which the reconstruction operators are elliptic for the visible singularities. If the filters are chosen according to those conditions, we show that almost all visible singularities can be recovered reliably. Our work generalizes the results for the classical line transforms in $\mathbb{R}^2$ and the classical reconstruction operators (that use specific filters). In our proofs, we employ a general paradigm that is based on the calculus of Fourier integral operators. Since this technique does not rely on explicit expressions of the reconstruction operators, it enables us to analyze more general imaging situations.
Methods and Algorithms for Economic MPC in Power Production Planning

This thesis concerns methods and algorithms for power production planning in contemporary and future power systems. Power production planning is a task that involves decisions across different time scales and planning horizons. Hours-ahead to days-ahead planning is handled by solving a mixed-integer linear program for unit commitment and economic dispatch of the system power generators. We focus on a minutes-ahead planning horizon, where unit commitment decisions are fixed. Economic model predictive control (EMPC) is employed to determine an optimal dispatch for a portfolio of power generators in real-time. A generator can represent a producer of electricity, a consumer of electricity, or possibly both. Examples of generators are heat pumps, electric vehicles, wind turbines, virtual power plants, solar cells, and conventional fuel-fired thermal power plants. Although this thesis is mainly concerned with EMPC for minutes-ahead production planning, we show that the proposed EMPC scheme can be extended to days-ahead planning (including unit commitment) as well.

The power generation from renewable energy sources such as wind and solar power is inherently uncertain and variable. A portfolio with a high penetration of renewable energy is therefore a stochastic system. To accommodate the need for EMPC of stochastic systems, we generalize certainty-equivalent EMPC (CEEMPC) to mean-variance EMPC (MV-EMPC). In MV-EMPC, the objective function is a trade-off between the expected cost and the cost variance. Simulations show that MV-EMPC reduces cost and risk compared to CE-EMPC. The simulations also show that the economic performance of CE-EMPC can be much improved using a constraint back-off heuristic.

Efficient solution of the optimal control problems (OCPs) that arise in EMPC is important, as the OCPs are solved online. We present special-purpose algorithms for EMPC of linear systems that exploit the high degree of structure in the OCPs. A Riccati-based homogeneous and self-dual interior-point method is developed for the special case, where the OCP objective function is a linear function. We design an algorithm based on the alternating direction method of multipliers (ADMM) to solve input-constrained OCPs with convex objective functions. The OCPs that occur in EMPC of dynamically decoupled subsystems, e.g. power generators, have a block-angular structure. Subsystem decomposition algorithms based on ADMM and Dantzig-Wolfe decomposition are proposed to solve these OCPs. Subproblems that arise in the decomposition algorithms are solved using structure-exploiting algorithms. To reduce computation time of the EMPC algorithms further, warm-start and early-termination strategies are employed. Benchmarks show that the special-purpose algorithms are significantly faster than current state-of-the-art solvers.

As a potential application area of EMPC, we study power production planning in small isolated power systems. A critical part of power production planning in small isolated power systems is operational reserve planning. The operational reserves are activated to balance production and consumption in real-time. An EMPC scheme is presented for activation of operational reserves. Simulations based on a Faroe Islands case study show that significant cost savings can be achieved using this strategy. For efficient planning of the operational reserves, we present an optimal reserve planning problem (ORPP). The ORPP is a contingency-constrained unit commitment problem that addresses low inertia challenges in small isolated power systems.

In summary, the main contributions of this thesis are:
- A mean-variance optimization strategy for EMPC of linear stochastic systems.
- Tailored algorithms for solution of the OCPs that arise in EMPC of linear stochastic systems.
Methods for power production planning in small isolated power; the ORPP for unit commitment and economic dispatch, and an EMPC scheme for activation of operational reserves.

Model Identification using Continuous Glucose Monitoring Data for Type 1 Diabetes

This paper addresses model identification of continuous-discrete nonlinear models for people with type 1 diabetes using sampled data from a continuous glucose monitor (CGM). We compare five identification techniques: least squares, weighted least squares, Huber regression, maximum likelihood with extended Kalman filter and maximum likelihood with unscented Kalman filter. We perform the identification on a 24-hour simulation of a stochastic differential equation (SDE) version of the Medtronic Virtual Patient (MVP) model including process and output noise. We compare the fits with the actual CGM signal, as well as the short- and long-term predictions for each identified model. The numerical results show that the maximum likelihood-based identification techniques offer the best performance in terms of fitting and prediction. Moreover, they have other advantages compared to ODE-based modeling, such as parameter tracking, population modeling and handling of outliers.
Modeling and Control for Price Responsive Electricity Loads

This thesis deals with the development of model-based control architectures to facilitate renewable sources integration in the power system, focusing on residential buildings. Energy use in buildings in developed countries is increasing rapidly, and advanced model based techniques for control of thermal storages are becoming popular due to the high demand for solutions that improve energy efficiency and reduce operating costs.

This presents new challenges on how to integrate uncertain and intermittent energy sources. This work proposes methods for control of price responsive electricity loads in future energy systems and methods for handling stochasticity of, e.g., wind and solar power production. Hierarchies of aggregators and predictive controllers, in flexible demand side response, are implemented to achieve a balance with the non-dispatchable energy production.

Particular focus is given on producing models for control that facilitate better planning for an efficient integration of renewable energy into the power generation. Combining both data and statistical expertise, opens up new possibilities for designing models that describe thermal storages flexibility.

Finally, focus is also put on the problem of managing a virtual power plant equipped with stochastic energy sources and flexible consumers. Two distinct control approaches are described: direct control of the load consumption and indirect control by broadcasting a price signal. The advantages and challenges of these two approaches are discussed providing examples for suggested techniques.

General information

State: Submitted
Organisations: Department of Applied Mathematics and Computer Science, Dynamical Systems, Scientific Computing
Authors: Parvizi, J. (Intern), Madsen, H. (Intern), Jørgensen, J. B. (Intern)
Number of pages: 184
Publication date: 2016

Publication information

Place of publication: Kgs. Lyngby
Publisher: Technical University of Denmark (DTU)
Original language: English

Series: DTU Compute PHD-2016
Number: 427
ISSN: 0909-3192
Main Research Area: Technical/natural sciences

Relations

Projects:
Modeling and Control for Price Responsive Electricity Loads
Publication: Research › Ph.D. thesis – Annual report year: 2016

Modeling and Prediction Using Stochastic Differential Equations

Pharmacokinetic/pharmacodynamic (PK/PD) modeling for a single subject is most often performed using nonlinear models based on deterministic ordinary differential equations (ODEs), and the variation between subjects in a population of subjects is described using a population (mixed effects) setup that describes the variation between subjects. The ODE setup implies that the variation for a single subject is described by a single parameter (or vector), namely the variance (covariance) of the residuals. Furthermore the prediction of the states is given as the solution to the ODEs and hence assumed deterministic and can predict the future perfectly. A more realistic approach would be to allow for randomness in the model due to e.g., the model be too simple or errors in input. We describe a modeling and prediction setup which
better reflects reality and suggests stochastic differential equations (SDEs) for modeling and forecasting. It is argued that this gives models and predictions which better reflect reality. The SDE approach also offers a more adequate framework for modeling and a number of efficient tools for model building. A software package (CTSM-R) for SDE-based modeling is briefly described.

**General information**

State: Published
Organisations: Department of Applied Mathematics and Computer Science, Dynamical Systems, Copenhagen Center for Health Technology, Center for Energy Resources Engineering, Scientific Computing
Authors: Juhl, R. (Intern), Møller, J. K. (Intern), Jørgensen, J. B. (Intern), Madsen, H. (Intern)
Pages: 183-209
Publication date: 2016

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Title of host publication: Prediction Methods for Blood Glucose Concentration: Design, Use and Evaluation
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ISBN (Print): 978-3-319-25911-6
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Series: Lecture Notes in Bioengineering
ISSN: 2195-271X
Main Research Area: Technical/natural sciences
DOIs: 10.1007/978-3-319-25913-0_10
Publication: Research - peer-review › Book chapter – Annual report year: 2016

**Modelling of glucose-insulin-glucagon pharmacodynamics in man**
The purpose is to build a simulation model of the glucoregulatory system in man. We estimate individual human parameters of a physiological glucose-insulin-glucagon model. We report posterior probability distributions and correlations of model parameters.

**General information**

State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Zealand Pharma A/S, McGill University
Authors: Wendt, S. L. (Intern), Møller, J. K. (Intern), Haidar, A. (Ekstern), Knudsen, C. B. (Ekstern), Madsen, H. (Intern), Jørgensen, J. B. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions: ieee_1page_slw_final.pdf
Source: PublicationPreSubmission
Source-ID: 125477420
Publication: Research - peer-review › Paper – Annual report year: 2016

**Modelling the glucose-insulin-glucagon dynamics after subcutaneous administration of native glucagon and a novel glucagon analogue in dogs**
Zealand Pharma has invented a glucagon analogue, ZP-GA-1, with increased stability in liquid formulation for treatment of hypoglycemia. A pharmacodynamic (PD) model is needed to compare ZP-GA-1 with marketed glucagon. We aim to develop a model of the complex glucose-insulin-glucagon dynamics based on physiology and data.

**General information**

State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Copenhagen Center for Health Technology, Center for Energy Resources Engineering, Dynamical Systems, Zealand Pharma A/S, McGill University
Authors: Wendt, S. L. (Intern), Boye Knudsen, C. (Ekstern), Jørgensen, J. B. (Intern), Madsen, H. (Intern), Haidar, A. (Ekstern)
Number of pages: 1
Publication date: 2016
Modelling the glucose-insulin-glucagon dynamics after subcutaneous administration of native glucagon and a novel glucagon analogue in dogs

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Copenhagen Center for Health Technology, Center for Energy Resources Engineering, Dynamical Systems, Zealand Pharma A/S, McGill University
Authors: Wendt, S. L. (Intern), Boye Knudsen, C. (Ekstern), Jørgensen, J. B. (Intern), Madsen, H. (Intern), Haidar, A. (Ekstern)
Number of pages: 1
Publication date: 2016
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Main Research Area: Technical/natural sciences
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Abstract number: 342
Read By Title in Diabetes Technology & Therapeutics, Volume 18, Issue S1
Source: PublicationPreSubmission
Source-ID: 120892935
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Model of the Glucose-Insulin-Glucagon Dynamics after Subcutaneous Administration of a Glucagon Rescue Bolus in Healthy Humans

In healthy individuals, insulin and glucagon work in a complex fashion to maintain blood glucose levels within a narrow range. This regulation is distorted in patients with diabetes. The hepatic glucose response due to an elevated glucagon level depends on the current insulin concentration and thus endogenous glucose production (EGP) can not be modelled without knowledge of the concentration of both hormones in plasma. Furthermore, literature suggests an upper limit to EGP irrespective of glucagon levels. We build a simulation model of the glucose-insulin-glucagon dynamics in man including saturation effect of EGP.

Ten healthy subjects received a 1 mg subcutaneous (SC) glucagon bolus (GlucaGen®). Plasma samples were collected until 300 minutes post dose and analyzed for glucagon, insulin, and glucose concentrations. All observations were used to fit a physiological model of the glucose-insulin-glucagon dynamics using the Hovorka model with a novel multiplicative description of the effects of insulin and of glucagon on EGP.

Bayesian estimation by Maximum a Posteriori using prior knowledge reported in literature was used to estimate the model parameters for each subject. Profile likelihood plots were used to investigate parameter identifiability. Unidentifiable parameters were fixed at their prior mean values.

The new model enables simulations of the glucose-insulin-glucagon dynamics in humans at both low and high glucagon concentrations (180-8000 pg/mL) and physiologic insulin concentrations (1.2-81.9 mIU/L). The model can be used for simulation of glucagon bolus strategies for treatment of hypoglycemia and for in silico simulation of dual-hormone artificial pancreas algorithms.

General information
Model of the Glucose-Insulin-Glucagon Dynamics after Subcutaneous Administration of a Glucagon Rescue Bolus in Healthy Humans

In healthy individuals, insulin and glucagon work in a complex fashion to maintain blood glucose levels within a narrow range. This regulation is distorted in patients with diabetes. The hepatic glucose response due to an elevated glucagon level depends on the current insulin concentration and thus endogenous glucose production (EGP) can not be modelled without knowledge of the concentration of both hormones in plasma. Furthermore, literature suggests an upper limit to EGP irrespective of glucagon levels. We build a simulation model of the glucose-insulin-glucagon dynamics in man including saturation effect of EGP.

Ten healthy subjects received a 1 mg subcutaneous (SC) glucagon bolus (GlucaGen®). Plasma samples were collected until 300 minutes post dose and analyzed for glucagon, insulin, and glucose concentrations. All observations were used to fit a physiological model of the glucose-insulin-glucagon dynamics using the Hovorka model with a novel multiplicative description of the effects of insulin and of glucagon on EGP.

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General information

Multi-region Statistical Shape Model for Cochlear Implantation

Statistical shape models are commonly used to analyze the variability between similar anatomical structures and their use is established as a tool for analysis and segmentation of medical images. However, using a global model to capture the variability of complex structures is not enough to achieve the best results. The complexity of a proper global model increases even more when the amount of data available is limited to a small number of datasets. Typically, the anatomical variability between structures is associated to the variability of their physiological regions. In this paper, a complete pipeline is proposed for building a multi-region statistical shape model to study the entire variability from locally identified physiological regions of the inner ear. The proposed model, which is based on an extension of the Point Distribution Model
(PDM), is built for a training set of 17 high-resolution images (24.5 μm voxels) of the inner ear. The model is evaluated according to its generalization ability and specificity. The results are compared with the ones of a global model built directly using the standard PDM approach. The evaluation results suggest that better accuracy can be achieved using a regional modeling of the inner ear.

**General information**

State: Published


Authors: Romera, J. (Ekstern), Kjer, H. M. (Intern), Piella, G. (Ekstern), Ceresa, M. (Ekstern), González Ballester, M. A. (Ekstern)

Number of pages: 8

Publication date: 2016

**Host publication information**

Title of host publication: SPIE Medical Imaging 2016: Image Processing

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ISBN (Print): 9781510600195

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Main Research Area: Technical/natural sciences

Conference: SPIE Medical Imaging 2016, San Diego, California, United States, 27/02/2016 - 27/02/2016

Statistical Shape Model, Multi-Region, Anatomical Regions, Patient Specific Modeling, Inner ear, Cochlear Implantation

DOIs: 10.1117/12.2213305

Source: Findit

Source-ID: 2306908916

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**Noise robustness of a combined phase retrieval and reconstruction method for phase-contrast tomography**

Classical reconstruction methods for phase-contrast tomography consist of two stages: phase retrieval and tomographic reconstruction. A novel algebraic method combining the two was suggested by Kostenko et al. [Opt. Express 21, 12185 (2013) [CrossRef], and preliminary results demonstrated improved reconstruction compared with a given two-stage method. Using simulated free-space propagation experiments with a single sample-detector distance, we thoroughly compare the novel method with the two-stage method to address limitations of the preliminary results. We demonstrate that the novel method is substantially more robust toward noise; our simulations point to a possible reduction in counting times by an order of magnitude.

**General information**

State: Published

Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Physics, Neutrons and X-rays for Materials Physics

Authors: Kongskov, R. D. (Intern), Jørgensen, J. S. (Intern), Poulsen, H. F. (Intern), Hansen, P. C. (Intern)

Pages: 447-454

Publication date: 2016

Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of the Optical Society of America A

Volume: 33

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Ratings:

BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
BFI (2016): BFI-level 2

Scopus rating (2016): CiteScore 1.54
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Nonlinear Multigrid for Reservoir Simulation

A feasibility study is presented on the effectiveness of applying nonlinear multigrid methods for efficient reservoir simulation of subsurface flow in porous media. A conventional strategy modeled after global linearization by means of Newton’s method is compared with an alternative strategy modeled after local linearization, leading to a nonlinear multigrid method in the form of the full-approximation scheme (FAS). It is demonstrated through numerical experiments that, without loss of robustness, the FAS method can outperform the conventional techniques in terms of algorithmic and numerical efficiency for a black-oil model. Furthermore, the use of the FAS method enables a significant reduction in memory usage compared with conventional techniques, which suggests new possibilities for improved large-scale reservoir simulation and numerical efficiency. Last, nonlinear multilevel preconditioning in the form of a hybrid-FAS/Newton strategy is demonstrated to increase robustness and efficiency.

General information

State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Abingdon Technology Center, Technical University of Denmark
Authors: Christensen, M. L. C. (Intern), Eskildsen, K. L. (Ekstern), Engsig-Karup, A. P. (Intern), Wakefield, M. (Ekstern)
Pages: 888-898
Publication date: 2016
Main Research Area: Technical/natural sciences

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Journal: SPE Journal
Volume: 21
Issue number: 3
Article number: SPE-178428-PA
ISSN (Print): 1086-055X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
The paper introduces a nonlinear multigrid solver for mixed finite element discretizations based on the Full Approximation Scheme (FAS) and element-based Algebraic Multigrid (AMGe). The main motivation to use FAS for unstructured problems is the guaranteed approximation property of the AMGe coarse spaces that were developed recently at Lawrence Livermore National Laboratory. These give the ability to derive stable and accurate coarse nonlinear discretization problems. The previous attempts (including ones with the original AMGe method), were less successful due to lack of such good approximation properties of the coarse spaces. With coarse spaces with approximation properties, our FAS approach on unstructured meshes has the ability to be as powerful/successful as FAS on geometrically refined meshes. For comparison, Newton's method and Picard iterations with an inner state-of-the-art linear solver are compared to FAS.
on a nonlinear saddle point problem with applications to porous media flow. It is demonstrated that FAS is faster than Newton’s method and Picard iterations for the experiments considered here. Due to the guaranteed approximation properties of our AMGe, the coarse spaces are very accurate, providing a solver with the potential for mesh-independent convergence on general unstructured meshes.

**General information**
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Christensen, M. L. C. (Ekstern), Villa, U. (Ekstern), Engsig-Karup, A. P. (Intern), Vassilevski, P. (Ekstern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 14th Copper Mountain Conference on Iterative Methods (2016), Copper Mountain, Colorado, United States.
Main Research Area: Technical/natural sciences
Electronic versions: christensen_max097106.pdf
Links: http://grandmaster.colorado.edu/~copper/2016/abstract/christensen_max097106/
Source: PublicationPreSubmission
Source-ID: 127899165
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

On nonlinear wave-structure interaction using an immersed boundary method in 2D

**Introduction**
We present our progress on the development and preliminary benchmarking results of a new efficient methodology for solving fully non-linear potential flow wave-structure interaction problems. The new model utilises the efficiency of finite difference methods on structured grids. The structure geometry is introduced using an Immersed Boundary Method (IBM) and the body boundary condition (BC) is satisfied with a Weighted Least Squares (WLS) approximation [7]. This allows complex geometries to be represented with high accuracy. The stability of the scheme is ensured by adopting the Weighted Essentially Non-Oscillatory (WENO) scheme [8] together with a Lax-Friedrichs type flux applied to the free surface conditions in Hamilton-Jacobi form. This work can be viewed as a novel extension of the flexible order finite difference potential flow solver OceanWave3D [2] to include the presence of a structure. The method obtains an optimum scaling of the solution effort [2] and has been implemented on massively parallel GPU architectures using the CUDA API [3] making it suitable for high resolution flow simulations. This combination of novel and robust numerical methods aims at creating new efficient tools for non-linear wave-structure interaction problems. The scheme is validated using the forced heaving motion of a two-dimensional (2D) horizontal circular cylinder with promising results, although there are still challenges to be overcome in terms of properly capturing the behavior of the intersection between the body and the free-surface.

**General information**
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Kontos, S. (Intern), Bingham, H. B. (Intern), Lindberg, O. (Intern), Engsig-Karup, A. P. (Intern)
Number of pages: 4
Publication date: 2016

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Title of host publication: Proceedings of the 31th International Workshop on Water Waves and Floating Bodies (IWWFB 2016)
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Workshop: 31th International Workshop on Water Waves and Floating Bodies (IWWFB 2016), Plymouth, United States, 03/04/2016 - 03/04/2016
Links: http://www.iwwfb.org/Workshops/31.htm
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016

On the significance of the noise model for the performance of a linear MPC in closed-loop operation

This paper discusses the significance of the noise model for the performance of a Model Predictive Controller when operating in closed-loop. The process model is parametrized as a continuous-time (CT) model and the relevant sampled-data filtering and control algorithms are developed. Using CT models typically means less parameters to identify. Systematic tuning of such controllers is discussed. Simulation studies are conducted for linear time-invariant systems showing that choosing a noise model of low order is beneficial for closed-loop performance. (C) 2016, IFAC (International
PK/PD modelling of glucose-insulin-glucagon dynamics in healthy dogs after a subcutaneous bolus administration of native glucagon or a novel glucagon analogue

Objective  We aim to develop a simulation model of the complex glucose-insulin-glucagon dynamics based on physiology and data. Furthermore, we compare pharmacokinetic (PK) and pharmacodynamic (PD) characteristics of marketed reconstituted glucagon with a stable liquid glucagon analogue invented by Zealand Pharma A/S.

Research Design and Methods  We expanded a physiological model of endogenous glucose production with multiplicative effects of insulin and glucagon and combined it with the Hovorka glucoregulatory model. We used a Bayesian framework to perform multidimensional MAP estimation of model parameters given priors reported in the literature. We used profile likelihood analysis to investigate parameter identifiability and reduce the number of model variables. We estimated model parameters in pre-clinical data from one cross-over study with a total of 20 experiments in five dogs. The dogs received two subcutaneous (SC) bolus injections of low and high doses of glucagon and ZP-GA-1 (20 and 120 nmol/kg).

Results  We report posterior probability distributions and correlations for all identifiable model parameters. Based on visual inspection and residual analysis, the PD model described data satisfactorily for both glucagon and the analogue. Parameter estimates of the PD model were not significantly different between the two compounds.

Conclusions  The new PK/PD model enables simulations of the glucose-insulin-glucagon dynamics after a SC bolus of glucagon or glucagon analogue. The novel glucagon analogue by Zealand Pharma A/S shows PK and PD characteristics similar to marketed glucagon.
Prediction Methods for Blood Glucose Concentration: Design, Use and Evaluation

Standard diabetes insulin therapy for type 1 diabetes and late stages of type 2 is based on the expected development of blood glucose (BG) both as a consequence of the metabolic glucose consumption as well as of meals and exogenous insulin intake. Traditionally, this is not done explicitly, but the insulin amount is chosen using factors that account for this expectation.

The increasing availability of more accurate continuous blood glucose measurement (CGM) systems is attracting much interest to the possibilities of explicit prediction of future BG values. Against this background, in 2014 a two-day workshop on the design, use and evaluation of prediction methods for blood glucose concentration was held at the Johannes Kepler University Linz, Austria. One intention of the workshop was to bring together experts working in various fields on the same topic, in order to shed light from different angles on the underlying problem of modeling the glucose insulin dynamics of type 1 diabetes patients.

Among the international participants were continuous glucose monitoring developers, diabetologists, mathematicians and control engineers, both, from academia and industry. In total 18 talks were given followed by panel discussions which allowed to receive direct feedback from the point of view of different disciplines.

This book is based on the contributions of that workshop and is intended to convey an overview of the different aspects involved in the prediction. The individual chapters are based on the presentations given by the authors at the workshop but were written afterward which allowed to include the findings and conclusions of the various discussions and of course updates.

The chapter "Alternative Frameworks for Personalized Insulin-Glucose Models" by Harald Kirchsteiger et al. asks the question whether more and more detailed physiological descriptions of the glucose metabolism with an ever-increasing degree of sophistication and number of modeled phenomena are really what is needed for pushing the boundaries in glucose prediction for control. As an alternative, the chapter introduces two data-based approaches that focus not on the prediction of exact future blood glucose values, but rather on the prediction of changes in the patients' blood glucose range.

The chapter "Accuracy of BG Meters and CGM Systems: Possible Influence Factors for the Glucose Prediction Based on Tissue Glucose Concentrations" by Guido Freckmann et al. discusses performance metrics used to characterize the accuracy of continuous glucose measurement devices. This topic is highly relevant for prediction models since many of them rely on the data given by the continuous sensors which are previously calibrated with blood glucose meter measurements which are also subject to measurement errors. Inaccurate measurements will directly affect the performance of the corresponding predictions.

The chapter "CGM — How Good Is Good Enough?" by Michael Schoemaker and Christopher G. Parkin also tackles the problem of continuous glucose monitor performance evaluation. Several performance metrics used in different published studies are compared and their individual characteristics analyzed. The chapter reveals why the comparison of a sensor evaluated in two different clinical studies is not always straightforward.

The chapter "Can We Use Measurements to Classify Patients Suffering from Type 1 Diabetes into Subcategories and Does It Make Sense?" by Florian Reiterer et al. makes use of continuous time prediction models to describe the interaction between ingested carbohydrates, subcutaneously injected insulin, and continuously measured glucose concentration. The identified model parameters of 12 subjects were analyzed and statistically significant correlations between the parameters and patient characteristics such as weight and age could be found.

The chapter "Prevention of Severe Hypoglycemia by Continuous EEG Monitoring" by Claus Borg Juhl et al. shows how to use EEG signals to predict upcoming hypoglycemic situations in real-time by employing artificial neural networks. The results of a 30-day long clinical study with the implanted device and the developed algorithm are presented.

The chapter "Meta-Learning Based Blood Glucose Predictor for DiabeticSmartphone App" by Valeriya Naumova et al. demonstrates how a highly sophisticated glucose prediction model can be ported from a development language running
on a PC to a format such that it can be used conveniently by the patients. A unique feature of the algorithm is its independence of any user input other than historic CGM data which is automatically transmitted from a CGM device. No parameter estimation nor prediction model individualization is required.

The chapter “Predicting Glycemia in Type 1 Diabetes Mellitus with Subspace-Based Linear Multistep Predictors” by Marzia Cescon et al. uses data-based methods to develop individualized prediction models. The model can be considered as a combination of physiological models to precompute the rate of appearance of injected insulin and ingested carbohydrates in the bloodstream and of data-based models to combine this information and compute predictions up to 120 min in the future. The results show the performance on data from 14 type 1 diabetes patients in a clinical trial.

The chapter “Empirical Representation of Blood Glucose Variability in a Compartmental Model” by Stephen D. Patek et al. shows a modeling technique designed to extract the information on the net effect of meals on the blood glucose concentration. By assuming that all major unexplained glycemic excursions can be vi Preface attributed to oral glucose ingestion, a meal vector is estimated which significantly improves the mathematical model. Results are shown on three patients during a clinical trial and on virtual patients where it is shown how the method can be used for adjustments of the basal insulin rate.

The chapter “Physiology-Based Interval Models: A Framework for Glucose Prediction Under Intra-patient Variability” by Jorge Bondia and Josep Vehi tries to cope with the large intrasubject variability by using the concept of interval predictions. Instead of predicting a single blood glucose value in the future, a whole solution envelope is determined. With the presented theory it can be guaranteed that the real value is always inside of the envelope and moreover the envelope is not conservative. The method is evaluated on a physiological diabetes model.

The chapter “Modeling and Prediction Using Stochastic Differential Equations” by Rune Juhl et al. considers uncertainty in the dynamics between different patients as well as within a patient by making use of stochastic differential equations. It is shown how the mixed effects modeling methodology can be applied such that the underlying information of several datasets from different patients is extracted to form the model.

The chapter “Uncertainties and Modeling Errors of Type 1 Diabetes Models” by Levente Kovács and Péter Szalay analyzes the effect of prediction model uncertainties on the control system during a design procedure involving the steps model reduction by elimination of state variables, state estimation using extended Kalman Filters and Sigma Point filters and linear parameter-varying control synthesis.

The chapter “Recent Results on Glucose–Insulin Predictions by Means of a State Observer for Time-Delay Systems” by Pasquale Palumbo et al. introduces a prediction model which in real time predicts the insulin concentration in blood which in turn is used in a control system. The method is tested in simulation on a time-delay system representing the glucose–insulin system.

The chapter “Performance Assessment of Model-Based Artificial Pancreas Control Systems” by Jianyuan Feng et al. makes use of prediction models to compute treatment advices. The novelty of the proposed algorithm consists in explicitly considering (among others) the model prediction error and model error elimination speed. A retuning of the advisory system is done in case the prediction model does not perform well. Results on 30 virtual patients show the performance of the control system.

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Prior Information in Inverse Boundary Problems
This thesis gives a threefold perspective on the inverse problem of inclusion detection in electrical impedance tomography: depth dependence, monotonicity-based reconstruction, and sparsity-based reconstruction.

The depth dependence is given in terms of explicit bounds on the datum norm, which shows the change in distinguishability of inclusions (support of an inhomogeneity) as they are placed closer towards the measurement boundary. This is done by determining eigenvalue bounds for differences of pseudodifferential operators on the boundary of the domain. Ultimately, the bounds serves as insight into how much noise that can be allowed in the datum before an inclusion cannot be detected.

The monotonicity method is a direct reconstruction method that utilizes a monotonicity property of the forward problem in order to characterize the inclusions. Here we rigorously prove that the method can be regularized against noise with a uniform regularization parameter, and that the method can be generalized to discrete electrode models. We give examples in 2D and 3D with noisy simulated data as well as real measurements, and give a comparison of reconstructions based on a non-linear and a linear formulation of the method.

Sparsity-based reconstruction is an iterative method, that through an optimization problem with a sparsity prior, approximates the inhomogeneities. Here we make use of prior information, that can cheaply be obtained from the monotonicity method, to improve both the contrast and resolution of the reconstruction. Numerical examples are given in both 2D and 3D for partial data using noisy simulated data as well as real measurements.

Protein Structure Refinement by Optimization
Proteins are the main active elements of life whose chemical activities regulate cellular activities. A protein is characterized by having a sequence of amino acids and a three dimensional structure. The three-dimensional structure has only been determined experimentally for 50000 of the seven million sequences that are known. Determining the protein structure from its sequence of amino acids is therefore a major problem in computational structural biology and is referred to as the protein folding problem. The folding problem is solved using de novo methods or comparative methods depending on whether the three-dimensional structure of a homologous sequence is known. Whether or not a protein model can be used for industrial purposes depends on the quality of the predicted structure. A model can be used to design a drug when the quality is high.

The overall goal of this project is to assess and improve the quality of a predicted structure. The starting point of this work is a technique called metric training where a knowledge-based protein potential, for a fixed set of native protein structures and a set of deformed decoys for each native structure, is designed to have native-decoy energy gaps that correlates maximally to a native-decoy distance. The main contribution of this thesis is methods developed for analyzing the performance of metrically trained knowledge-based potentials and for optimizing their performance while making them less dependent on the decoy set used to define them. We focus on using the gradient and the Hessian in the analysis and present a novel smooth solvation potential but otherwise the studied potential is kept close to standard coarse grained potentials.
We analyze the importance of the choice of metric both when used in metric training and when used in the evaluation of the performance of the resulting potential and find a significant improvement by using a metric based on intrinsic geometry. It is well-known that energy minimization of a potential that is efficient in ordering a fixed set of decoys need not bring the decoys closer to the native state. The next part of the work is focused on improving the convergence of decoy structures and we present a method that significantly improves the results of shorter energy minimizations of a metrically trained potential and discuss its limitations. In an ideal potential all nearnative decoys will converge toward the native structure being at-least a local minimum of the potential. To address how far the current functional form of the potential is from an ideal potential we present two methods for finding the optimal metrically trained potential that simultaneous has a number of native structures as a local minimum. Our results generally indicate that a more fine-grained potential is needed to meet desired model accuracies but even with our coarse-grained model we obtain good results and there is an unexplored possibility to combine it with comparative modeling.

To allow fast energy minimization in Matlab a new set of more sparse formulas to calculate the first and second derivatives of a molecular potential is derived and implemented.

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Random walks with shape prior for cochlea segmentation in ex vivo μCT
Purpose
Cochlear implantation is a safe and effective surgical procedure to restore hearing in deaf patients. However, the level of restoration achieved may vary due to differences in anatomy, implant type and surgical access. In order to reduce the variability of the surgical outcomes, we previously proposed the use of a high-resolution model built from μCT images and then adapted to patient-specific clinical CT scans. As the accuracy of the model is dependent on the precision of the original segmentation, it is extremely important to have accurate μCT segmentation algorithms.

Methods
We propose a new framework for cochlea segmentation in ex vivo μCT images using random walks where a distance-based shape prior is combined with a region term estimated by a Gaussian mixture model. The prior is also weighted by a confidence map to adjust its influence according to the strength of the image contour. Random walks is performed iteratively, and the prior mask is aligned in every iteration.

Results
We tested the proposed approach in ten μCT data sets and compared it with other random walks-based segmentation techniques such as guided random walks (Eslami et al. in Med Image Anal 17(2):236–253, 2013) and constrained random walks (Li et al. in Advances in image and video technology. Springer, Berlin, pp 215–226, 2012). Our approach demonstrated higher accuracy results due to the probability density model constituted by the region term and shape prior information weighed by a confidence map.

Conclusion
The weighted combination of the distance-based shape prior with a region term into random walks provides accurate segmentations of the cochlea. The experiments suggest that the proposed approach is robust for cochlea segmentation.
Robust Numerical Methods for Nonlinear Wave-Structure Interaction in a Moving Frame of Reference

This project is focused on improving the state of the art for predicting the interaction between nonlinear ocean waves and marine structures. To achieve this goal, a flexible order finite difference potential flow solver has been extended to calculate for fully nonlinear wave-structure interaction problems at forward speed. The model utilises the efficiency of finite difference methods on structured grids and exploits the flexibility of a novel Immersed Boundary Method (IBM) based on Weighted Least Squares (WLS) for the approximation of the no-flux boundary condition on the body surface. As a result, the grid generation is very simple and the need for regridding when considering moving body problems is avoided. The temporal oscillations related to the IBM method and moving boundaries are minimized by sufficient spatial resolution and an increased time-step size.

The time-dependent physical domain is mapped to a time-invariant computational domain with a sigma transformation. For a smooth and continuous transformation a $C^2$ continuous free surface is required over the entire domain. Thus, an artificial free surface that respects this property is created in the interior of the body using a seventh order polynomial. The forward speed problem is formulated in a moving coordinate system attached to the mean position of the body. Robust approximations for all combinations of forward speed and wave velocity are obtained by expressing the free surface boundary conditions in Hamilton-Jacobi form and using a Weighted Essentially Non-Oscillatory (WENO) scheme for the convective derivatives. The linear WENO weights are derived with a new procedure that is suitable for numerical implementation and avoids the limitations of existing tabulated WENO coefficients. Furthermore, a simplified smoothness indicator that performs as well as the tabulated versions is proposed. Explicit high-order Runge-Kutta time integration and a Lax-Friedrichs-type numerical flux complete the scheme. The solver was tested on the two-dimensional zero speed wave radiation problem and the steady forward speed problem with satisfactory results and thus, the proof of concept for extending the methodology to three dimensions is established.
Simultaneous Reconstruction and Segmentation with Class-Specific Priors

Studying the interior of objects using tomography often require an image segmentation, such that different material properties can be quantified. This can for example be volume or surface area. Segmentation is typically done as an image analysis step after the image has been reconstructed. This thesis investigates computing the reconstruction and segmentation simultaneously. The advantage of this is that because the reconstruction and segmentation are computed jointly, reconstruction errors are not propagated to the segmentation step. Furthermore the segmentation procedure can be used for regularizing the reconstruction process. The thesis provides models and algorithms for simultaneous reconstruction and segmentation and their performance is empirically validated.

Two method of simultaneous reconstruction and segmentation are described in the thesis. Also, a method for parameter selection is given. The reconstruction and segmentation are modeled as two parts: the image that is reconstructed and a so-called Hidden Markov Measure Field Model (HMMFM). Pixel values in the image contain material attenuation coefficients and the HMMFM contains pixelwise probabilities for material classes. The number of material classes and their parameters are assumed known a priori. These parameters are the mean value of the class attenuation coefficients and their standard deviations. Given this input together with projection data, the problem is to find the image and HMMFM. The segmentation is obtained from the HMMFM as the most probable class in each pixel.

The solution for the reconstruction and segmentation problem is found using an algorithm that simultaneously minimizes the reprojection error, deviation of the grey levels of pixels from known mean values and the spatial differences in the class probabilities.

In the first Simultaneous Reconstruction and Segmentation (SRS) method data is assumed Gaussian distributed and the minimization is done using standard optimization techniques in two stages. Experimental validation on both phantom and real data shows that modeling the reconstruction and segmentation simultaneously has superior performance, especially when the problem is underdetermined, i.e. when the number of unknowns in the reconstruction exceeds the number of observations.

The second SRS method assumes Poisson distributed data, which is the case for data originating from discrete events like photon counts. The algorithm is again based on solving a minimization problem. In addition a relaxation strategy is employed in order to avoid being stuck in local minimum. This model is also validated on artificial data.

Selecting appropriate regularization parameters can be difficult, so the last thing that we consider is a parameter selection approach. The most promising approach was a modified L-curve algorithm, which was empirically analyzed.

This thesis contributes with methods for simultaneous reconstruction and segmentation and demonstrates the benefits of this approach in situations where only few projections are available and data is noisy. Here a higher precision image as well as segmentation can be computed.
Sparsity prior for electrical impedance tomography with partial data

This paper focuses on prior information for improved sparsity reconstruction in electrical impedance tomography with partial data, i.e. Cauchy data measured on subsets of the boundary. Sparsity is enforced using an (Formula presented.) norm of the basis coefficients as the penalty term in a Tikhonov functional, and prior information is incorporated by applying a spatially distributed regularization parameter. The resulting optimization problem allows great flexibility with respect to the choice of measurement subsets of the boundary and incorporation of prior knowledge. In fact, the measurement subsets can be chosen completely arbitrary. The problem is solved using a generalized conditional gradient method applying soft thresholding. Numerical examples with noisy simulated data show that the addition of prior information in the proposed algorithm gives vastly improved reconstructions, even for the partial data problem. Moreover, numerical examples show that a reliable reconstruction for the partial data problem can only be found close to the measurement subsets. The method is in addition compared to a total variation approach.

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Spectral Tensor-Train Decomposition

The accurate approximation of high-dimensional functions is an essential task in uncertainty quantification and many other fields. We propose a new function approximation scheme based on a spectral extension of the tensor-train (TT) decomposition. We first define a functional version of the TT decomposition and analyze its properties. We obtain results on the convergence of the decomposition, revealing links between the regularity of the function, the dimension of the input space, and the TT ranks. We also show that the regularity of the target function is preserved by the univariate functions (i.e., the “cores”) comprising the functional TT decomposition. This result motivates an approximation scheme employing polynomial approximations of the cores. For functions with appropriate regularity, the resulting spectral tensor-train decomposition combines the favorable dimension-scaling of the TT decomposition with the spectral convergence rate of polynomial approximations, yielding efficient and accurate surrogates for high-dimensional functions. To construct these decompositions, we use the sampling algorithm `TT-DMRG-cross` to obtain the TT decomposition of tensors resulting from suitable discretizations of the target function. We assess the performance of the method on a range of numerical examples: a modified set of Genz functions with dimension up to 100, and functions with mixed Fourier modes or with local features. We observe significant improvements in performance over an anisotropic adaptive Smolyak approach. The method is also used to approximate the solution of an elliptic PDE with random input data. The open source software and examples presented in this work are available online (http://pypi.python.org/pypi/TensorToolbox/).
**Time-explicit methods for joint economical and geological risk mitigation in production optimization**

Real-life applications of production optimization face challenges of risks related to unpredictable fluctuations in oil prices and sparse geological data. Consequently, operating companies are reluctant to adopt model-based production
optimization into their operations. Conventional production optimization methods focus on mitigation of geological risks related to the long-term net present value (NPV). A major drawback of such methods is that the time-dependent and exceedingly growing uncertainty of oil prices implies that long-term predictions become highly unreliable. Conventional methods therefore leave the oil production subject to substantial economical risk. To address this challenge, this paper introduces a novel set of time-explicit (TE) methods, which combine ideas of multi-objective optimization and ensemble-based risk mitigation into a computationally tractable joint effort of mitigating economical and geological risks. As opposed to conventional strategies that focus on a single long-term objective, TE methods seek to reduce risks and promote returns over the entire reservoir life by optimization of a given ensemble-based geological risk measure over time. By explicit involvement of time, economical risks are implicitly addressed by balancing short-term and long-term objectives throughout the reservoir life. Open-loop simulations of a two-phase synthetic reservoir demonstrate that TE methods may significantly improve short-term risk measures such as expected return, standard deviation and conditional value-at-risk compared to nominal, robust and mean-variance optimization. The gains in short-term objectives are obtained with none or only slight deterioration of long-term objectives.

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Unstructured Spectral Element Model for Dispersive and Nonlinear Wave Propagation

We introduce a new stabilized high-order and unstructured numerical model for modeling fully nonlinear and dispersive water waves. The model is based on a nodal spectral element method of arbitrary order in space and a -transformed formulation due to Cai, Langtangen, Nielsen and Tveito (1998). In the present paper we use a single layer of quadratic (in 2D) and prismatic (in 3D) elements. The model has been stabilized through a combination of over-integration of the Galerkin projections and a mild modal filter. We present numerical tests of nonlinear waves serving as a proof-of-concept validation for this new high-order model. The model is shown to exhibit exponential convergence even for very steep waves and there is a good agreement to analytic and experimental data.

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3D reconstruction for partial data electrical impedance tomography using a sparsity prior

In electrical impedance tomography the electrical conductivity inside a physical body is computed from electro-static boundary measurements. The focus of this paper is to extend recent results for the 2D problem to 3D: prior information about the sparsity and spatial distribution of the conductivity is used to improve reconstructions for the partial data problem with Cauchy data measured only on a subset of the boundary. A sparsity prior is enforced using the r1 norm in the penalty term of a Tikhonov functional, and spatial prior information is incorporated by applying a spatially distributed regularization parameter. The optimization problem is solved numerically using a generalized conditional gradient method with soft
thresholding. Numerical examples show the effectiveness of the suggested method even for the partial data problem with measurements affected by noise.

A Bolus Calculator Based on Continuous-Discrete Unscented Kalman Filtering for Type 1 Diabetics

In patients with type 1 diabetes, the effects of meals intake on blood glucose level are usually mitigated by administering a large amount of insulin (bolus) at mealtime or even slightly before. This strategy assumes, among other things, a prior knowledge of the meal size and the postprandial glucose dynamics. On the other hand, administering the meal bolus during or after mealtime could benefit from the information provided by the postprandial meal dynamics at the expense of a delayed meal bolus. The present paper investigates different bolus administration strategies (at mealtime, 15 minutes after or 30 minutes after the beginning of the meal). We implement a continuous-discrete unscented Kalman filter to estimate the states and insulin sensitivity. These estimates are used in a bolus calculator. The numerical results demonstrate that administering the meal bolus 15 minutes after mealtime both reduces the risk of hypoglycemia in case of an overestimated meal and the time spent in hyperglycemia if the meal size is underestimated. Faster insulin and the use of glucagon will have the potential to encourage postprandial meal bolus administration and hence will not require to accurately estimate the meal size.
A Continuous-Discrete Extended Kalman Filter for State and Parameter Estimation in People with Type 1 Diabetes

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Adaptive spectral tensor-strain decomposition for the construction of surrogate models
The construction of surrogate models is important as a mean of acceleration in computational methods for uncertainty quantification (UQ). When the forward model is particularly expensive, surrogate models can be used for the forward propagation of uncertainty [4] and the solution of inference problems [5]. An adaptive construction is necessary to meet the prescribed accuracy tolerances with the lowest computational effort.
A dynamic mathematical model for packed columns in carbon capture plants

In this paper, we present a dynamic mathematical model for the absorption and desorption columns in a carbon capture plant. Carbon capture plants must be operated in synchronization with the operation of thermal power plants. Dynamic and flexible operation of the carbon capture plant is important as thermal plants must be operated very flexibly to accommodate large shares of intermittent energy sources such as wind and solar in the energy system. To facilitate such operation, dynamic models for simulation, optimization and control system design are crucial. The dynamic model developed in this paper is suitable for gas-liquid packed columns, e.g. for CO2 absorption and desorption. The model is based on rigorous thermodynamic and conservation principles and it is set up to preserve these properties upon numerical integration in time. The developed model is applied for CO2 absorption and desorption simulation using monoethanolamine (MEA) and piperazine (PZ) as solvent. MEA is considered as the base-case solvent in the carbon capture business. The effect of changes in the flue gas flow rate and changes in the available steam are investigated to determine their influence on the performance of the capture process. The response of the model is shown in terms of capture efficiency and purity of the CO2 product stream. The model is aimed for rigorous dynamic simulation in the context of optimization and control strategy development.

A Homogeneous and Self-Dual Interior-Point Linear Programming Algorithm for Economic Model Predictive Control

We develop an efficient homogeneous and self-dual interior-point method (IPM) for the linear programs arising in economic model predictive control of constrained linear systems with linear objective functions. The algorithm is based on a Riccati iteration procedure, which is adapted to the linear system of equations solved in homogeneous and self-dual IPMs. Fast convergence is further achieved using a warm-start strategy. We implement the algorithm in MATLAB and C. Its performance is tested using a conceptual power management case study. Closed loop simulations show that 1) the proposed algorithm is significantly faster than several state-of-the-art IPMs based on sparse linear algebra, and 2) warm-start reduces the average number of iterations by 35-40%.
Algorithms for Electromagnetic Scattering Analysis of Electrically Large Structures

Accurate analysis of electrically large antennas is often done using either Physical Optics (PO) or Method of Moments (MoM), where the former typically requires fewer computational resources but has a limited application regime. This study has focused on fast variants of these two methods, with the goal of reducing the computational complexity while maintaining accuracy.

Regarding MoM, the complexity is reduced by applying the Multi-Level Fast Multipole Method (MLFMM) in combination with an iterative solver. Using MLFMM with a MoM implementation based on Higher-Order (HO) basis functions has, by several authors, been dismissed as being too memory intensive. In the present work, we demonstrate for the first time that by including a range of both novel and previously presented modifications to the standard MLFMM implementation, HO MLFMM can achieve both memory reduction and significant speed increase compared to Lower-Order (e.g., RWG) based MLFMM. Further, issues surrounding an iterative solution, such as the iterative solver and preconditioning, are discussed. Numerical results demonstrate the performance and stability of the algorithm for very large problems, including full satellites at Ku band.

Accelerating PO is an entirely different matter. A few authors have discussed applying the Fast-PO technique to far fields, achieving relative errors of 0.1%–1% for moderately sized scatterers. For near-fields, the state-of-the-art implementation of Fast-PO has several difficulties, in particular low accuracy and limited application regime. For the problems considered in this thesis, the error limit for PO is ≈ 0.01%, and the application limitations of the published Fast-PO are too prohibitive for our use. Therefore, results based on an improved Fast-PO implementation for far-fields, as well as a novel algorithm for near-fields, are presented. These results demonstrate that it is possible to achieve very accurate results, with relative errors around $10^{-5}$, at a much reduced time consumption. The method behind this part of the code is deemed confidential by TICRA.

Analysis of Electrically Large Antennas using Fast Physical Optics

The design of electrically large antennas can be a significant challenge for computational electromagnetics (CEM) tools, particularly during the final stages of the design process where there are strict requirements for the accuracy. In the present paper, we consider the use of a newly developed accelerated Physical Optics (Fast-PO) and show that this approach allows for a timely and accurate solution of realistic designs. Several examples, ranging from canonical tests of the scaling of the method against the wavelength to real-life applications, illustrate the performance of the approach in practice.
An artificial pancreas for automated blood glucose control in patients with Type 1 diabetes
Automated glucose control in patients with Type 1 diabetes is much-coveted by patients, relatives and healthcare professionals. It is the expectation that a system for automated control, also known as an artificial pancreas, will improve glucose control, reduce the risk of diabetes complications and markedly improve patient quality of life. An artificial pancreas consists of portable devices for glucose sensing and insulin delivery which are controlled by an algorithm residing on a computer. The technology is still under development and currently no artificial pancreas is commercially available. This review gives an introduction to recent progress, challenges and future prospects within the field of artificial pancreas research.

A novel tuning approach for offset-free MPC
Since the beginnings in the chemical and process industry, model based predictive control strategies have become widely accepted. Often mentioned success factors for MPC are the use of optimization based on a plant model, the consideration of constraints, and an intuitive tuning. Indeed, if a nominal plant and overall objective are known, the tuning can become straightforward. However, as soon as disturbances have to be taken into account, the tuning effort increases and becomes less intuitive. Against this background, a novel strategy to address the issues with unknown disturbances is proposed. The idea is to separate the nominal tuning process and extend the control by an outer loop, which ensures offset-free control. The inner, nominal loop decouples the system and essentially leads to a first order response. This inner loop addresses the performance targets in the nominal case, and the outer loop provides offset-free control in case of unknown disturbances. The outer loop consists of feedback controllers adapting the reference, which due to the decoupling can be tuned by known guidelines. The proposed strategy is presented and evaluated using a simulated case study.
A Parameter Choice Method for Simultaneous Reconstruction and Segmentation

The problem of finding good regularization parameters for the reconstruction problems without knowledge of the ground truth is a non-trivial task. We overview the existing parameter choice methods and present the modified L-curves approach for a good regularization parameters selection that is suited for our Simultaneous Reconstruction and Segmentation method. We verify the validity of this approach with numerical experiments based on reconstructions of artificial phantoms from noisy data, and the problems in our numerical experiments are underdetermined.

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A Spectral Element Method for Nonlinear and Dispersive Water Waves

The use of flexible mesh discretisation methods are important for simulation of nonlinear wave-structure interactions in offshore and marine settings such as harbour and coastal areas. For real applications, development of efficient models for wave propagation based on unstructured discretisation methods is of key interest. We present a high-order general-purpose three-dimensional numerical model solving fully nonlinear and dispersive potential flow equations with a free surface.

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Bihormonal control of blood glucose in people with type 1 diabetes

This paper presents a bihormonal artificial pancreas (AP) for people with type 1 diabetes (T1D) designed to provide a safe blood glucose control with minimal use of glucagon. The control algorithm uses insulin as well as glucagon to prevent hyper- and hypoglycemia. We employ a novel prediction-based activation of glucagon administration. The control algorithm consists of a Kalman filter, an insulin infusion model predictive controller (MPC), a proportional-derivative (PD) controller for glucagon infusion, and a meal time insulin bolus calculator. The PD controller is activated if the Kalman filter predicts hypoglycemia. Predictions utilize an ARMAX model describing glucose-insulin and glucose-glucagon dynamics. The model parameters are estimated from basic patient-specific data. A continuous glucose monitor provides feedback. We test the control algorithm using a simulation model with time-varying parameters available for 3 patients. We consider a simulation scenario where meals are estimated correctly as well as overestimated by 30%. The simulation results demonstrate that during normal operation, the controller only needs insulin and does not need glucagon. During unexpected events, such as insulin overdose due to an overestimated meal, the control algorithm uses glucagon efficiently to avoid severe hypoglycemia.

Characterization of nano-textured samples in a production environment

Nano-textured surfaces have been characterized by optical diffraction techniques using an adapted commercial light microscope with two detectors, a CCD camera and a spectrometer. We demonstrate that the microscope has a resolution in the nanometer range, also in an environment with many vibrations, such as a machine floor. The acquisition and analysing time for the topological parameters height, width and sidewall angle is only a few milliseconds. It is demonstrated that by simple adaptions to an optical microscope we can measure nano-textured surfaces with an uncertainty of a few nanometers for the height and width of the structures. The microscope has been validated by measuring on certified transfer artefact and 1D gratings. The measurements are very robust, such that vibrations of the sample and/or the microscope do not affect the results. The sample can be translated during acquisition, as long as the beam spot is kept inside an area with homogenous structures, which makes the proposed microscope well suited for implementation in a production environment.
Chordal Graphs and Semidefinite Optimization

Chordal graphs play a central role in techniques for exploiting sparsity in large semidefinite optimization problems and in related convex optimization problems involving sparse positive semidefinite matrices. Chordal graph properties are also fundamental to several classical results in combinatorial optimization, linear algebra, statistics, signal processing, machine learning, and nonlinear optimization. This survey covers the theory and applications of chordal graphs, with an emphasis on algorithms developed in the literature on sparse Cholesky factorization. These algorithms are formulated as recursions on elimination trees, supernodal elimination trees, or clique trees associated with the graph. The best known example is the multifrontal Cholesky factorization algorithm, but similar algorithms can be formulated for a variety of related problems, including the computation of the partial inverse of a sparse positive definite matrix, positive semidefinite and Euclidean distance matrix completion problems, and the evaluation of gradients and Hessians of logarithmic barriers for cones of sparse positive semidefinite matrices and their dual cones. The purpose of the survey is to show how these techniques can be applied in algorithms for sparse semidefinite optimization, and to point out the connections with related topics outside semidefinite optimization, such as probabilistic networks, matrix completion problems, and partial separability in nonlinear optimization.

Comparison of Linear and Nonlinear Model Predictive Control for Optimization of Spray Dryer Operation

In this paper, we compare the performance of an economically optimizing Nonlinear Model Predictive Controller (E-NMPC) to a linear tracking Model Predictive Controller (MPC) for a spray drying plant. We find in this simulation study, that the economic performance of the two controllers are almost equal. We evaluate the economic performance with an industrially recorded disturbance scenario, where unmeasured disturbances and model mismatch are present. The state of the spray dryer, used in the E-NMPC and MPC, is estimated using Kalman Filters with noise covariances estimated by a maximum likelihood (ML) method.
Comparison of Prediction Models for a Dual-Hormone Artificial Pancreas

In this paper we compare the performance of five different continuous time transfer function models used in closed-loop model predictive control (MPC). These models describe the glucose-insulin and glucose-glucagon dynamics. They are discretized into a state-space description and used as prediction models in the MPC algorithm. We simulate a scenario including meals and daily variations in the model parameters. The numerical results do not show significant changes in the glucose traces for any of the models, excepted for the first order model. From the present study, we can conclude that the second order model without delay should provide the best trade-off between sensitivity to uncertainties and practical usability for in vivo clinical studies.
Computational Hydrodynamics: How Portable and Scalable Are Heterogeneous Programming Paradigms?

New many-core era applications at the interface of mathematics and computer science adopt modern parallel programming paradigms and expose parallelism through proper algorithms. We present new performance results for a novel massively parallel free surface wave model suitable for advanced simulations in arbitrary size Numerical Wave Tanks.

The application has already been studied in a series of works (see References) and is demonstrated to exhibit excellent performance portability and scalability using hybrid MPI-OpenCL/CUDA. Furthermore, it can be executed on arbitrary heterogeneous multi-device system sizes from desktops to large HPC systems such as superclusters and in the cloud utilizing heterogeneous devices like multi-core CPUs, GPUs, and Xeon Phi coprocessors.

The numerical efficiency is evaluated on heterogeneous devices like multi-core CPUs, GPUs and Xeon Phi coprocessors to test the performance with respect to both portability and scalability. This study contributes to investigating the potential of code acceleration for reducing turn-around times of industrial CFD applications on heterogeneous hardware.

General information
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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Technical University of Denmark, Lloyd's Register Consulting
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Contingency-Constrained Unit Commitment in Meshed Isolated Power Systems

This paper presents a mixed-integer linear optimization problem for unit commitment and economic dispatch of power generators in a meshed isolated power system. The optimization problem is referred to as the optimal reserve planning problem (ORPP). The ORPP guarantees that the system frequency is kept above a predefined limit in the event of a contingency. The minimum frequency constraints are formulated using novel sufficient conditions that take into account the system inertia and the dynamics of the power generators. The proposed sufficient conditions are attractive from both a computational and a modelling point of view. We compare the ORPP to a unit commitment problem that only considers the stationary behavior of the frequency. Simulations based on a Faroe Islands case study show that, without being overly conservative, potential blackouts and power outages can be avoided using the ORPP. In the particular case study, the cost increase associated with the additional security provided by the ORPP is less than 3%.

General information
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Authors: Sokoler, L. E. (Intern), Vinter, P. (Ekstern), Bærentsen, R. (Ekstern), Edlund, K. (Ekstern), Jørgensen, J. B. (Intern)
Control of a post-combustion CO₂ capture plant during process start-up and load variations

Dynamic and flexible operation of a carbon capture plant is important as thermal power plants must be operated very flexibly to accommodate large shares of intermittent energy sources such as wind and solar energy. To facilitate such operation, dynamic models for simulation, optimization and control system design are crucial. In this paper, we present a dynamic mathematical model for the absorption and desorption columns in a carbon capture plant. Moreover, we implement a decentralized proportional-integral (PI) based control scheme and we evaluate the performance of the control structure for various operational procedures, e.g. start-up, load changes, noise on the flue gas flow rate and composition. Note that the carbon capture plant is based on the solvent storage configuration. To the authors knowledge, this is the first paper addressing the issue of start-up operation and control of carbon capture. The study demonstrates that the implemented control structure keeps the carbon capture process at 90% CO₂ removal rate with a deviation up to 8% during load variations. In addition, it reveals that the control structure brings the process to the desired set point in approximately 10 min during process start-up. [All rights reserved Elsevier].

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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
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Control of a post-combustion CO₂ capture plant during process start-up and load variations

Dynamic and flexible operation of a carbon capture plant is important as thermal power plants must be operated very flexibly to accommodate large shares of intermittent energy sources such as wind and solar energy. To facilitate such operation, dynamic models for simulation, optimization and control system design are crucial. In this paper, we present a dynamic mathematical model for the absorption and desorption columns in a carbon capture plant. Moreover, we implement a decentralized proportional-integral (PI) based control scheme and we evaluate the performance of the control structure for various operational procedures, e.g. start-up, load changes, noise on the flue gas flow rate and composition. Note that the carbon capture plant is based on the solvent storage configuration. To the authors knowledge, this is the first paper addressing the issue of start-up operation and control of carbon capture. The study demonstrates that the implemented control structure keeps the carbon capture process at 90% CO₂ removal rate with a deviation up to 8% during load variations. In addition, it reveals that the control structure brings the process to the desired set point in approximately 10 min during process start-up.

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Organisations: Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Copenhagen Center for Health Technology, Department of Applied
Control of Electricity Load in Future Smart Cities

General information
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Organisations: Department of Applied Mathematics and Computer Science, Dynamical Systems, Scientific Computing
Authors: Madsen, H. (Intern), Parvizi, J. (Intern), Halvgaard, R. (Intern), Jørgensen, J. B. (Intern)
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Control of Electricity Loads in Future Electric Energy Systems

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Chapter: 24
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Book chapter – Annual report year: 2015
Economic Model Predictive Control for Large-Scale and Distributed Energy Systems

In this thesis, we consider control strategies for large and distributed energy systems that are important for the implementation of smart grid technologies. An electrical grid has to ensure reliability and avoid long-term interruptions in the power supply. Moreover, the share of Renewable Energy Sources (RESs) in the smart grids is increasing. These energy sources bring uncertainty to the production due to their fluctuations. Hence, smart grids need suitable control systems that are able to continuously balance power production and consumption. We apply the Economic Model Predictive Control (EMPC) strategy to optimise the economic performances of the energy systems and to balance the power production and consumption. In the case of large-scale energy systems, the electrical grid connects a high number of power units. Because of this, the related control problem involves a high number of variables and constraints and its solution requires high computational times. Energy systems have a hierarchical control framework and the controllers have to work in the time-scale required by their hierarchy level. Dedicated optimisation techniques efficiently solve the control problem and reduce computational time. We implement the Dantzig-Wolfe decomposition technique to efficiently solve the EMPC problem.

The contributions of this thesis are primarily on:

**Large-scale energy system**

Smart-grids connect a high number of energy units. In such a large-scale scenario the energy units are independent and dynamically decoupled. The mathematical model of the large-scale energy system embodies the decoupled dynamics of each power units. Moreover, all units of the grid contribute to the overall power production.

**Economic Model Predictive Control (EMPC)**

This control strategy is an extension of the Model Predictive Control (MPC) strategy. Energy systems often involve stochastic variables due to the share of fluctuating Renewable Energy Sources (RESs). Moreover, the related control problems are multi variables and they are hard, or impossible, to split into single-input-single-output control systems. MPC strategy can handle multi variables control problems and it can embody stochastic variables. The Economic MPC (EMPC) policy optimises the economic performances of the process. In this work, we apply the EMPC to energy systems and it computes the control trajectory for each energy unit. This control policy minimises production costs and ensures that the power production satisfies the customers' demand. The EMPC designs a linear control problem that has a block-angular constraints matrix and it has two sets of constraints. The independent dynamics of the energy units define the decoupling constraints sited on the diagonal. The coupling constraints represent the common goal of all power units in the energy system and this is to satisfy the customers' demand. The Dantzig-Wolfe optimisation technique applies to this structure of the constraints matrix in the view of fastening the control algorithm and increase its applicability.

**Dantzig-Wolfe decomposition**

The Dantzig-Wolfe decomposition solves the EMPC problem through a distributed optimisation technique. The EMPC problem via Dantzig-Wolfe decomposition algorithm computes the optimal input trajectory for each energy unit and reduces the computation times. Moreover, such a control algorithm applies to large-scale energy systems and the number of energy units does not affect the performances of the controller. In this thesis, we also investigate suboptimal solutions of the EMPC problem via modified versions of the Dantzig-Wolfe decomposition algorithms. The feasibility of the suboptimal solutions suffices for stability. The goal of these modified Dantzig-Wolfe decomposition algorithms is to reduce computation time in the solution of the EMPC problem.

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Economic Optimization of Spray Dryer Operation using Nonlinear Model Predictive Control with State Estimation

In this paper, we develop an economically optimizing Nonlinear Model Predictive Controller (E-NMPC) for a complete spray drying plant with multiple stages. In the E-NMPC the initial state is estimated by an extended Kalman Filter (EKF) with noise covariances estimated by an autocovariance least squares method (ALS). We present a model for the spray drying plant and use this model for simulation as well as for prediction in the E-NMPC. The open-loop optimal control problem in the E-NMPC is solved using the single-shooting method combined with a quasi-Newton Sequential Quadratic
programming (SQP) algorithm and the adjoint method for computation of gradients. We evaluate the economic performance when unmeasured disturbances are present. By simulation, we demonstrate that the E-NMPC improves the profit of spray drying by 17% compared to conventional PI control.

**General information**

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**Edge-promoting reconstruction of absorption and diffusivity in optical tomography**

In optical tomography a physical body is illuminated with near-infrared light and the resulting outward photon flux is measured at the object boundary. The goal is to reconstruct internal optical properties of the body, such as absorption and diffusivity. In this work, it is assumed that the imaged object is composed of an approximately homogeneous background with clearly distinguishable embedded inhomogeneities. An algorithm for finding the maximum a posteriori estimate for the absorption and diffusion coefficients is introduced assuming an edge-preferring prior and an additive Gaussian measurement noise model. The method is based on iteratively combining a lagged diffusivity step and a linearization of the measurement model of diffuse optical tomography with prior-conditioned LSQR. The performance of the reconstruction technique is tested via three-dimensional numerical experiments with simulated data.

**General information**

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Aalto University
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Scopus rating (2016): CiteScore 1.84 SJR 1.502 SNIP 1.386
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Web of Science (2015): Indexed yes
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Scopus rating (2013): SJR 1.19 SNIP 1.566 CiteScore 2.13
Efficient solvers for soft-constrained MPC
In this work, integrated design and control of reactive distillation processes is presented. Simple graphical design methods that are similar in concept to non-reactive distillation processes are used, such as reactive McCabe-Thiele method and driving force approach. The methods are based on the element concept, which is used to translate a system of compounds into elements. The operation of the reactive distillation column at the highest driving force and other candidate points is analyzed through analytical solution as well as rigorous open-loop and closed-loop simulations. By application of this approach, it is shown that designing the reactive distillation process at the maximum driving force results in an optimal design in terms of controllability and operability. It is verified that the reactive distillation design option is less sensitive to the disturbances in the feed at the highest driving force and has the inherent ability to reject disturbances.

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Authors: Frison, G. (Intern), Jørgensen, J. B. (Intern)
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Empirical average-case relation between undersampling and sparsity in X-ray CT

In X-ray computed tomography (CT) it is generally acknowledged that reconstruction methods exploiting image sparsity allow reconstruction from a significantly reduced number of projections. The use of such reconstruction methods is inspired by recent progress in compressed sensing (CS). However, the CS framework provides neither guarantees of accurate CT reconstruction, nor any relation between sparsity and a sufficient number of measurements for recovery, i.e., perfect reconstruction from noise-free data. We consider reconstruction through 1-norm minimization, as proposed in CS, from data obtained using a standard CT fan-beam sampling pattern. In empirical simulation studies we establish quantitatively a relation between the image sparsity and the sufficient number of measurements for recovery within image classes motivated by tomographic applications. We show empirically that the specific relation depends on the image class and in many cases exhibits a sharp phase transition as seen in CS, i.e., same-sparse images require the same number of projections for recovery. Finally we demonstrate that the relation holds independently of image size and is robust to small amounts of additive Gaussian white noise.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, University of Chicago
Authors: Jørgensen, J. S. (Intern), Sidky, E. Y. (Ekstern), Hansen, P. C. (Intern), Pan, X. (Ekstern)
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.872 SNIP 0.852 CiteScore 1.24
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.103 SNIP 1.054 CiteScore 1.34
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.835 SNIP 1.307 CiteScore 1.61
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.772 SNIP 1.15 CiteScore 1.3
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.437 SNIP 1.026 CiteScore 0.96
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Fast Characterization of Moving Samples with Nano-Textured Surfaces
Characterization of structures using conventional optical microscopy is restricted by the diffraction limit. Techniques like atomic force and scanning electron microscopy can investigate smaller structures but are very time consuming. We show that using scatterometry, a technique based on optical diffraction, integrated into a commercial light microscope we can characterize nano-textured surfaces in a few milliseconds. The adapted microscope has two detectors, a CCD camera used to easily find an area of interest and a spectrometer for the measurements. We demonstrate that the microscope has a resolution in the nanometer range for the topographic parameters: height, width, and sidewall angle of a periodic grating, also in an environment with many vibrations, such as a production facility with heavy equipment.

High-Performance Small-Scale Solvers for Moving Horizon Estimation
In this paper we present a moving horizon estimation (MHE) formulation suitable to easily describe the quadratic programs (QPs) arising in constrained and nonlinear MHE. We propose algorithms for factorization and solution of the underlying Karush-Kuhn-Tucker (KKT) system, as well as the efficient implementation techniques focusing on small-scale problems. The proposed MHE solver is implemented using custom linear algebra routines and is compared against implementations using BLAS libraries. Additionally, the MHE solver is interfaced to a code generation tool for nonlinear model predictive control (NMPC) and nonlinear MHE (NMHE). On an example problem with 33 states, 6 inputs and 15 estimation intervals execution times below 500 microseconds are reported for the QP underlying the NMHE.
High-resolution imaging methods in array signal processing

The purpose of this study is to develop methods in array signal processing which achieve accurate signal reconstruction from limited observations resulting in high-resolution imaging. The focus is on underwater acoustic applications and sonar signal processing both in active (transmit and receive) and passive (only receive) mode. The study addresses the limitations of existing methods and shows that, in many cases, the proposed methods overcome these limitations and outperform traditional methods for acoustic imaging.

The project comprises two parts; The first part deals with computational methods in active sonar signal processing for detection and imaging of submerged oil contamination in sea water from a deep-water oil leak. The submerged oil field is modeled as a fluid medium exhibiting spatial perturbations in the acoustic parameters from their mean ambient values which cause weak scattering of the incident acoustic energy. A high frequency active sonar is selected to insonify the medium and receive the backscattered waves. High-frequency acoustic methods can both overcome the optical opacity of water (unlike methods based on electromagnetic waves) and resolve the small-scale structure of the submerged oil field (unlike low-frequency acoustic methods). The study shows that high-frequency acoustic methods are suitable not only for large-scale localization of the oil contamination in the water column but also for statistical characterization of the submerged oil field through inference of the spatial covariance of its acoustic parameters.

The second part of the project investigates methods that exploit sparsity in order to achieve super-resolution in sound source localization with passive sonars. Sound source localization with sensor arrays involves the estimation of the direction-of-arrival (DOA) of the associated wavefronts from a limited number of observations. Usually, there are only a few sources generating the acoustic wavefield such that DOA estimation is essentially a sparse signal reconstruction problem. Conventional methods for DOA estimation (i.e., beamforming) suffer from resolution limitations related to the physical size and the geometry of the array. DOA estimation methods that are developed up-to-date in order to overcome the resolution limitations of conventional methods involve the estimation or the eigendecomposition of the data cross-spectral matrix. The cross-spectral methods require many snapshots (i.e., observation windows of the recorded wavefield) hence are suitable only for stationary incoherent sources. In this study, the DOA estimation problem is formulated both for single and multiple snapshots in the compressive sensing framework (CS), which achieves sparsity, thus improved resolution, and can be solved efficiently with convex optimization. It is shown that CS has superior performance compared to traditional DOA estimation methods especially under challenging scenarios such as coherent arrivals, single-snapshot data and random array configurations. The high-resolution performance and the robustness of CS in DOA estimation are validated with experimental array data from ocean acoustic measurements.
How little data is enough? Phase-diagram analysis of sparsity-regularized X-ray computed tomography

We introduce phase-diagram analysis, a standard tool in compressed sensing (CS), to the X-ray computed tomography (CT) community as a systematic method for determining how few projections suffice for accurate sparsity-regularized reconstruction. In CS, a phase diagram is a convenient way to study and express certain theoretical relations between sparsity and sufficient sampling. We adapt phase-diagram analysis for empirical use in X-ray CT for which the same theoretical results do not hold. We demonstrate in three case studies the potential of phase-diagram analysis for providing quantitative answers to questions of undersampling. First, we demonstrate that there are cases where X-ray CT empirically performs comparably with a near-optimal CS strategy, namely taking measurements with Gaussian sensing matrices. Second, we show that, in contrast to what might have been anticipated, taking randomized CT measurements does not lead to improved performance compared with standard structured sampling patterns. Finally, we show preliminary results of how well phase-diagram analysis can predict the sufficient number of projections for accurately reconstructing a large-scale image of a given sparsity by means of total-variation regularization.
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Web of Science (2006): Indexed yes
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Improving the efficiency of deconvolution algorithms for sound source localization
The localization of sound sources with delay-and-sum (DAS) beamforming is limited by a poor spatial resolution - particularly at low frequencies. Various methods based on deconvolution are examined to improve the resolution of the beamforming map, which can be modeled by a convolution of the unknown acoustic source distribution and the beamformer's response to a point source, i.e., point-spread function. A significant limitation of deconvolution is, however, an additional computational effort compared to beamforming. In this paper, computationally efficient deconvolution algorithms are examined with computer simulations and experimental data. Specifically, the deconvolution problem is solved with a fast gradient projection method called Fast Iterative Shrinkage-Thresholding Algorithm (FISTA), and compared with a Fourier-based non-negative least squares algorithm. The results indicate that FISTA tends to provide an improved spatial resolution and is up to 30% faster and more robust to noise. In the spirit of reproducible research, the source code is available online.

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Authors: Lylloff, O. A. (Intern), Fernandez Grande, E. (Intern), Agerkvist, F. T. (Intern), Hald, J. (Ekstern), Tiana Roig, E. (Ekstern), Andersen, M. S. (Intern)
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
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Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 0.705 SNIP 1.966 CiteScore 2
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.763 SNIP 1.622 CiteScore 1.75
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.695 SNIP 1.642 CiteScore 1.68
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.754 SNIP 1.528
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 0.783 SNIP 1.717
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.848 SNIP 1.633
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.865 SNIP 1.647
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.752 SNIP 1.559
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.954 SNIP 1.749
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.77 SNIP 1.787
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.882 SNIP 1.712
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.87 SNIP 1.501
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.719 SNIP 1.467
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.621 SNIP 1.411
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.591 SNIP 1.319
Original language: English
Acoustic generators, Acoustics, Algorithms, Beamforming, Image resolution, Iterative methods, Least squares approximations, Optical transfer function, Computationally efficient, Deconvolution algorithm, Deconvolution problem, Gradient projection methods, Least squares algorithm, Reproducible research, Sound source localization, Thresholding algorithms, Deconvolution
DOIs: 10.1121/1.4922516
Source: FindIt
Source-ID: 275417279
Publication: Research - peer-review › Journal article – Annual report year: 2015
In the fall of 2014 I taught ‘02601 Introduction to Numerical Algorithms’ to a class of 86 engineering students at Technical University of Denmark. The course employed basic calculus and linear algebra to elucidate and analyse canonical algorithms of scientific computing. A major part of the course was hands-on MATLAB programming, where the algorithms were tested and applied to solve physical model-based problems. To encourage a deep approach, and discourage a surface approach to learning, I introduced into the lectures a basic but rigorous mathematical treatment of crucial theoretical points, emphasising the beauty of the underlying mathematical structure. Into this I integrated frequent and activating dialogue with the students. In section 1 I describe the course and the students in more detail. Section 2 details and justifies the pedagogical elements I introduced into the lectures; my central hypothesis is also given there. The results of the experiment are presented and discussed in section 3.

**General information**

State: Published  
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Physics, Neutrons and X-rays for Materials Physics  
Authors: Karamehmedovic, M. (Intern)  
Number of pages: 8  
Publication date: 2015

**Host publication information**

Title of host publication: Proceedings of the 43rd Annual SEFI Conference (2015)  
Article number: 55856  
BFI conference series: European Society for Engineering Education. Annual Conference proceedings (5010018)  
Main Research Area: Technical/natural sciences  
Conference: 43rd Annual Conference of the European Society for Engineering Education (SEFI 2015), Orléans, France, 29/06/2015 - 29/06/2015  
Mathematics, Engineering  
Electronic versions:  
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Links:  
http://www.sefi.be/?page_id=6043

**Bibliographical note**

CHAPTER 3. Mathematics and Engineering Education  
Source: PublicationPreSubmission  
Source-ID: 112235359  
Publication: Research - peer-review › Article in proceedings – Annual report year: 2015

**Modeling and Simulation of a Modified Quadruple Tank System**

Quadruple tank process is a non-linear system, have multiple manipulated and controlled variables and have significant cross binding parameters. Furthermore, the modified system is affected by some unknown measurement noise and stochastic disturbance variables which make it more complicated to model and control. In this paper, a modified quadruple-tank system has been described, all the important variables has been outlined and a mathematical model has been presented. We developed deterministic and stochastic models using differential equations and simulate the models using Matlab. Subsequently, steady state analysis is included to determine the operating window for the set points. The purpose to have an operating window for the system is to distinguish the range of feasible region to select the set points for optimum operations. Therefore, in this paper a virtual process plant is created, we investigate the operating window and construct the model in an appropriate form for future controller design.

**General information**

State: Published  
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing  
Authors: Mohd. Azam, S. N. (Intern), Jørgensen, J. B. (Intern)  
Pages: 365-370  
Publication date: 2015

**Host publication information**

Title of host publication: Proceedings of the 5th International Conference on Control Systems, Computing and Engineering (ICCSCE 2015)  
Publisher: IEEE  
ISBN (Print): 978-1-4799-8251-6  
Main Research Area: Technical/natural sciences
Model predictive control for wind power gradients

We consider the operation of a wind turbine and a connected local battery or other electrical storage device, taking into account varying wind speed, with the goal of maximizing the total energy generated while respecting limits on the time derivative (gradient) of power delivered to the grid. We use the turbine inertia as an additional energy storage device, by varying its speed over time, and coordinate the flows of energy to achieve the goal. The control variables are turbine pitch, generator torque and charge/discharge rates for the storage device, each of which can be varied over given ranges. The system dynamics are quite non-linear, and the constraints and objectives are not convex functions of the control inputs, so the resulting optimal control problem is difficult to solve globally. In this paper, we show that by a novel change of variables, which focuses on power flows, we can transform the problem to one with linear dynamics and convex constraints. Thus, the problem can be globally solved, using robust, fast solvers tailored for embedded control applications. We implement the optimal control problem in a receding horizon manner and provide extensive closed-loop tests with real wind data and modern wind forecasting methods. The simulation results using real wind data demonstrate the ability to reject the disturbances from fast changes in wind speed, ensuring certain power gradients, with an insignificant loss in energy production.
MPC Related Computational Capabilities of ARMv7A Processors

In recent years, the mass market of mobile devices has pushed the demand for increasingly fast but cheap processors. ARM, the world leader in this sector, has developed the Cortex-A series of processors with focus on computationally intensive applications. If properly programmed, these processors are powerful enough to solve the complex optimization problems arising in MPC in real-time, while keeping the traditional low-cost and low-power consumption. This makes these processors ideal candidates for use in embedded MPC. In this paper, we investigate the floating-point capabilities of Cortex A7, A9 and A15 and show how to exploit the unique features of each processor to obtain the best performance, in the context of a novel implementation method for the linear-algebra routines used in MPC solvers. This method adapts high-performance computing techniques to the needs of embedded MPC. In particular, we investigate the performance of matrix-matrix and matrix-vector multiplications, which are the backbones of second- and first-order methods for convex optimization. Finally, we test the performance of MPC solvers implemented using these optimized linear-algebra routines.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering
Authors: Frison, G. (Intern), Jørgensen, J. B. (Intern)
Pages: 3414-3421
Publication date: 2015

Host publication information
Title of host publication: Proceedings of the European Control Conference (ECC 2015)
Publisher: IEEE
ISBN (Print): 978-3-9524269-3-7
BFI conference series: European Control Conference (5010925)
Multilevel techniques lead to accurate numerical upscaling and scalable robust solvers for reservoir simulation

This paper demonstrates an application of element-based Algebraic Multigrid (AMGe) technique developed at LLNL to the numerical upscaling and preconditioning of subsurface porous media flow problems. The upscaling results presented here are further extension of our recent work in . The AMGe approach is well suited for the solution of large problems coming from finite element discretizations of systems of partial differential equations. The AMGe technique from allows for the construction of operator-dependent coarse (upscaled) models and guarantees approximation properties of the coarse velocity spaces by introducing additional degrees of freedom associated with non-planar interfaces between agglomerates. This leads to coarse spaces which maintain the specific desirable properties of the original pair of Raviart-Thomas and piecewise discontinuous polynomial spaces. These coarse spaces can be used both as an upscaling tool and as a robust and scalable solver. The methods employed in the present paper have provable O(N) scaling and are particularly well suited for modern multicores architectures, because the construction of the coarse spaces by solving many small local problems offers a high level of concurrency in the computations. Numerical experiments demonstrate the accuracy of using AMGe as an upscaling tool and comparisons are made to more traditional flow-based upscaling techniques. The efficient solution of both the original and upscaled problem is also addressed, and a specialized AMGe preconditioner for saddle point problems is compared to state-of-the-art algebraic multigrid block preconditioners. In particular, we show that for the algebraically upscaled systems, our AMGe preconditioner outperforms traditional solvers. Lastly, parallel strong scaling of a distributed memory implementation of the reservoir simulator is demonstrated.

Multiple and single snapshot compressive beamforming

For a sound field observed on a sensor array, compressive sensing (CS) reconstructs the direction of arrival (DOA) of multiple sources using a sparsity constraint. The DOA estimation is posed as an underdetermined problem by expressing the acoustic pressure at each sensor as a phase-lagged superposition of source amplitudes at all hypothetical DOAs. Regularizing with an ‘1-norm constraint renders the problem solvable with convex optimization, and promoting sparsity gives highresolution DOA maps. Here the sparse source distribution is derived using maximum a posteriori estimates for both single and multiple snapshots. CS does not require inversion of the data covariance matrix and thus works well even for a single snapshot where it gives higher resolution than conventional beamforming. For multiple snapshots, CS outperforms conventional high-resolution methods even with coherent arrivals and at low signal-to-noise ratio. The superior resolution of CS is demonstrated with vertical array data from the SWellEx96 experiment for coherent multi-paths.
Noise properties of CT images reconstructed by use of constrained total-variation, data-discrepancy minimization

Purpose: The authors develop and investigate iterative image reconstruction algorithms based on data-discrepancy minimization with a total-variation (TV) constraint. The various algorithms are derived with different data-discrepancy measures reflecting the maximum likelihood (ML) principle. Simulations demonstrate the iterative algorithms and the resulting image statistical properties for low-dose CT data acquired with sparse projection view angle sampling. Of particular interest is to quantify improvement of image statistical properties by use of the ML data fidelity term.

Methods: An incremental algorithm framework is developed for this purpose. The instances of the incremental algorithms are derived for solving optimization problems including a data fidelity objective function combined with a constraint on the image TV. For the data fidelity term the authors, compare application of the maximum likelihood principle, in the form of weighted least-squares (WLSQ) and Poisson-likelihood (PL), with the use of unweighted least-squares (LSQ).

Results: The incremental algorithms are applied to projection data generated by a simulation modeling the breast computed tomography (bCT) imaging application. The only source of data inconsistency in the bCT projections is due to noise, and a Poisson distribution is assumed for the transmitted x-ray photon intensity. In the simulations involving the incremental algorithms an ensemble of images, reconstructed from 1000 noise realizations of the x-ray transmission data, is used to estimate the image statistical properties. The WLSQ and PL incremental algorithms are seen to reduce image variance as compared to that of LSQ without sacrificing image bias. The difference is also seen at few iterations-short of numerical convergence of the corresponding optimization problems.

Conclusions: The proposed incremental algorithms prove effective and efficient for iterative image reconstruction in low-dose CT applications particularly with sparse-view projection data.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science , Scientific Computing, University of Chicago
Authors: Rose, S. (Ekstern), Andersen, M. S. (Intern), Sidky, E. Y. (Ekstern), Pan, X. (Ekstern)
Pages: 2690-2698
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Medical Physics
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.227 SNIP 1.299 CiteScore 2.46
Web of Science (2016): Indexed yes
Numerical Modeling of Microelectrochemical Systems

The PhD dissertation is concerned with mathematical modeling and simulation of electrochemical systems. The first three chapters of the thesis consist of the introductory part, the model development chapter and the chapter on the summary of the main results. The remaining three chapters report three independent papers and manuscripts.

As a preliminary to the study, we describe a general model for electrochemical systems and study their underlying mechanisms through electroanalytical techniques. We then extend the model to a more realistic model for microelectrochemical systems which incorporates the finite size of ionic species in the transport equation. The model presents a more appropriate boundary conditions which describe the modified Butler-Volmer reaction kinetics and account
for the surface capacitance of the thin electric double layer. We also have found analytical solution for the reactants in the bulk electrolyte that are traveling waves.

The first paper presents the mathematical model which describes an electrochemical system and simulates an electroanalytical technique called cyclic voltammetry. The model is governed by a system of advection–diffusion equations with a nonlinear reaction term at the boundary. We investigate the effect of flow rates, scan rates, and concentration on the cyclic voltammetry. We establish that high flow rates lead to the reduced hysteresis in the cyclic voltammetry curves and increasing scan rates lead to more pronounced current peaks. The final part of the paper shows that the response current in a cyclic voltammetry increases proportionally to the electrolyte concentration.

In the second paper we present an experiment of an electrochemical system in a microfluidic system and compare the result to the numerical solutions. We investigate how the position of the electrodes in the system affects the recorded cyclic voltammetry. The result shows that convection influences the charge transfer dynamics on the electrode surface and hence the cyclic voltammetry recorded. In terms of relative high flow to scan rates, the current response is dominated by the convection due to the fresh supply of reactants towards the electrode surface and quick removal of the products. We also establish that at high scan rates and modest flow rates, peak currents are recorded. Finally, the results show that the position of the electrodes is critical when performing cyclic voltammetry under the flow condition. The numerical results show promising agreement with experimental findings which could be critical in designing highly sensitive electrochemical systems.

The last paper explores the numerical solution which describes the non-linear transient responses to a large applied potential at the electrode in a microelectrochemical system. In our analysis, we account for the finite size properties of ions in the mass and the charge transport of ionic species in an electrochemical system. This term characterizes the saturation of the ionic species close to the electrode surface. We then analyse the responses of the system on the charging of the electric double layer. We consider an arbitrary electrolyte solution that is sandwiched between electrodes and allow for electrochemical reactions at the electrode/electrolyte interface. One of the electrodes is biased with a potential which triggers the reaction and the dynamics of the system. We establish that there is a quick build up of boundary layers in the double layer, but the finite size constraint on the ionic species prevents overcrowding of the ionic species. The result also shows that reactants which undergo charge transfer at the electrode/electrolyte interface crowded the electric double layer and the dynamics of the electric double layer is controlled by the charge transfer.
On artifacts in limited data spherical Radon transform: curved observation surface

We study the limited data problem of the spherical Radon transform in two and three-dimensional spaces with general acquisition surfaces. In such situations, it is known that the application of filtered-backprojection reconstruction formulas might generate added artifacts and degrade the quality of reconstructions. In this article, we explicitly analyze a family of such inversion formulas, depending on a smoothing function that vanishes to order k on the boundary of the acquisition surfaces. We show that the artifacts are k orders smoother than their generating singularity. Moreover, in two-dimensional space, if the generating singularity is conormal satisfying a generic condition then the artifacts are even orders smoother than the generating singularity. Our analysis for three-dimensional space contains an important idea of lifting up space. We also explore the theoretical findings in a series of numerical experiments. Our experiments show that a good choice of the smoothing function leads to a significant improvement of reconstruction quality.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, University of Idaho
Authors: Barannyk, L. L. (Ekstern), Frikel, J. (Intern), Nguyen, L. V. (Ekstern)
Number of pages: 32
Publication date: 2015
Main Research Area: Technical/natural sciences

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Journal: Inverse Problems
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ISSN (Print): 0266-5611
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Web of Science (2016): Indexed yes
Scopus rating (2016): CiteScore 1.84 SJR 1.502 SNIP 1.386
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.389 SNIP 1.411 CiteScore 1.82
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.257 SNIP 1.346 CiteScore 1.63
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.19 SNIP 1.566 CiteScore 2.13
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.239 SNIP 1.838 CiteScore 2.15
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.127 SNIP 1.6 CiteScore 1.9
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.365 SNIP 1.587
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.33 SNIP 1.759
On Devising Boussinesq-type Equations with Bounded Eigenspectra: Two Horizontal Dimensions

Boussinesq-type equations are used to describe the propagation and transformation of free-surface waves in the nearshore region. The nonlinear and dispersive performance of the equations are determined by tunable parameters. Recently the authors presented conditions on the free parameters under which a Nwogu-type equations would yield bounded eigenspectra [5]. This leads to a global conditional CFL time-step restriction which is shown to not be affected by the discretisation method and in this sense the CFL condition is tamed to impose a minimal constraint. In this paper we extend the previous study and provide numerical experiments which confirms the theoretical results also is valid in two horizontal dimensions.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Chalmers University of Technology
Authors: Eskilsson, C. (Ekstern), Engsig-Karup, A. P. (Intern)
Number of pages: 7
Publication date: 2015

Host publication information
Title of host publication: Proceedings of the 18th European Conference on Mathematics for Industry (ECMI 2014)
Publisher: Springer
Main Research Area: Technical/natural sciences
Conference: 18th European Conference on Mathematics for Industry, Taormina, Italy, 09/06/2014 - 09/06/2014

Pairs of dual Gabor frames generated by functions of Hilbert-Schmidt type

We show that any two functions which are real-valued, bounded, compactly supported and whose integer translates each form a partition of unity lead to a pair of windows generating dual Gabor frames for (Formula presented.). In particular we show that any such functions have families of dual windows where each member may be written as a linear combination of integer translates of any B-spline. We introduce functions of Hilbert-Schmidt type along with a new method which allows us to associate to certain such functions finite families of recursively defined dual windows of arbitrary smoothness. As a special case we show that any exponential B-spline has finite families of dual windows, where each member may be conveniently written as a linear combination of another exponential B-spline. Unlike results known from the literature we avoid the usual need for the partition of unity constraint in this case.

General information
State: Published
Pharmacokinetics Modeling of Glucagon and a Novel Glucagon Analogue after Subcutaneous Administration in Dogs

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Zealand Pharma A/S
Authors: Wendt, S. L. (Intern), Valeur, A. (Ekstern), Madsen, H. (Intern), Jørgensen, J. B. (Intern), Boye Knudsen, C. (Ekstern)
Number of pages: 1
Publication date: 2015
Event: Poster session presented at The 8th International Conference on Advanced Technologies and Treatments for Diabetes (ATTD 2015), Paris, France.
Main Research Area: Technical/natural sciences
Electronic versions:
Eposter_final2_comp.pdf
Source: PublicationPreSubmission
Source-ID: 106095949
Publication: Research › Poster – Annual report year: 2015

Profit and Risk Measures in Oil Production Optimization
In oil production optimization, we usually aim to maximize a deterministic scalar performance index such as the profit over the expected reservoir lifespan. However, when uncertainty in the parameters is considered, the profit results in a random variable that can assume a range of values depending on the value of the uncertain parameters. In this case, a problem reformulation is needed to properly define the optimization problem. In this paper we describe the concept of risk and we explore how to handle the risk by using appropriate risk measures. We provide a review on various risk measures reporting pro and cons for each of them. Finally, among the presented risk measures, we identify two of them as appropriate risk measures when minimizing the risk.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Center for Energy Resources Engineering, Scientific Computing, Technical University of Denmark, Norwegian University of Science and Technology
Authors: Capolei, A. (Intern), Foss, B. (Ekstern), Jørgensen, J. B. (Ekstern)
Pages: 214-220
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Host publication information
Title of host publication: Proceedings of the 2nd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production OOGP 2015
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ISSN: 1474-6670
Main Research Area: Technical/natural sciences
Conference: 2nd IFAC Workshop on Automatic Control in Offshore Oil and Gas Production, Florianópolis, Brazil, 27/05/2015 - 27/05/2015
Production optimization, Oil production, Risk measures, Stochastic problems
Electronic versions:
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DOIs:
10.1016/j.ifacol.2015.08.034
Publication: Research - peer-review › Article in proceedings – Annual report year: 2016

Real-time nonlinear MPC and MHE for a large-scale mechatronic application
Progress in optimization algorithms and in computational hardware made deployment of Nonlinear Model Predictive Control (NMPC) and Moving Horizon Estimation (MHE) possible to mechatronic applications. This paper aims to assess
the computational performance of NMPC and MHE for rotational start-up of Airborne Wind Energy systems. The capabilities offered by an automatic code generation tool are experimentally verified on a real physical system, using a model comprising 27 states and 4 inputs at a sampling frequency of 25 Hz. The results show the feedback times less than 5 ms for the NMPC with more than 1500 variables.
Reconstruction Methods for Inverse Problems with Partial Data
This thesis presents a theoretical and numerical analysis of a general mathematical formulation of hybrid inverse problems in impedance tomography. This includes problems from several existing hybrid imaging modalities such as Current Density Impedance Imaging, Magnetic Resonance Electrical Impedance Tomography, and Ultrasound Modulated Electrical Impedance Tomography. After giving an introduction to hybrid inverse problems in impedance tomography and the mathematical tools that facilitate the related analysis, we explain in detail the stability properties associated with the classification of a linearised hybrid inverse problem. This is done using pseudo-differential calculus and theory for overdetermined boundary value problem. Using microlocal analysis we then present novel results on the propagation of singularities, which give a precise description of the distinct features of solutions in the case of a non-elliptic problem. To conduct a numerical analysis, we develop four iterative reconstruction methods using the Picard and Newton iterative schemes, and the unified approach to the reconstruction problem encompasses several algorithms suggested in the literature. The algorithms are implemented numerically in two dimensions and the properties of the algorithms and their implementations are investigated theoretically. Novel numerical results are presented for both the full and partial data problem, and they show similarities and differences between the proposed algorithms, which are closely linked to the results of the theoretical analysis. The findings in this thesis justify that the choice of algorithm should be based on a theoretical analysis of the underlying inverse problem.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Hoffmann, K. (Intern), Knudsen, K. (Intern)
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Original language: English

Series: DTU Compute PHD-2014
Number: 344
ISSN: 0909-3192
Main Research Area: Technical/natural sciences
Electronic versions:
phd344_Hoffmann_K.pdf
Publication: Research - Ph.D. thesis – Annual report year: 2015

Relaxed Simultaneous Tomographic Reconstruction and Segmentation with Class Priors for Poisson Noise
This work is a continuation of work on algorithms for simultaneous reconstruction and segmentation. In our previous work we developed an algorithm for data with Gaussian noise, and in that algorithm the coefficient matrix for the system is explicitly stored. We improve this algorithm in two ways: our new algorithm can handle Poisson noise in the data, and it can solve much larger problems since it does not store the matrix. We formulate this algorithm and test it on artificial test problems. Our results show that the algorithm performs well, and that we are able to produce reconstructions and segmentations with small errors.

General information
State: Published
Remarks on models for estimating the carbohydrate to insulin ratio and insulin sensitivity in T1DM
In this paper we estimate linear models for prediction of the interstitial glucose concentration in response to meals and bolus insulin. Parameters of these models can be directly used in simple bolus calculation rules. In contrast to models proposed in the literature, we present a model without an integrator. This model maintains the benefits of the existing empirical models and allows simulation of a longer time period than the post-prandial period, i.e. the couple of hours following a meal. Furthermore, the new model proposed in this paper does not require any re-initialization before meals.

Simultaneous tomographic reconstruction and segmentation with class priors
We consider tomographic imaging problems where the goal is to obtain both a reconstructed image and a corresponding segmentation. A classical approach is to first reconstruct and then segment the image; more recent approaches use a discrete tomography approach where reconstruction and segmentation are combined to produce a reconstruction that is identical to the segmentation. We consider instead a hybrid approach that simultaneously produces both a reconstructed image and segmentation. We incorporate priors about the desired classes of the segmentation through a Hidden Markov Measure Field Model, and we impose a regularization term for the spatial variation of the classes across neighbouring pixels. We also present an efficient implementation of our algorithm based on state-of-the-art numerical optimization algorithms. Simulation experiments with artificial and real data demonstrate that our combined approach can produce better results than the classical two-step approach.
Sparse acoustic imaging with a spherical array

In recent years, a number of methods for sound source localization and sound field reconstruction with spherical microphone arrays have been proposed. These arrays have properties that are potentially very useful, e.g. omnidirectionality, robustness, compensable scattering, etc. This paper proposes a plane wave expansion method based on
measurements with a spherical microphone array, and solved in the framework provided by Compressed Sensing. The proposed methodology results in a sparse solution, i.e. few non-zero coefficients, and it is suitable for both source localization and sound field reconstruction. In general it provides fine spatial resolution for localization (delta-like functions), and robust reconstruction (the noisy components are naturally suppressed). The validity and performance of the proposed method is examined, and its limitations as well as the underlying assumptions are addressed.

**Sparse DOA estimation with polynomial rooting**

Direction-of-arrival (DOA) estimation involves the localization of a few sources from a limited number of observations on an array of sensors. Thus, DOA estimation can be formulated as a sparse signal reconstruction problem and solved efficiently with compressive sensing (CS) to achieve high-resolution imaging. Utilizing the dual optimal variables of the CS optimization problem, it is shown with Monte Carlo simulations that the DOAs are accurately reconstructed through polynomial rooting (Root-CS). Polynomial rooting is known to improve the resolution in several other DOA estimation methods. However, traditional methods involve the estimation of the cross-spectral matrix hence they require many snapshots and stationary incoherent sources and are suitable only for uniform linear arrays (ULA). Root-CS does not have these limitations as demonstrated on experimental towed array data from ocean acoustic measurements.

**Spectral element modelling of floating bodies in a Boussinesq framework**

The wave energy sector relies heavily on the use of linear hydrodynamic models for the assessment of motions, loads and power production. The linear codes are computationally efficient and produce good results if applied within their application window. However, recent studies using two-phase VOF-RANS simulations of point-absorbers close to resonance have indicated that there might be significant differences between the power production using linear hydrodynamics and VOF-RANS. At present VOF-RANS simulations are too computational expensive to be used in the design cycle. In shallow and intermediate waters a possible middle way between the highly simplified and fast linear
hydrodynamics and the very complete but slow VOF-RANS simulations is to use nonlinear, dispersive wave equations of Boussinesq-type. Jiang (2001) presented a unified approach for including bodies into the Boussinesq framework and solved the system with finite differences. In this study we will outline how to implement the approach of Jiang in a spectral/hp element setting, and simulate the heave motion of a body using different asymptotic wave equations. We will especially focus on the stabilization of the coupled system.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, INRIA Bordeaux-Sud-Ouest, Chalmers University of Technology
Authors: Engsig-Karup, A. P. (Intern), Eskilsson, C. (Ekstern), Ricchiuto, M. (Ekstern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
engsig_karup_etalFrontiers2015.pdf

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Source-ID: 118278184
Publication: Research › Conference abstract for conference – Annual report year: 2015

Stability patterns for a size-structured population model and its stage-structured counterpart
In this paper we compare a general size-structured population model, where a size-structured consumer feeds upon an unstructured resource, to its simplified stage-structured counterpart in terms of equilibrium stability. Stability of the size-structured model is understood in terms of an equivalent delayed system consisting of a renewal equation for the consumer population birth rate and a delayed differential equation for the resource. Results show that the size- and stage-structured models differ considerably with respect to equilibrium stability, although the two models have completely identical equilibrium solutions. First, when adult consumers are superior foragers to juveniles, the size-structured model is more stable than the stagestructured model while the opposite occurs when juveniles are the superior foragers. Second, relatively large juvenile (adult) mortality tends to stabilise (destabilise) the size-structured model but destabilise (stabilise) the stage-structured model. Third, the stability pattern is sensitive to the adult-offspring size ratio in the sizestructured model but much less sensitive in the stage-structured model. Finally, unless the adult-offspring size ratio is sufficiently small, the stage-structured model cannot satisfactorily capture the dynamics of the size-structured model. We conclude that caution must be taken when the stage-structured population model is applied, although it can consistently translate individual life history and stage-specific differences to the population level.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Umeå University, Yangzhou University
Authors: Zhang, L. (Ekstern), Pedersen, M. (Intern), Lin, Z. (Ekstern)
Pages: 109-123
Publication date: 2015
Main Research Area: Technical/natural sciences

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Journal: Mathematical Biosciences
Volume: 267
ISSN (Print): 0025-5564
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Web of Science (2015): Indexed yes
In this report, we address the problem of low-dose tomographic image reconstruction using dictionary priors learned from training images. In our recent work [22] dictionary learning is used to incorporate priors from training images and construct a dictionary, and then the reconstruction problem is formulated in a convex optimization framework by looking for a solution with a sparse representation in the subspace spanned by the dictionary. The work in [22] has shown that using learned dictionaries in computed tomography can lead to superior image reconstructions comparing to classical methods. Our formulation in [22] enforces that the solution is an exact representation by the dictionary; in this report, we investigate this requirement. Furthermore, the underlying assumption that the scale and orientation of the training images are consistent with the unknown image of interest may not be realistic. We investigate the sensitivity and robustness of the reconstruction to variations of the scale and orientation in the training images and we suggest algorithms to estimate the correct relative scale and orientation of the unknown image to the training images from the data.
Testable uniqueness conditions for empirical assessment of undersampling levels in total variation-regularized X-ray CT

We study recoverability in fan-beam computed tomography (CT) with sparsity and total variation priors: how many underdetermined linear measurements suffice for recovering images of given sparsity? Results from compressed sensing (CS) establish such conditions for example for random measurements, but not for CT. Recoverability is typically tested by checking whether a computed solution recovers the original. This approach cannot guarantee solution uniqueness and the recoverability decision therefore depends on the optimization algorithm. We propose new computational methods to test recoverability by verifying solution uniqueness conditions. Using both reconstruction and uniqueness testing, we empirically study the number of CT measurements sufficient for recovery on new classes of sparse test images. We demonstrate an average-case relation between sparsity and sufficient sampling and observe a sharp phase transition as known from CS, but never established for CT. In addition to assessing recoverability more reliably, we show that uniqueness tests are often the faster option.
The contribution of glucagon in an Artificial Pancreas for people with type 1 diabetes

The risk of hypoglycemia is one of the main concerns in treatment of type 1 diabetes (T1D). In this paper we present a head-to-head comparison of a currently used insulin-only controller and a prospective bihormonal controller for blood glucose in people with T1D. The bihormonal strategy uses insulin to treat hyperglycemia as well as glucagon to ensure fast recovery from hypoglycemic episodes. Two separate model predictive controllers (MPC) based on patient-specific models handle insulin and glucagon infusion. In addition, the control algorithm consists of a Kalman filter and a meal time insulin bolus calculator. The feedback is obtained from a continuous glucose monitor (CGM). We implement a bihormonal simulation model with time-varying parameters available for 3 subjects to compare the strategies. We consider a protocol with 3 events - a correct mealtime insulin bolus, a missed bolus and a bolus overestimated by 60%. During normal operation both strategies provide similar results. The contribution of glucagon becomes evident after administration of the overestimated insulin bolus. In a 10h period following an overbolused meal, the bihormonal strategy reduces time spent in hypoglycemia in the most severe case by almost 15% (1.5h), outperforming the insulin-only control. Therefore, glucagon contributes to the safety of an Artificial Pancreas.
The equivalent source method as a sparse signal reconstruction

This study proposes an acoustic holography method for sound field reconstruction based on a point source model, which uses the Compressed Sensing (CS) framework to provide a sparse solution. Sparsity implies that the sound field can be represented by a minimal number of non-zero terms, point sources in the case of this model. Sparse solutions can be achieved by l-1 norm minimization, providing accurate reconstruction and robustness to noise, because favouring sparsity suppresses noisy components. The study addresses the influence of the ill-conditioning of the propagation matrix, which can be a challenge for inverse problems where the energy in the solution vector is much greater than the energy in the observations (particularly in acoustic near-fields). Finally, the study examines the case of spatially extended sources and problems where the sparsity condition is not certainly guaranteed.

Tomographic Image Reconstruction Using Training Images with Matrix and Tensor Formulations

Reducing X-ray exposure while maintaining the image quality is a major challenge in computed tomography (CT); since the imperfect data produced from the few view and/or low intensity projections results in low-quality images that are suffering from severe artifacts when using conventional reconstruction methods. Incorporating a priori information about the solution is a necessity to improve the reconstruction. For example, Total Variation (TV) regularization method –assuming a piecewise constant image model – has been shown to allow reducing X-ray exposure significantly, while maintaining the image resolution compared to a classical reconstruction method such as Filtered Back Projection (FBP).

Some priors for the tomographic reconstruction take the form of cross-section images of similar objects, providing a set of the so-called training images, that hold the key to the structural information about the solution. The training images must be reliable and application-specific. This PhD project aims at providing a mathematical and computational framework for the use of training sets as non-parametric priors for the solution in tomographic image reconstruction. Through an unsupervised machine learning technique (here, the dictionary learning), prototype elements from the training images are extracted and then incorporated in the tomographic reconstruction problem both with matrix and tensor representations of the training images.

First, an algorithm for the tomographic image reconstruction using training images, where the training images are represented as vectors in a training matrix, is described. The dictionary learning problem is formulated as a regularized non-negative matrix factorization in order to compute a nonnegative dictionary. Then a tomographic solution with a sparse representation in the dictionary is obtained through a convex optimization formulation. Computational experiments clarify the choice and interplay of the model parameters and the regularization parameters. Furthermore, the assumptions in the tomographic problem formulation are analyzed. The sensitivity and robustness of the reconstruction to variations of the scale and rotation in the training images is investigated and algorithms to estimate the correct relative scale and orientation of the unknown image to the training images are suggested.

Then, a third-order tensor representation for the training images images is used. The dictionary and image reconstruction problem are reformulated using the tensor representation. The dictionary learning problem is presented as a nonnegative tensor factorization problem with sparsity constraints and the reconstruction problem is formulated in a convex optimization framework by looking for a solution with a sparse representation in the tensor dictionary. Numerical results show considering a tensor formulation over a matrix formulation significantly reduces the approximation error by the dictionary as well as leads to very sparse representations of both the training images and the reconstructions.

Further computational experiments show that in few-projection and low-dose settings our algorithm is while (not surprisingly) being superior to the classical reconstruction methods, is competitive with (or even better of) the TV regularization and tends to include more texture and sharper edges in the reconstructed images.
The focus of the thesis is the study of mathematical and algorithmic prospectives and thus the training images and tomographic scenarios are mostly simulation based. More studies are however needed for implementing the proposed algorithm in a routine use for clinical applications and materials testing.

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TV-constrained incremental algorithms for low-intensity CT image reconstruction
Low-dose X-ray computed tomography (CT) has garnered much recent interest as it provides a method to lower patient dose and simultaneously reduce scan time. In non-medical applications the possibility of preventing sample damage makes low-dose CT desirable. Reconstruction in low-dose CT poses a significant challenge due to the high level of noise in the data. Here we propose an iterative method for reconstruction which minimizes the transmission Poisson likelihood subject to a total-variation constraint. This formulation accommodates efficient methods of parameter selection because the choice of TV constraint can be guided by an image reconstructed by filtered backprojection (FBP). We apply our algorithm to low-dose synchrotron X-ray CT data from the Advanced Photon Source (APS) at Argonne National Labs (ANL) to demonstrate its potential utility. We find that the algorithm provides a means of edge-preserving regularization with the potential to generate useful images at low iteration number in low-dose CT.

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, University of Chicago
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Uncertainty Quantification with Applications to Engineering Problems
The systematic quantification of the uncertainties affecting dynamical systems and the characterization of the uncertainty of their outcomes is critical for engineering design and analysis, where risks must be reduced as much as possible. Uncertainties stem naturally from our limitations in measurements, predictions and manufacturing, and we can say that any dynamical system used in engineering is subject to some of these uncertainties.

The first part of this work presents an overview of the mathematical framework used in Uncertainty Quantification (UQ) analysis and introduces the spectral tensor-train (STT) decomposition, a novel high-order method for the effective
propagation of uncertainties which aims at providing an exponential convergence rate while tackling the curse of dimensionality. The curse of dimensionality is a problem that afflicts many methods based on meta-models, for which the computational cost increases exponentially with the number of inputs of the approximated function – which we will call dimension in the following.

The STT-decomposition is based on the Polynomial Chaos (PC) approximation and the low-rank decomposition of the function describing the Quantity of Interest of the considered problem. The low-rank decomposition is obtained through the discrete tensor-train decomposition, which is constructed using an optimization algorithm for the selection of the relevant points on which the function needs to be evaluated. The selection of these points is informed by the approximated function and thus it is able to adapt to its features. The number of function evaluations needed for the construction grows only linearly with the dimension and quadratically with the rank.

In this work we will present and use the functional counterpart of this low-rank decomposition and, after proving some auxiliary properties, we will apply PC on it, obtaining the STT-decomposition. This will allow the decoupling of each dimension, leading to a much cheaper construction of the PC surrogate. In the associated paper, the capabilities of the STT-decomposition are checked on commonly used test functions and on an elliptic problem with random inputs.

This work will also present three active research directions aimed at improving the efficiency of the STT-decomposition. In this context, we propose three new strategies for solving the ordering problem suffered by the tensor-train decomposition, for computing better estimates with respect to the norms usually employed in UQ and for the anisotropic adaptivity of the method.

The second part of this work presents engineering applications of the UQ framework. Both the applications are characterized by functions whose evaluation is computationally expensive and thus the UQ analysis of the associated systems will benefit greatly from the application of methods which require few function evaluations.

We first consider the propagation of the uncertainty and the sensitivity analysis of the non-linear dynamics of railway vehicles with suspension components whose characteristics are uncertain. These analysis are carried out using mostly PC methods, and resorting to random sampling methods for comparison and when strictly necessary.

The second application of the UQ framework is on the propagation of the uncertainties entering a fully non-linear and dispersive model of water waves. This computationally challenging task is tackled with the adoption of state-of-the-art software for its numerical solution and of efficient PC methods. The aim of this study is the construction of stochastic benchmarks where to test UQ methodologies before being applied to full-scale problems, where efficient methods are necessary with today’s computational resources.

The outcome of this work was also the creation of several freely available Python modules for Uncertainty Quantification, which are listed and described in the appendix.

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Variational approach for restoring blurred images with cauchy noise
The restoration of images degraded by blurring and noise is one of the most important tasks in image processing. In this paper, based on the total variation (TV) we propose a new variational method for recovering images degraded by Cauchy noise and blurring. In order to obtain a strictly convex model, we add a quadratic penalty term, which guarantees the uniqueness of the solution. Due to the convexity of our model, the primal dual algorithm is employed to solve the minimization problem. Experimental results show the effectiveness of the proposed method for simultaneously deblurring and denoising images corrupted by Cauchy noise. Comparison with other existing and well-known methods is provided as
A Branch and Bound Algorithm for a Class of Biobjective Mixed Integer Programs

Most real-world optimization problems are multiobjective by nature, involving noncomparable objectives. Many of these problems can be formulated in terms of a set of linear objective functions that should be simultaneously optimized over a class of linear constraints. Often there is the complicating factor that some of the variables are required to be integral. The resulting class of problems is named multiobjective mixed integer programming (MOMIP) problems. Solving these kinds of optimization problems exactly requires a method that can generate the whole set of nondominated points (the Pareto-optimal front). In this paper, we first give a survey of the newly developed branch and bound methods for solving MOMIP problems. After that, we propose a new branch and bound method for solving a subclass of MOMIP problems, where only
two objectives are allowed, the integer variables are binary, and one of the two objectives has only integer variables. The proposed method is able to find the full set of nondominated points. It is tested on a large number of problem instances, from six different classes of MOMIP problems. The results reveal that the developed biobjective branch and bound method performs better on five of the six test problems, compared with a generic two-phase method. At this time, the two-phase method is the most preferred exact method for solving MOMIP problems with two criteria and binary variables.

**General information**

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Organisations: Department of Management Engineering, Management Science, Department of Applied Mathematics and Computer Science, Scientific Computing, Aarhus University
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BFI (2016): BFI-level 2
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 3.662 SNIP 2.575 CiteScore 3.4
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.32 SNIP 2.301 CiteScore 2.79
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.08 SNIP 2.274 CiteScore 2.84
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.983 SNIP 2.394
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.951 SNIP 2.519
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 3.993 SNIP 2.784
Scopus rating (2006): SJR 3.255 SNIP 2.564
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Scopus rating (2002): SJR 2.859 SNIP 2.208
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OPERATIONS, MANAGEMENT, ASSIGNMENT PROBLEM, OPTIMIZATION, POINTS, biobjective optimization, integer programming, branch and bound, Biobjective optimization, Branch and bound, Integer programming, Algorithms, Branch
A computationally efficient tool for assessing the depth resolution in large-scale potential-field inversion

In potential-field inversion, careful management of singular value decomposition components is crucial for obtaining information about the source distribution with respect to depth. In principle, the depth-resolution plot provides a convenient visual tool for this analysis, but its computational complexity has hitherto prevented application to large-scale problems. To analyze depth resolution in such problems, we developed a variant ApproxDRP, which is based on an iterative algorithm and therefore suited for large-scale problems because we avoid matrix factorizations and the associated demands on memory and computing time. We used the ApproxDRP to study retrievable depth resolution in inversion of the gravity field of the Neapolitan Volcanic Area. Our main contribution is the combined use of the Lanczos bidiagonalization algorithm, established in the scientific computing community, and the depth-resolution plot defined in the geoscience community.

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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.413 SNIP 1.434 CiteScore 1.9
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Scopus rating (2013): SJR 1.658 SNIP 2.105 CiteScore 2.25
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.693 SNIP 1.837 CiteScore 2.04
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.141 SNIP 1.729 CiteScore 2.51
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Web of Science (2011): Indexed yes
A Computationally Efficient Tool for Assessing the Depth Resolution in Potential-Field Inversion

In potential-field inversion problems, it can be difficult to obtain reliable information about the source distribution with respect to depth. Moreover, spatial resolution of the reconstructions decreases with depth, and in fact the more ill-posed the problem - and the more noisy the data - the less reliable the depth information. Based on earlier work using the singular value decomposition, we introduce a tool ApproxDRP which uses approximations of the singular vectors obtained by the iterative Lanczos bidiagonalization algorithm, making it well suited for large-scale problems. This tool allows a computational/visual analysis of how much the depth resolution in a computational potential-field inversion problem can be obtained from the given data. Through synthetic and real data examples we demonstrate that ApproxDRP, when used in combination with a plot of the approximate SVD quantities, may successfully show the limitations of depth resolution resulting from noise in the data. This allows a reliable analysis of the retrievable depth information and effectively guides the user in choosing the optimal number of iterations, for a given problem.

General information
State: Published
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Number of pages: 25
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A Dantzig-Wolfe decomposition algorithm for linear economic model predictive control of dynamically decoupled subsystems

This paper presents a warm-started Dantzig–Wolfe decomposition algorithm tailored to economic model predictive control of dynamically decoupled subsystems. We formulate the constrained optimal control problem solved at each sampling instant as a linear program with state space constraints, input limits, input rate limits, and soft output limits. The objective function of the linear program is related directly to the cost of operating the subsystems, and the cost of violating the soft output constraints. Simulations for large-scale economic power dispatch problems show that the proposed algorithm is significantly faster than both state-of-the-art linear programming solvers, and a structure exploiting implementation of the alternating direction method of multipliers. It is also demonstrated that the control strategy presented in this paper can be tuned using a weighted ℓ1-regularization term. In the presence of process and measurement noise, such a regularization term is critical for achieving a well-behaved closed-loop performance.
Adaptive grouping for the higher-order multilevel fast multipole method
An alternative parameter-free adaptive approach for the grouping of the basis function patterns in the multilevel fast multipole method is presented, yielding significant memory savings compared to the traditional Octree grouping for most discretizations, particularly when using higher-order basis functions. Results from both a uniformly and nonuniformly meshed scatterer are presented, showing how the technique is worthwhile even for regular meshes, and demonstrating that there is no loss of accuracy in spite of the large reduction in memory requirements and the relatively low computational cost.

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, TICRA
Authors: Borries, O. P. (Intern), Jørgensen, E. (Ekstern), Meincke, P. (Ekstern), Hansen, P. C. (Intern)
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.362 SNIP 0.594 CiteScore 0.71
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BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.371 SNIP 0.639 CiteScore 0.75
A Decomposition Algorithm for Mean-Variance Economic Model Predictive Control of Stochastic Linear Systems

This paper presents a decomposition algorithm for solving the optimal control problem (OCP) that arises in Mean-Variance Economic Model Predictive Control of stochastic linear systems. The algorithm applies the alternating direction method of multipliers to a reformulation of the OCP that decomposes into small independent subproblems. We test the decomposition algorithm using a simple power management case study, in which the OCP is formulated as a convex quadratic program. Simulations show that the decomposition algorithm scales linearly in the number of uncertainty scenarios. Moreover, a parallel implementation of the algorithm is several orders of magnitude faster than state-of-the-art convex quadratic programming algorithms, provided that the number of uncertainty scenarios is large.

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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Center for Energy Resources Engineering, Centre for IT-Intelligent Energy Systems in Cities
Authors: Sokoler, L. E. (Intern), Dammann, B. (Ekstern), Madsen, H. (Intern), Jørgensen, J. B. (Intern)
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Publication date: 2014
A Family of High-Performance Solvers for Linear Model Predictive Control

In Model Predictive Control (MPC), an optimization problem has to be solved at each sampling time, and this has traditionally limited the use of MPC to systems with slow dynamic. In this paper, we propose an efficient solution strategy for the unconstrained sub-problems that give the search-direction in Interior-Point (IP) methods for MPC, and that usually are the computational bottle-neck. This strategy combines a Riccati-like solver with the use of high-performance computing techniques: in particular, in this paper we explore the performance boost given by the use of single precision computation, and techniques such as inexact search direction and mixed precision computation. Finally, we test our HPMPC toolbox, a family of high-performance solvers tailored for MPC and implemented using these techniques, that is shown to be several times faster than current state-of-the-art solvers for linear MPC.

A Mean-Variance Criterion for Economic Model Predictive Control of Stochastic Linear Systems

Stochastic linear systems arise in a large number of control applications. This paper presents a mean-variance criterion for economic model predictive control (EMPC) of such systems. The system operating cost and its variance is approximated based on a Monte-Carlo approach. Using convex relaxation, the tractability of the resulting optimal control problem is addressed. We use a power management case study to compare different variations of the mean-variance strategy with EMPC based on the certainty equivalence principle. The certainty equivalence strategy is much more computationally efficient than the mean-variance strategies, but it does not account for the variance of the uncertain parameters. Openloop simulations suggest that a single-stage mean-variance approach yields a significantly lower operating cost than the certainty equivalence strategy. In closed-loop, the single-stage formulation is overly conservative, which results in a high operating cost. For this case, a two-stage extension of the mean-variance approach provides the best trade-off between the expected cost and its variance. It is demonstrated that by using a constraint back-off technique in the specific case study, certainty equivalence EMPC can be modified to perform almost as well as the two-stage mean-variance formulation. Nevertheless, we argue that the mean-variance approach can be used both as a strategy for evaluating less computational demanding methods such as the certainty equivalence method, and as an individual control strategy when heuristics such as constraint back-off do not perform well.
A mean–variance objective for robust production optimization in uncertain geological scenarios

In this paper, we introduce a mean–variance criterion for production optimization of oil reservoirs and suggest the Sharpe ratio as a systematic procedure to optimally trade-off risk and return. We demonstrate by open-loop simulations of a two-phase synthetic oil field that the mean–variance criterion is able to mitigate the significant inherent geological uncertainties better than the alternative certainty equivalence and robust optimization strategies that have been suggested for production optimization. In production optimization, the optimal water injection profiles and the production borehole pressures are computed by solution of an optimal control problem that maximizes a financial measure such as the Net Present Value (NPV). The NPV is a stochastic variable as the reservoir parameters, such as the permeability field, are stochastic. In certainty equivalence optimization, the mean value of the permeability field is used in the maximization of the NPV of the reservoir over its lifetime. This approach neglects the significant uncertainty in the NPV. Robust optimization maximizes the expected NPV over an ensemble of permeability fields to overcome this shortcoming of certainty equivalence optimization. Robust optimization reduces the risk compared to certainty equivalence optimization because it considers an ensemble of permeability fields instead of just the mean permeability field. This is an indirect mechanism for risk mitigation as the risk does not enter the objective function directly. In the mean–variance bi-criterion objective function risk appears directly, it also considers an ensemble of reservoir models, and has robust optimization as a special extreme case. The mean–variance objective is common for portfolio optimization problems in finance. The Markowitz portfolio optimization problem is the original and simplest example of a mean–variance criterion for mitigating risk. Risk is mitigated in oil production by including both the expected NPV (mean of NPV) and the risk (variance of NPV) for the ensemble of possible reservoir models. With the inclusion of the risk in the objective function, the Sharpe ratio can be used to compute the optimal water injection and production borehole pressure trajectories that give the optimal return–risk ratio. By simulation, we investigate and compare the performance of production optimization by mean–variance optimization, robust optimization, certainty equivalence optimization, and the reactive strategy. The optimization strategies are simulated in open-loop without feedback while the reactive strategy is based on feedback. The simulations demonstrate that certainty equivalence optimization and robust optimization are risky strategies. At the same computational effort as robust optimization, mean–variance optimization is able to reduce risk significantly at the cost of slightly smaller return. In this way, mean–variance optimization is a powerful tool for risk management and uncertainty mitigation in production optimization.
An algorithm for total variation regularized photoacoustic imaging

Recovery of image data from photoacoustic measurements asks for the inversion of the spherical mean value operator. In contrast to direct inversion methods for specific geometries, we consider a semismooth Newton scheme to solve a total variation regularized least squares problem. During the iteration, each matrix vector multiplication is realized in an efficient way using a recently proposed spectral discretization of the spherical mean value operator. All theoretical results are
illustrated by numerical experiments.

**General information**

- **State:** Published
- **Organisations:** Department of Applied Mathematics and Computer Science, Scientific Computing, University of Osnabrück, Helmholtz Zentrum München
- **Authors:** Dong, Y. (Intern), Görner, T. (Ekstern), Kunis, S. (Ekstern)
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  - Web of Science (2014): Indexed yes
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  - ISI indexed (2012): ISI indexed yes
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  - Scopus rating (2011): SJR 0.946 SNIP 1.347 CiteScore 1.11
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  - BFI (2010): BFI-level 1
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  - Web of Science (2010): Indexed yes
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  - Scopus rating (2008): SJR 0.761 SNIP 1.071
  - Web of Science (2008): Indexed yes
  - Scopus rating (2007): SJR 0.92 SNIP 1.08
  - Web of Science (2007): Indexed yes
  - Scopus rating (2006): SJR 1.062 SNIP 1.119
  - Scopus rating (2005): SJR 1.148 SNIP 1.745
  - Scopus rating (2004): SJR 0.875 SNIP 0.984
  - Scopus rating (2003): SJR 1.013 SNIP 1.489
  - Scopus rating (2002): SJR 1.108 SNIP 1.374
Analysis of efficient preconditioned defect correction methods for nonlinear water waves

Robust computational procedures for the solution of non-hydrostatic, free surface, irrotational and inviscid free-surface water waves in three space dimensions can be based on iterative preconditioned defect correction (PDC) methods. Such methods can be made efficient and scalable to enable prediction of free-surface wave transformation and accurate wave kinematics in both deep and shallow waters in large marine areas or for predicting the outcome of experiments in large numerical wave tanks. We revisit the classical governing equations are fully nonlinear and dispersive potential flow equations. We present new detailed fundamental analysis using finite-amplitude wave solutions for iterative solvers. We demonstrate that the PDC method in combination with a high-order discretization method enables efficient and scalable solution of the linear system of equations arising in potential flow models. Our study is particularly relevant for fast and efficient simulation of non-breaking fully nonlinear water waves over varying bottom topography that may be limited by computational resources or requirements. To gain insight into algorithmic properties and proper choices of discretization parameters for different PDC strategies, we study systematically limits of accuracy, convergence rate, algorithmic and numerical efficiency and scalability of the most efficient known PDC methods. These strategies are of interest, because they enable generalization of geometric multigrid methods to high-order accurate discretizations and enable significant improvement in numerical efficiency while incurring minimal storage requirements. We demonstrate robustness using such PDC methods for practical ranges of interest for coastal and maritime engineering, that is, from shallow to deep water, and report details of numerical experiments that can be used for benchmarking purposes.
Anomaly detection in homogenous populations: A sparse multiple kernel-based regularization method

A problem of anomaly detection in homogenous populations consisting of linear stable systems is studied. The recently introduced sparse multiple kernel based regularization method is applied to solve the problem. A common problem with the existing regularization methods is that there lacks an efficient and systematic way to tune the involved regularization parameters. In contrast, the hyper-parameters (some of them can be interpreted as regularization parameters) involved in the proposed method are tuned in an automatic way, and in fact estimated by using the empirical Bayes method. What's more, both the parameter and hyper-parameter estimation problems can be cast as convex and sequential convex optimization problems. It is possible to derive scalable solutions to both the parameter and hyper-parameter estimation problems and thus provide a scalable solution to the anomaly detection.

General information
State: Published
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Pages: 265-270
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BFI conference series: IEEE Conference on Decision and Control (5010888)
Main Research Area: Technical/natural sciences
Conference: 53rd IEEE Conference on Decision and Control (CDC 2014), Los Angeles, United States, 15/12/2014 - 15/12/2014
A non-linear wave decomposition model for efficient wave–structure interaction. Part A: Formulation, validations and analysis

This paper deals with the development of an enhanced model for solving wave–wave and wave–structure interaction problems. We describe the application of a non-linear splitting method originally suggested by Di Mascio et al. [1], to the high-order finite difference model developed by Bingham et al. [2] and extended by Engsig-Karup et al. [3] and [4]. The enhanced strategy is based on splitting all solution variables into incident and scattered fields, where the incident field is assumed to be known and only the scattered field needs to be computed by the numerical model. Although this splitting technique has been applied to both potential flow and Navier–Stokes solvers in the past, it has not been thoroughly described and analyzed, nor has it been presented in widely read journals. Here we describe the method in detail and carefully analyze its performance using several 2D linear and non-linear test cases. In particular, we consider the extreme case of non-linear waves up to the point of breaking reflecting from a vertical wall; and conclude that no limitations are imposed by adopting this splitting. The advantages of this strategy in terms of robustness, accuracy and efficiency are also demonstrated by comparison with the more common strategy of solving the incident and scattered fields together.
Application of Constrained Linear MPC to a Spray Dryer

In this paper we develop a linear model predictive control (MPC) algorithm for control of a two stage spray dryer. The states are estimated by a stationary Kalman filter. A non-linear first-principle engineering model is developed to simulate the spray drying process. The model is validated against experimental data and able to precisely predict the temperatures, the air humidity and the residual moisture in the dryer. The MPC controls these variables to the target and reject disturbances. Spray drying is a cost-effective method to evaporate water from liquid foods and produces a free flowing powder. The main challenge of spray drying is to meet the residual moisture specification and prevent powder from sticking to the chamber walls. By simulation we compare the performance of the MPC against the conventional PID control strategy. During an industrially recorded disturbance scenario, the MPC increases the production rate by 7.9%, profit of production by 8.2% and the energy efficiency by 4.1% on average.
Application of incremental algorithms to CT image reconstruction for sparse-view, noisy data

This conference contribution adapts an incremental framework for solving optimization problems of interest for sparse-view CT. From the incremental framework two algorithms are derived: one that combines a damped form of the algebraic reconstruction technique (ART) with a total-variation (TV) projection, and one that employs a modified damped ART, accounting for a weighted-quadratic data fidelity term, combined with TV projection. The algorithms are demonstrated on simulated, noisy, sparse-view CT data.

General information
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Conference: 3rd International Conference on Image Formation in X-Ray Computed Tomography, Salt Lake City, Utah, United States, 22/06/2014 - 22/06/2014
Electronic versions:
Application_of_incremental_algorithms_to_CT_image_reconstruction_for_sparse_view_noisy_data.pdf
Links:
http://www.ucair.med.utah.edu/CTmeeting/
Source: PublicationPreSubmission
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2014

A Realistic Process Example for MIMO MPC based on Autoregressive Models

Advanced controllers such as model predictive control are in use for a wide range of application in the process industry. The potential utilization of such advanced predictive controllers is far from exhausted. One barrier for more widespread implementation is the lack of simple methodologies for advanced control design development which may be used by non-experts in control theory. This paper presents and illustrates the use of a simple methodology to design an offset-free MPC based on ARX models. Hence a mechanistic process model is not required. The forced circulation evaporator by Newell and Lee is used to illustrate the offset-free MPC based on ARX models for a nonlinear multivariate process.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
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Pages: 3086-3091
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Publisher: International Federation of Automatic Control
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Chemical Process Control, Model Predictive Control, Autoregressive Models
DOIs:
10.3182/20140824-6-ZA.1003.00461
Source: PublicationPreSubmission
Source-ID: 101282811
A Reduced Dantzig-Wolfe Decomposition for a Suboptimal Linear MPC

Linear Model Predictive Control (MPC) is an efficient control technique that repeatedly solves online constrained linear programs. In this work we propose an economic linear MPC strategy for operation of energy systems consisting of multiple and independent power units. These systems cooperate to meet the supply of power demand by minimizing production costs. The control problem can be formulated as a linear program with block-angular structure. To speed-up the solution of the optimization control problem, we propose a reduced Dantzig-Wolfe decomposition. This decomposition algorithm computes a suboptimal solution to the economic linear MPC control problem and guarantees feasibility and stability. Finally, six scenarios are performed to show the decrease in computation time in comparison with the classic Dantzig-Wolfe algorithm.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science , Scientific Computing, Dynamical Systems, Department of Chemical and Biochemical Engineering, Center for Energy Resources Engineering, Centre for IT-Intelligent Energy Systems in Cities
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Pages: 2207-2212
Publication date: 2014

Assessment of Model Predictive and Adaptive Glucose Control Strategies for People with Type 1 Diabetes

This paper addresses overnight blood glucose stabilization in people with type 1 diabetes using a Model Predictive Controller (MPC). We use a control strategy based on an adaptive ARMAX model in which we use a Recursive Extended Least Squares (RELS) method to estimate parameters of the stochastic part. We compare this model structure with an autoregressive integrated moving average with exogenous input (ARIMAX) structure, and with an autoregressive moving average with exogenous input (ARMAX) model, i.e. without an integrator. Additionally, safety layers improve the controller robustness and reduce the risk of hypoglycemia. We test our control strategies on a virtual clinic of 100 randomly generated patients with a representative inter-subject variability. This virtual clinic is based on the Hovorka model. We consider the case where only half of the meal bolus is administered at mealtime, and the case where the insulin sensitivity varies during the night. The simulation results demonstrate that the adaptive control strategy can reduce the risks of hypoglycemia and hyperglycemia during the night.

General information
State: Published
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Pages: 231-236
Publication date: 2014
A tuning approach for offset-free MPC with conditional reference adaptation

Model predictive control has become a widely accepted strategy in industrial applications in the recent years. Often mentioned reasons for the success are the optimization based on a system model, consideration of constraints and an intuitive tuning process. However, as soon as unknown disturbances or model plant mismatch have to be taken into account the tuning effort to achieve offset-free tracking increases. In this work a novel approach for offset-free MPC is presented, which divides the tuning in two steps, the setup of a nominal MPC loop and an external reference adaptation. The inner nominal loop addresses the performance targets in the nominal case, decouples the system and essentially leads to a first order response. The second outer loop enables offset-free tracking in case of unknown disturbances and consists of feedback controllers adapting the reference. Due to the mentioned properties these controllers can be tuned separate and by known guidelines. To address conditions with active input constraints, additionally a conditional reference adaptation scheme is introduced. The tuning strategy is evaluated on a simulated linear Wood-Berry binary distillation column example.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Chemical and Biochemical Engineering, Centre for IT-Intelligent Energy Systems in Cities, Johannes Kepler University of Linz
Authors: Waschl, H. (Ekstern), Jørgensen, J. B. (Intern), Huusom, J. K. (Intern), Del Re, L. (Ekstern)
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Publication date: 2014

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DOIs: 10.3182/20140824-6-ZA-1003.02369
Source: FindIt
Source-ID: 2288854873
Publication: Research - peer-review › Article in proceedings – Annual report year: 2015

A Tuning Approach for Offset-free MPC with Conditional Reference Adaptation.
Model predictive control has become a widely accepted strategy in industrial applications in the recent years. Often mentioned reasons for the success are the optimization based on a system model, consideration of constraints and an intuitive tuning process. However, as soon as unknown disturbances or model plant mismatch have to be taken into account the tuning effort to achieve offset-free tracking increases. In this work a novel approach for offset-free MPC is presented, which divides the tuning in two steps, the setup of a nominal MPC loop and an external reference adaptation. The inner nominal loop addresses the performance targets in the nominal case, decouples the system and essentially leads to a first order response. The second outer loop enables offset-free tracking in case of unknown disturbances and consists of feedback controllers adapting the reference. Due to the mentioned properties these controllers can be tuned separate and by known guidelines. To address conditions with active input constraints, additionally a conditional reference adaptation scheme is introduced. The tuning strategy is evaluated on a simulated linear Wood-Berry binary distillation column example.

General information
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Publisher: International Federation of Automatic Control
Bihormonal model predictive control of blood glucose in people with type 1 diabetes

In this paper we present a bihormonal control system that controls blood glucose in people with type 1 diabetes (T1D). We use insulin together with glucagon to mitigate the negative effects of hyper- and hypoglycemia. The system consists of a Kalman filter, a micro-bolus insulin and glucagon infusion MPC, a mealtime bolus calculator and a CGM providing feedback to the controller. The controller employs a patient data-based prediction model with ARMAX structure. We test the controller using a bihormonal model with time-varying parameters for 3 subjects and compare its performance to a system with an identical insulin MPC, but a glucagon PD controller. The key contribution of the bihormonal MPC is the efficiency of glucagon use. We consider scenarios where the meals are estimated correctly or overestimated and where the insulin sensitivity increases. Both solutions provide tight glucose control. According to the simulations, the bihormonal MPC requires on average 30% less glucagon than the system with a PD controller.

Conditional Reference Adaptation for Offset-free MPC

Model predictive control has become a widely accepted strategy in industrial applications in the recent years. Often mentioned reasons for the success are the optimization based on a system model, consideration of constraints and an intuitive tuning process. However, as soon as unknown disturbances or model plant mismatch have to be taken into account the tuning sort to achieve offset-free tracking increases. In this work a novel approach for offset-free MPC is presented, which divides the tuning in two steps, the setup of a nominal MPC loop and an external reference adaptation. The inner nominal loop addresses the performance targets in the nominal case, decouples the system and essentially leads to a first order response. The second outer loop enables offset-free tracking in case of unknown disturbances and consists of feedback controllers adapting the reference. Due to the mentioned properties these controllers can be tuned separate and by known guidelines. To address conditions with active input constraints, additionally a conditional reference adaptation scheme is introduced. The tuning strategy is evaluated on a simulated linear Wood-Berry binary distillation column example.
Decomposition in conic optimization with partially separable structure

Decomposition techniques for linear programming are difficult to extend to conic optimization problems with general nonpolyhedral convex cones because the conic inequalities introduce an additional nonlinear coupling between the variables. However in many applications the convex cones have a partially separable structure that allows them to be characterized in terms of simpler lower-dimensional cones. The most important example is sparse semidefinite programming with a chordal sparsity pattern. Here partial separability derives from the clique decomposition theorems that characterize positive semidefinite and positive-semidefinite-completable matrices with chordal sparsity patterns. The paper describes a decomposition method that exploits partial separability in conic linear optimization. The method is based on Spingarn’s method for equality constrained convex optimization, combined with a fast interior-point method for evaluating proximal operators.

General information

State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, University of California
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.22 SJR 2.902 SNIP 2.237
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.388 SNIP 2.373 CiteScore 3.32
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.851 SNIP 2.513 CiteScore 2.98
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.267 SNIP 2.701 CiteScore 3.44
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.529 SNIP 2.773 CiteScore 3.05
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.339 SNIP 2.217 CiteScore 2.4
ISI indexed (2011): ISI indexed yes
Distributed Interior-point Method for Loosely Coupled Problems

In this paper, we put forth distributed algorithms for solving loosely coupled unconstrained and constrained optimization problems. Such problems are usually solved using algorithms that are based on a combination of decomposition and first order methods. These algorithms are commonly very slow and require many iterations to converge. In order to alleviate this issue, we propose algorithms that combine the Newton and interior-point methods with proximal splitting methods for solving such problems. Particularly, the algorithm for solving unconstrained loosely coupled problems, is based on Newton’s method and utilizes proximal splitting to distribute the computations for calculating the Newton step at each iteration. A combination of this algorithm and the interior-point method is then used to introduce a distributed algorithm for solving constrained loosely coupled problems. We also provide guidelines on how to implement the proposed methods efficiently, and briefly discuss the properties of the resulting solutions.
Distributed Robustness Analysis of Interconnected Uncertain Systems Using Chordal Decomposition

Large-scale interconnected uncertain systems commonly have large state and uncertainty dimensions. Aside from the heavy computational cost of performing robust stability analysis in a centralized manner, privacy requirements in the network can also introduce further issues. In this paper, we utilize IQC analysis for analyzing large-scale interconnected uncertain systems and we evade these issues by describing a decomposition scheme that is based on the interconnection structure of the system. This scheme is based on the so-called chordal decomposition and does not add any conservativeness to the analysis approach. The decomposed problem can be solved using distributed computational algorithms without the need for a centralized computational unit. We further discuss the merits of the proposed analysis approach using a numerical experiment.

General information
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Publication date: 2014

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Robustness analysis, Networked systems, Convex optimization

Distributed Solutions for Loosely Coupled Feasibility Problems Using Proximal Splitting Methods

In this paper, we consider convex feasibility problems (CFPs) where the underlying sets are loosely coupled, and we propose several algorithms to solve such problems in a distributed manner. These algorithms are obtained by applying proximal splitting methods to convex minimization reformulations of CFPs. We also put forth distributed convergence tests which enable us to establish feasibility or infeasibility of the problem distributedly, and we provide convergence rate results. Under the assumption that the problem is feasible and boundedly linearly regular, these convergence results are given in terms of the distance of the iterates to the feasible set, which are similar to those of classical projection methods. In case the feasibility problem is infeasible, we provide convergence rate results that concern the convergence of certain error bounds.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Linköping University
Authors: Pakazad, S. K. (Ekstern), Andersen, M. S. (Intern), Hansson, A. (Ekstern)
Number of pages: 34
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication Information
Journal: Optimization Methods and Software
ISSN (Print): 1055-6788
Ratings:
In this paper we investigate an economically optimizing Nonlinear Model Predictive Control (E-NMPC) for a spray drying process. By simulation we evaluate the economic potential of this E-NMPC compared to a conventional PID based control strategy. Spray drying is the preferred process to reduce the water content for many liquid foodstuffs and produces a free flowing powder. The main challenge in controlling the spray drying process is to meet the residual moisture specifications and avoid that the powder sticks to the chamber walls of the spray dryer. We present a model for a spray dryer that has been validated on experimental data from a pilot plant. We use this model for simulation as well as for prediction in the E-NMPC. The E-NMPC is designed with hard input constraints and soft output constraints. The open-loop optimal control problem in the E-NMPC is solved using the single-shooting method combined with a quasi-Newton Sequential Quadratic Programming (SQP) algorithm and the adjoint method for computation of gradients. The E-NMPC improves the cost of spray drying by 26.7% compared to conventional PI control in our simulations.
Efficient Implementation of Solvers for Linear Model Predictive Control on Embedded Devices

This paper proposes a novel approach for the efficient implementation of solvers for linear MPC on embedded devices. The main focus is to explain in detail the approach used to optimize the linear algebra for selected low-power embedded devices, and to show how the high-performance implementation of a single routine (the matrix-matrix multiplication gemm) can speed-up an interior-point method for linear MPC. The results show that the high-performance MPC obtained using the proposed approach is several times faster than the current state-of-the-art IP method for linear MPC on embedded devices.

Gaussian translation operator for Multi-Level Fast Multipole Method

Results using a new translation operator for the Multi-Level Fast Multipole Method are presented. Based on Gaussian beams, the translation operator allows a significant portion of the plane-wave directions to be neglected, resulting in a much faster translation step.
Generalized Row-Action Methods for Tomographic Imaging

Row-action methods play an important role in tomographic image reconstruction. Many such methods can be viewed as incremental gradient methods for minimizing a sum of a large number of convex functions, and despite their relatively poor global rate of convergence, these methods often exhibit fast initial convergence which is desirable in applications where a low-accuracy solution is acceptable. In this paper, we propose relaxed variants of a class of incremental proximal gradient methods, and these variants generalize many existing row-action methods for tomographic imaging. Moreover, they allow us to derive new incremental algorithms for tomographic imaging that incorporate different types of prior information via regularization. We demonstrate the efficacy of the approach with some numerical examples.
High-performance small-scale solvers for linear Model Predictive Control

In Model Predictive Control (MPC), an optimization problem needs to be solved at each sampling time, and this has traditionally limited use of MPC to systems with slow dynamic. In recent years, there has been an increasing interest in the area of fast small-scale solvers for linear MPC, with the two main research areas of explicit MPC and tailored on-line MPC. State-of-the-art solvers in this second class can outperform optimized linear-algebra libraries (BLAS) only for very small problems, and do not explicitly exploit the hardware capabilities, relying on compilers for that. This approach can attain only a small fraction of the peak performance on modern processors. In our paper, we combine high-performance computing techniques with tailored solvers for MPC, and use the specific instruction sets of the target architectures. The resulting software (called HPMPC) can solve linear MPC problems 2 to 8 times faster than the current state-of-the-art solver for this class of problems, and the high-performance is maintained for MPC problems with up to a few hundred states.

General information

State: Published
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Pages: 128-133
Publication date: 2014
Improved Multilevel Fast Multipole Method for Higher-Order discretizations

The Multilevel Fast Multipole Method (MLFMM) allows for a reduced computational complexity when solving electromagnetic scattering problems. Combining this with the reduced number of unknowns provided by Higher-Order discretizations has proven to be a difficult task, with the general conclusion being that going above 2nd order is not worthwhile. In this paper, we challenge this conclusion, providing results that demonstrate the potential performance gains with Higher-Order MLFMM and showing some modifications to the traditional MLFMM that can benefit both Higher-Order and standard discretizations.

Input-constrained model predictive control via the alternating direction method of multipliers

This paper presents an algorithm, based on the alternating direction method of multipliers, for the convex optimal control problem arising in input-constrained model predictive control. We develop an efficient implementation of the algorithm for the extended linear quadratic control problem (LQCP) with input and input-rate limits. The algorithm alternates between solving an extended LQCP and a highly structured quadratic program. These quadratic programs are solved using a Riccati iteration procedure, and a structure-exploiting interior-point method, respectively. The computational cost per iteration is quadratic in the dimensions of the controlled system, and linear in the length of the prediction horizon. Simulations show that the approach proposed in this paper is more than an order of magnitude faster than several state-of-the-art quadratic programming algorithms, and that the difference in computation time grows with the problem size. We improve the method further using a warm-start procedure.
Interior Point Methods on GPU with application to Model Predictive Control

The goal of this thesis is to investigate the application of interior point methods to solve dynamical optimization problems, using a graphical processing unit (GPU) with a focus on problems arising in Model Predictive Control (MPC). Multi-core processors have been available for over ten years now, and manycore processors, such as GPUs, have also become a standard component in any consumer computer. The GPU offers faster floating point operations and higher memory bandwidth than the CPU, but requires algorithms to be redesigned and implemented, to match the underlying architecture. A large number of different optimization algorithms are available for solving optimization problems. Some of the most common method are the simplex method and interior point methods. We focus on interior point methods in this thesis, due to its polynomial complexity, and since the use of the simplex method with GPUs have been investigated by several other authors already. The main computational task in interior point methods is the solution of a linear system to compute the Newton direction in each iteration. Direct interior point methods use a direct method such as Cholesky factorization to factorize the normal equations of the Hessian matrix. The use of a GPU has been shown to be very efficient in the factorization of dense matrices, and several numeric libraries, which utilize the GPU, have become available during the course of this thesis. We have developed a direct interior point method, which utilizes the GPU, and demonstrate that our implementation can reduce the solution time substantially.

There are multiple software packages available for solving optimization problems with interior point methods, such as GLPK, IPOPT, MOSEK and many more. However, none of these support the GPU yet. With this thesis, we include a new software package called GPUOPT, available under the non-restrictive MIT license. GPUOPT includes includes a primal-dual interior-point method, which supports both the CPU and the GPU. It is implemented as multiple components, where the matrix operations and solver for the Newton directions is separated from the core interior point method. This makes it possible to replace the matrix operations and solver with alternative, and potentially problem-specific, implementations. In this thesis, we include different implementations of the matrix operations, including general dense, general sparse and problem-specific implementation of a test problem from model predictive control. Multiple solvers are implemented as well, including a direct solver based on CHOLMOD, and an iterative solver which uses preconditioned conjugate gradient. The iterative solver is based on the matrix-free iterative interior point method.

Iso-geometric shape optimization of magnetic density separators

Purpose
The waste recycling industry increasingly relies on magnetic density separators. These devices generate an upward magnetic force in ferro-fluids allowing to separate the immersed particles according to their mass density. Recently, a new separator design has been proposed that significantly reduces the required amount of permanent magnet material. The purpose of this paper is to alleviate the undesired end-effects in this design by altering the shape of the ferromagnetic covers of the individual poles.

Design/methodology/approach
The paper represents the shape of the ferromagnetic pole covers with B-splines and defines a cost functional that measures the non-uniformity of the magnetic field in an area above the poles. The authors apply an iso-geometric shape optimization procedure, which allows us to accurately represent, analyze and optimize the geometry using only a few design variables. The design problem is regularized by imposing constraints that enforce the convexity of the pole cover shapes and is solved by a non-linear optimization procedure. The paper validates the implementation of the algorithm using a simplified variant of the design problem with a known analytical solution. The algorithm is subsequently applied to the problem posed.

Findings
The shape optimization attains its target and yields pole cover shapes that give rise to a magnetic field that is uniform over a larger domain.

Research limitations/implications
This increased magnetic field uniformity is obtained at the cost of a pole cover shape that differs per pole. This limitation has negligible impact on the manufacturing of the separator. The new pole cover shapes therefore lead to improved performance of the density separation.

Practical implications
Due to the larger uniformity the generated field, these shapes should enable larger amounts of waste to be processed than the previous design.

Originality/value
This paper treats the shapes optimization of magnetic density separators systematically and presents new shapes for the ferromagnetic poles covers.

**General information**
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Web of Science (2016): Indexed yes
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Scopus rating (2014): SJR 0.29 SNIP 0.693 CiteScore 0.63
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 0.202 SNIP 0.53 CiteScore 0.55
ISI indexed (2013): ISI indexed yes
Scopus rating (2012): SJR 0.21 SNIP 0.513 CiteScore 0.5
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): SJR 0.214 SNIP 0.708 CiteScore 0.5
ISI indexed (2011): ISI indexed yes
Scopus rating (2010): SJR 0.235 SNIP 0.83
Scopus rating (2009): SJR 0.245 SNIP 0.817
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.298 SNIP 0.858
Scopus rating (2007): SJR 0.266 SNIP 0.453
Scopus rating (2006): SJR 0.301 SNIP 0.676
Scopus rating (2005): SJR 0.22 SNIP 0.54
Web of Science (2005): Indexed yes
Iterative Reconstruction Methods for Hybrid Inverse Problems in Impedance Tomography

For a general formulation of hybrid inverse problems in impedance tomography the Picard and Newton iterative schemes are adapted and four iterative reconstruction algorithms are developed. The general problem formulation includes several existing hybrid imaging modalities such as current density impedance imaging, magnetic resonance electrical impedance tomography, and ultrasound modulated electrical impedance tomography, and the unified approach to the reconstruction problem encompasses several algorithms suggested in the literature. The four proposed algorithms are implemented numerically in two dimensions and the properties of the algorithms and the implementations are investigated, both theoretically and on simulated data obtained from a numerical phantom. The numerical results show similarities and differences between the proposed algorithms, and they justify that the choice of algorithm should be based on a theoretical analysis of the underlying inverse problem.
Mathematical Modeling and Dimension Reduction in Dynamical Systems

Processes that change in time are in mathematics typically described by differential equations. These may be applied to model everything from weather forecasting, brain patterns, reaction kinetics, water waves, finance, social dynamics, structural dynamics and electrodynamics to name only a few. These systems are generically nonlinear and the studies of them often become enormously complex. The framework in which such systems are best understood is via the theory of dynamical systems, where the critical behavior is systematically analyzed by performing bifurcation theory. In that context the current thesis is attacking two problems.

The first is concerned with the mathematical modelling and analysis of an experiment of a vibro-impacting beam. This type of dynamical system has received much attention in the recent years and they occur frequently in mechanical applications, where they induce noise and wear which decrease the life time of machines. From the modelling point of view these systems are often particularly rich in nonlinear dynamics. In the present study a mathematical model is derived. Amongst other outcomes the model was successfully applied to predict a nonlinear phenomenon, namely the existence of isolas of subharmonic orbits. These were then verified in the practical experiment in the lab. The second problem that is addressed in the current thesis is a problem that has developed as a consequence of the increasing power of computers which has created the demand for analysis of ever more advanced and complex systems. These complex systems are computationally very demanding and proper analysis of the qualitative behavior of the systems becomes difficult. In order to overcome this obstacle much research is going into the direction of development of robust methods to perform dimension and model reduction such as to pave the way for a qualitative analysis of the high-dimensional problems by analyzing the low-dimensional models.

In this thesis we demonstrate how to reduce the dimension of a certain class of dynamical systems by construction of k-dimensional submanifolds using the so-called graph transform. The method is suitable for a specific class of problems with spectral gaps, these are often observed. In particular the method is applied to a mechanical system. Furthermore the method has some unique and promising properties compared to other methods.
In this thesis, we consider control strategies for flexible distributed energy resources in the future intelligent energy system – the Smart Grid. The energy system is a large-scale complex network with many actors and objectives in different hierarchical layers. Specifically, the power system must supply electricity reliably to both residential and industrial consumers around the clock. More and more fluctuating renewable energy sources, like wind and solar, are integrated in the power system. Consequently, uncertainty in production starts to affect an otherwise controllable power production significantly. A Smart Grid calls for flexible consumers that can adjust their consumption based on the amount of green energy in the grid. This requires coordination through new large-scale control and optimization algorithms. Trading of flexibility is key to drive power consumption in a sustainable direction. In Denmark, we expect that distributed energy resources such as heat pumps, and batteries in electric vehicles will mobilize part of the needed flexibility.

Our primary objectives in the thesis were threefold:

1. Simulate the components in the power system based on simple models from literature (e.g. heat pumps, heat tanks, electrical vehicle battery charging/discharging, wind farms, power plants).

2. Embed forecasting methodologies for the weather (e.g. temperature, solar radiation), the electricity consumption, and the electricity price in a predictive control system.

3. Develop optimization algorithms for large-scale dynamic systems. This includes decentralized optimization and simulation on realistic large-scale dynamic systems.

Chapter 1 introduces the power system, the markets, and the main actors. The objectives and control hierarchy is outlined while Aggregators are introduced as new actors.

Chapter 2 provides linear dynamical models of Smart Grid units: Electric Vehicles, buildings with heat pumps, refrigeration systems, solar collectors, heat storage tanks, power plants, and wind farms. The models can be realized as discrete time state space models that fit into a predictive control system.

Chapter 3 introduces Model Predictive Control (MPC) including state estimation, filtering and prediction for linear models.

Chapter 4 simulates the models from Chapter 2 with the certainty equivalent MPC from Chapter 3. An economic MPC minimizes the costs of consumption based on real electricity prices that determined the flexibility of the units. A predictive control system easily handles constraints, e.g. limitations in power consumption, and predicts the future behavior of a unit by integrating predictions of electricity prices, consumption, and weather variables. The simulations demonstrate the expected load shifting capabilities of the units that adapts to the given price predictions. We furthermore evaluated control performance in terms of economic savings for different control strategies and forecasts.

Chapter 5 describes and compares the proposed large-scale Aggregator control strategies. Aggregators are assumed to play an important role in the future Smart Grid and coordinate a large portfolio of units. The developed economic MPC controllers interfaces each unit directly to an Aggregator. We developed several MPC-based aggregation strategies that
coordinates the global behavior of a portfolio of units by solving a large-scale optimization and control problem. We applied decomposition methods based on convex optimization, such as dual decomposition and operator splitting, and developed price-based aggregator strategies.

Chapter 6 provides conclusions, contributions and future work.

The main scientific contributions can be summarized to:

- Linear dynamical models of flexible Smart Grid units: heat pumps in buildings, heat storage tanks, and electric vehicle batteries.
- Economic MPC that integrates forecasts in the control of these flexible units.
- Large-scale distributed control strategies based on economic MPC, convex optimization, and decomposition methods.
- A Matlab toolbox including the modeled units for simulating a Smart Energy System with MPC.

General information
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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering, Dynamical Systems
Authors: Halvgaard, R. (Intern), Jørgensen, J. B. (Intern), Poulsen, N. K. (Intern), Madsen, H. (Intern)
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Model_Predictive_Control.pdf
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Multicore Performance of Block Algebraic Iterative Reconstruction Methods
Algebraic iterative methods are routinely used for solving the ill-posed sparse linear systems arising in tomographic image reconstruction. Here we consider the algebraic reconstruction technique (ART) and the simultaneous iterative reconstruction techniques (SIRT), both of which rely on semiconvergence. Block versions of these methods, based on a partitioning of the linear system, are able to combine the fast semiconvergence of ART with the better multicore properties of SIRT. These block methods separate into two classes: those that, in each iteration, access the blocks in a sequential manner, and those that compute a result for each block in parallel and then combine these results before the next iteration. The goal of this work is to demonstrate which block methods are best suited for implementation on modern multicore computers. To compare the performance of the different block methods, we use a fixed relaxation parameter in each method, namely, the one that leads to the fastest semiconvergence. Computational results show that for multicore computers, the sequential approach is preferable.

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Multilevel Fast Multipole Method for Higher Order Discretizations

The multi-level fast multipole method (MLFMM) for a higher order (HO) discretization is demonstrated on high-frequency (HF) problems, illustrating for the first time how an efficient MLFMM for HO can be achieved even for very large groups. Applying several novel ideas, beneficial to both lower order and higher order discretizations, results from a low-memory, high-speed MLFMM implementation of a HO hierarchical discretization are shown. These results challenge the general view that the benefits of HO and HF-MLFMM cannot be combined.
Numerical nonlinear complex geometrical optics algorithm for the 3D Calderón problem

The Calderon problem is the mathematical formulation of the inverse problem in Electrical Impedance Tomography and asks for the uniqueness and reconstruction of an electrical conductivity distribution in a bounded domain from the knowledge of the Dirichlet-to-Neumann map associated to the generalized Laplace equation. The 3D problem was solved in theory in late 1980s using complex geometrical optics solutions and a scattering transform. Several approximations to the reconstruction method have been suggested and implemented numerically in the literature, but here, for the first time, a complete computer implementation of the full nonlinear algorithm is given. First a boundary integral equation is solved by a Nystrom method for the traces of the complex geometrical optics solutions, second the scattering transform is computed and inverted using fast Fourier transform, and finally a boundary value problem is solved for the conductivity distribution.

To test the performance of the algorithm highly accurate data is required, and to this end a boundary element method is developed and implemented for the forward problem. The numerical reconstruction algorithm is tested on simulated data and compared to the simpler approximations. In addition, convergence of the numerical solution towards the exact solution of the boundary integral equation is proved.
On devising Boussinesq-type models with bounded eigenspectra: One horizontal dimension

The propagation of water waves in the nearshore region can be described by depth-integrated Boussinesq-type equations. The dispersive and nonlinear characteristics of the equations are governed by tuneable parameters. We examine the associated linear eigenproblem both analytically and numerically using a spectral element method of arbitrary spatial order p. It is shown that existing sets of parameters, found by optimising the linear dispersion relation, give rise to unbounded eigenspectra which govern stability. For explicit time-stepping schemes the global CFL time-step restriction typically requires $\Delta t \propto p^{-2}$. We derive and present conditions on the parameters under which implicitly-implicit Boussinesq-type equations will exhibit bounded eigenspectra. Two new bounded versions having comparable nonlinear and dispersive properties as the equations of Nwogu (1993) and Schäffer and Madsen (1995) are introduced. Using spectral element simulations of stream function waves it is illustrated that (i) the bounded equations capture the physics of the wave motion as well as the standard unbounded equations, and (ii) the bounded equations are computationally more efficient when explicit time-stepping schemes are used. Thus the bounded equations were found to lead to more robust and efficient numerical schemes without compromising the accuracy.
On the importance of the distance measures used to train and test knowledge-based potentials for proteins

Knowledge-based potentials are energy functions derived from the analysis of databases of protein structures and sequences. They can be divided into two classes. Potentials from the first class are based on a direct conversion of the distributions of some geometric properties observed in native protein structures into energy values, while potentials from the second class are trained to mimic quantitatively the geometric differences between incorrectly folded models and native structures. In this paper, we focus on the relationship between energy and geometry when training the second class of knowledge-based potentials. We assume that the difference in energy between a decoy structure and the corresponding native structure is linearly related to the distance between the two structures. We trained two distance-based knowledge-based potentials accordingly, one based on all inter-residue distances (PPD), while the other had the set of all distances filtered to reflect consistency in an ensemble of decoys (PPE). We tested four types of metric to characterize the distance between the decoy and the native structure, two based on extrinsic geometry (RMSD and GTD-
TS*), and two based on intrinsic geometry (Q* and MT). The corresponding eight potentials were tested on a large collection of decoy sets. We found that it is usually better to train a potential using an intrinsic distance measure. We also found that PPE outperforms PPD, emphasizing the benefits of capturing consistent information in an ensemble. The relevance of these results for the design of knowledge-based potentials is discussed.
Planar Parametrization in Isogeometric Analysis

Before isogeometric analysis can be applied to solving a partial differential equation posed over some physical domain, one needs to construct a valid parametrization of the geometry. The accuracy of the analysis is affected by the quality of the parametrization. The challenge of computing and maintaining a valid geometry parametrization is particularly relevant in applications of isogeometric analysis to shape optimization, where the geometry varies from one optimization iteration to another. We propose a general framework for handling the geometry parametrization in isogeometric analysis and shape optimization. It utilizes an expensive non-linear method for constructing/updating a high quality reference parametrization, and an inexpensive linear method for maintaining the parametrization in the vicinity of the reference one. We describe several linear and non-linear parametrization methods, which are suitable for our framework. The non-linear methods we consider are based on solving a constrained optimization problem numerically, and are divided into two classes, geometry-oriented methods and analysis-oriented methods. Their performance is illustrated through a few numerical examples.

*Plug-and-play* edge-preserving regularization

In many inverse problems it is essential to use regularization methods that preserve edges in the reconstructions, and many reconstruction models have been developed for this task, such as the Total Variation (TV) approach. The associated algorithms are complex and require a good knowledge of large-scale optimization algorithms, and they involve certain tolerances that the user must choose. We present a simpler approach that relies only on standard computational building blocks in matrix computations, such as orthogonal transformations, preconditioned iterative solvers, Kronecker products, and the discrete cosine transform. Hence the term *plug-and-play*. We do not attempt to improve on TV reconstructions, but rather provide an easy-to-use approach to computing reconstructions with similar properties.
Predicting Plasma Glucose From Interstitial Glucose Observations Using Bayesian Methods

One way of constructing a control algorithm for an artificial pancreas is to identify a model capable of predicting plasma glucose (PG) from interstitial glucose (IG) observations. Stochastic differential equations (SDEs) make it possible to
account both for the unknown influence of the continuous glucose monitor (CGM) and for unknown physiological influences. Combined with prior knowledge about the measurement devices, this approach can be used to obtain a robust predictive model. A stochastic-differential-equation-based gray box (SDE-GB) model is formulated on the basis of an identifiable physiological model of the glucoregulatory system for type 1 diabetes mellitus (T1DM) patients. A Bayesian method is used to estimate robust parameters from clinical data. The models are then used to predict PG from IG observations from 2 separate study occasions on the same patient. First, all statistically significant diffusion terms of the model are identified using likelihood ratio tests, yielding inclusion of $\sigma_{Isc}$, $\sigma_{Gp}$, and $\sigma_{Gsc}$. Second, estimates using maximum likelihood are obtained, but prediction capability is poor. Finally, a Bayesian method is implemented. Using this method the identified models are able to predict PG using only IG observations. These predictions are assessed visually. We are also able to validate these estimates on a separate data set from the same patient. This study shows that SDE-GBs and a Bayesian method can be used to identify a reliable model for prediction of PG using IG observations obtained with a CGM. The model could eventually be used in an artificial pancreas.

**General information**

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Web of Science (2017): Indexed yes
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.855 SNIP 0.897 CiteScore 1.99
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.871 SNIP 0.971 CiteScore 1.84
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.78 SNIP 0.918 CiteScore 2.19
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.69 SNIP 0.972 CiteScore 1.33
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.687 SNIP 0.916 CiteScore 0.6
ISI indexed (2011): ISI indexed no
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Scopus rating (2010): SJR 0.452 SNIP 0.683
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R3GMRES: including prior information in GMRES-type methods for discrete inverse problems

Lothar Reichel and his collaborators proposed several iterative algorithms that augment the underlying Krylov subspace with an additional low-dimensional subspace in order to produce improved regularized solutions. We take a closer look at this approach and investigate a particular Regularized Range-Restricted GMRES method, R3GMRES, with a subspace that represents prior information about the solution. We discuss the implementation of this approach and demonstrate its advantage by means of several test problems.

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Authors: Dong, Y. (Intern), Garde, H. (Intern), Hansen, P. C. (Intern)
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BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.945 SNIP 1.099 CiteScore 1.15
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.641 SNIP 0.738 CiteScore 0.76
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.783 SNIP 0.898 CiteScore 0.99
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.975 SNIP 1.287 CiteScore 1.33
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.836 SNIP 1.313 CiteScore 1.13
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.659 SNIP 0.772 CiteScore 0.75
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.583 SNIP 0.874
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.703 SNIP 0.827
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.56 SNIP 0.69
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.435 SNIP 0.918
Scopus rating (2006): SJR 0.729 SNIP 1.526
Scopus rating (2005): SJR 1.201 SNIP 1.269
Scopus rating (2004): SJR 0.878 SNIP 1.33
Scopus rating (2003): SJR 1.316 SNIP 1.942
Scopus rating (2002): SJR 0.867 SNIP 1.034
Real-time economic optimization for a fermentation process using Model Predictive Control

Fermentation is a widely used process in production of many foods, beverages, and pharmaceuticals. The main goal of the control system is to maximize profit of the fermentation process, and thus this is also the main goal of this paper. We present a simple dynamic model for a fermentation process and demonstrate its usefulness in economic optimization. The model is formulated as an index-1 differential algebraic equation (DAE), which guarantees conservation of mass and energy in discrete form. The optimization is based on recent advances within Economic Nonlinear Model Predictive Control (E-NMPC), and also utilizes the index-1 DAE model. The E-NMPC uses the single-shooting method and the adjoint method for computation of the optimization gradients. The process constraints are relaxed to soft-constraints on the outputs. Finally we derive the analytical solution to the economic optimization problem and compare it with the numerically determined solution.

Reduced-Complexity Semidefinite Relaxations of Optimal Power Flow Problems

We propose a new method for generating semidefinite relaxations of optimal power flow problems. The method is based on chordal conversion techniques: by dropping some equality constraints in the conversion, we obtain semidefinite relaxations that are computationally cheaper, but potentially weaker, than the standard semidefinite relaxation. Our numerical results show that the new relaxations often produce the same results as the standard semidefinite relaxation, but at a lower computational cost.
Reflector antenna analysis using physical optics on Graphics Processing Units

The Physical Optics approximation is a widely used asymptotic method for calculating the scattering from electrically large bodies. It requires significant computational work and little memory, and is thus well suited for application on a Graphics Processing Unit. Here, we investigate the performance of an implementation and demonstrate that while there are some implementational pitfalls, a careful implementation can result in impressive improvements.

General information
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Organisations: Department of Applied Mathematics and Computer Science , Scientific Computing, TICRA
Authors: Borries, O. P. (Intern), Sørensen, H. H. B. (Intern), Dammann, B. (Ekstern), Jorgensen, E. (Intern), Meincke, P. (Intern), Sorensen, S. B. (Ekstern), Hansen, P. C. (Intern)
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Rotational image deblurring with sparse matrices
We describe iterative deblurring algorithms that can handle blur caused by a rotation along an arbitrary axis (including the common case of pure rotation). Our algorithms use a sparse-matrix representation of the blurring operation, which allows us to easily handle several different boundary conditions. We also include robust stopping rules for the iterations. The performance of our algorithms is illustrated with examples.

General information
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Organisations: Department of Applied Mathematics and Computer Science , Scientific Computing, Emory University, Fraunhofer Gesellschaft
Authors: Hansen, P. C. (Intern), Nagy, J. G. (Ekstern), Tigkos, K. (Intern)
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 1.535 SNIP 1.312 CiteScore 1.41
Web of Science (2016): Indexed yes
Kaczmarz’s method—sometimes referred to as the algebraic reconstruction technique—is an iterative method that is widely used in tomographic imaging due to its favorable semi-convergence properties. Specifically, when applied to a problem with noisy data, during the early iterations it converges very quickly toward a good approximation of the exact solution, and thus produces a regularized solution. While this property is generally accepted and utilized, there is surprisingly little theoretical justification for it. The purpose of this paper is to present insight into the semi-convergence of Kaczmarz’s method as well as its projected counterpart (and their block versions). To do this we study how the data errors propagate into the iteration vectors and we derive upper bounds for this noise propagation. Our bounds are compared with numerical results obtained from tomographic imaging.

**Semi-convergence properties of Kaczmarz’s method**

Kaczmarz’s method—sometimes referred to as the algebraic reconstruction technique—is an iterative method that is widely used in tomographic imaging due to its favorable semi-convergence properties. Specifically, when applied to a problem with noisy data, during the early iterations it converges very quickly toward a good approximation of the exact solution, and thus produces a regularized solution. While this property is generally accepted and utilized, there is surprisingly little theoretical justification for it. The purpose of this paper is to present insight into the semi-convergence of Kaczmarz’s method as well as its projected counterpart (and their block versions). To do this we study how the data errors propagate into the iteration vectors and we derive upper bounds for this noise propagation. Our bounds are compared with numerical results obtained from tomographic imaging.

**General information**

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**Organisations:** Department of Applied Mathematics and Computer Science, Scientific Computing, Linköping University, Iran University of Science and Technology

**Authors:** Elfving, T. (Ekstern), Hansen, P. C. (Intern), Nikazad, T. (Ekstern)

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Sensitivity Analysis of the Critical Speed in Railway Vehicle Dynamics

We present an approach to global sensitivity analysis aiming at the reduction of its computational cost without compromising the results. The method is based on sampling methods, cubature rules, High-Dimensional Model Representation and Total Sensitivity Indices. The approach has a general applicability in many engineering fields and does not require the knowledge of the particular solver of the dynamical system. This analysis can be used as part of the virtual homologation procedure and to help engineers during the design phase of complex systems. The method is applied to a half car with a two-axle Cooperider bogie, in order to study the sensitivity of the critical speed with respect to suspension parameters. The importance of a certain suspension component is expressed by the variance in critical speed that is ascribable to it. This proves to be useful in the identification of parameters for which the exactness of their values is critically important.

General information

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BFI (2015): BFI-level 1
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Scopus rating (2013): SJR 0.715 SNIP 2.22 CiteScore 1.57
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 0.723 SNIP 2.109 CiteScore 1.44
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.749 SNIP 1.996 CiteScore 1.38
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.669 SNIP 2.099
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.588 SNIP 1.261
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.744 SNIP 2.057
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.386 SNIP 0.898
Scopus rating (2006): SJR 0.485 SNIP 1.523
Size-based predictions of food web patterns

We employ size-based theoretical arguments to derive simple analytic predictions of ecological patterns and properties of natural communities: size-spectrum exponent, maximum trophic level, and susceptibility to invasive species. The predictions are brought about by assuming that an infinite number of species are continuously distributed on a size-trait axis. It is, however, an open question whether such predictions are valid for a food web with a finite number of species embedded in a network structure. We address this question by comparing the size-based predictions to results from dynamic food web simulations with varying species richness. To this end, we develop a new size- and trait-based food web model that can be simplified into an analytically solvable size-based model. We confirm existing solutions for the size distribution and derive novel predictions for maximum trophic level and invasion resistance. Our results show that the predicted size-spectrum exponent is borne out in the simulated food webs even with few species, albeit with a systematic bias. The predicted maximum trophic level turns out to be an upper limit since simulated food webs may have a lower number of trophic levels, especially for low species richness, due to structural constraints. The size-based model possesses an evolutionary stable state and is therefore un-invadable. In contrast, the food web simulations show that all communities, irrespective of number of species, are equally open to invasions. We use these results to discuss the validity of size-based predictions in the light of the structural constraints imposed by food webs.

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Scopus rating (2014): SJR 1.468 SNIP 0.981 CiteScore 1.86
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Scopus rating (2013): SJR 1.456 SNIP 0.914 CiteScore 2.2
ISI indexed (2013): ISI indexed yes
**Sparse data structures in 3DXRD**

In 3D X-ray diffraction tomography (3DXRD) of polycrystals, the spatial and the orientational distribution of crystal grains are numerically reconstructed from the observed diffraction spots and rings. The high dimensionality of the solution space poses a significant computational challenge. In this talk I will present a sparsity-promoting mathematical framework for the 3DXRD and show supporting numerical results.

**Spectral Tensor-Train Decomposition for low-rank surrogate models**

The construction of surrogate models is very important as a mean of acceleration in computational methods for uncertainty quantification (UQ). When the forward model is particularly expensive compared to the accuracy loss due to the use of a surrogate – as for example in computational fluid dynamics (CFD) – the latter can be used for the forward propagation of uncertainty [7] and the solution of inference problems.
Stable finite difference discretizations of the forward speed seakeeping problem

General information
State: Published
Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Bingham, H. B. (Intern), Amini Afshar, M. (Intern), Read, R. (Intern), Engsig-Karup, A. P. (Intern)
Number of pages: 4
Publication date: 2014

Host publication information
Title of host publication: Proceedings of the International Workshop on Water Waves and Floating Bodies 2014
Publisher: IWWFB
Main Research Area: Technical/natural sciences
Conference: 29th International Workshop on Water Waves and Floating Bodies, Osaka, Japan, 30/03/2014 - 30/03/2014
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Stable_finite_difference_discretizations.pdf
Links:
http://www.iwwfb.org/Workshops/29.htm
Source: PublicationPreSubmission
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Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

State space Newton's method for topology optimization
We introduce a new algorithm for solving certain classes of topology optimization problems, which enjoys fast local convergence normally achieved by the full space methods while working in a smaller reduced space. The computational complexity of Newton's direction finding subproblem in the algorithm is comparable with that of finding the steepest descent direction in the traditional first order nested/reduced space algorithms for topology optimization. That is, the space reduction is computationally inexpensive, and more importantly it does not ruin the sparsity of the full-space system of optimality conditions.

The fast local convergence of the algorithm allows one to efficiently solve a sequence of optimization problems for varying parameters (numerical continuation). This can be utilized for eliminating the errors introduced by the approximate enforcement of the boundary conditions or 0/10/1-type constraints on the design field through penalties in many topology optimization approaches.

We test the algorithm on the benchmark problems of dissipated power minimization for Stokes flows, and in all cases the algorithm outperforms the traditional first order reduced space/nested approaches by a factor varying from two to almost twenty in terms of the number of iterations while attaining an almost unprecedented accuracy in solving the discretized topology optimization problem. Finally we present a few extensions to the algorithm, one involving computations on adaptively refined meshes and another related to solving topology optimization problems for non-Newtonian fluids.

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State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Evgrafov, A. (Intern)
Pages: 272-290
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Computer Methods in Applied Mechanics and Engineering
Volume: 278
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Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.31 SJR 2.743 SNIP 1.962
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.823 SNIP 2.126 CiteScore 3.91
Model estimation and structure detection with short data records are two issues that receive increasing interests in System Identification. In this paper, a multiple kernel-based regularization method is proposed to handle those issues. Multiple kernels are conic combinations of fixed kernels suitable for impulse response estimation, and equip the kernel-based regularization method with three features. First, multiple kernels can better capture complicated dynamics than single kernels. Second, the estimation of their weights by maximizing the marginal likelihood favors sparse optimal weights, which enables this method to tackle various structure detection problems, e.g., the sparse dynamic network identification and the segmentation of linear systems. Third, the marginal likelihood maximization problem is a difference of convex programming problem. It is thus possible to find a locally optimal solution efficiently by using a majorization minimization algorithm and an interior point method where the cost of a single interior-point iteration grows linearly in the number of fixed kernels. Monte Carlo simulations show that the locally optimal solutions lead to good performance for randomly
General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Linköping University, University of Padua
Authors: Chen, T. (Ekstern), Andersen, M. S. (Intern), Ljung, L. (Ekstern), Chiuso, A. (Ekstern), Pillonetto, G. (Ekstern)
Pages: 2933-2945
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
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Issue number: 11
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 4.174 SNIP 3.159 CiteScore 6.06
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.926 SNIP 2.884 CiteScore 5.08
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 4.196 SNIP 3.347 CiteScore 5.14
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 4.096 SNIP 3.13 CiteScore 5.24
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 4.143 SNIP 3.292 CiteScore 5.11
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.749 SNIP 2.961 CiteScore 4.11
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.939 SNIP 2.917
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.945 SNIP 3.449
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Scopus rating (2006): SJR 3.67 SNIP 2.917
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.968 SNIP 2.566
Scopus rating (2004): SJR 2.959 SNIP 2.708
Scopus rating (2003): SJR 3.359 SNIP 2.589
Scopus rating (2002): SJR 3.982 SNIP 2.349
Scopus rating (2001): SJR 4.161 SNIP 2.777
Scopus rating (2000): SJR 3.887 SNIP 2.772
Scopus rating (1999): SJR 1.93 SNIP 2.438
Original language: English
System identification, regularization methods, kernel methods, convex optimization, sparsity, structure detection, kernel

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, FORCE Technology
Authors: Lindberg, O. (Ekstern), Bingham, H. B. (Intern), Engsig-Karup, A. P. (Intern)
Number of pages: 4
Publication date: 2014

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Title of host publication: Proceedings of the International Workshop on Water Waves and Floating Bodies 2014
Publisher: IWWWFB
Main Research Area: Technical/natural sciences
Conference: 29th International Workshop on Water Waves and Floating Bodies, Osaka, Japan, 30/03/2014 - 30/03/2014
Electronic versions: iwwwfb29_34.pdf
Links:
http://www.iwwwfb.org/Workshops/29.htm

Using Operators to Expand the Block Matrices Forming the Hessian of a Molecular Potential

We derive compact expressions of the second-order derivatives of bond length, bond angle, and proper and improper torsion angle potentials, in terms of operators represented in two orthonormal bases. Hereby, simple rules to generate the Hessian of an internal coordinate or a molecular potential can be formulated. The algorithms we provide can be implemented efficiently in high-level programming languages using vectorization. Finally, the method leads to compact expressions for a second-order expansion of an internal coordinate or a molecular potential. © 2014 Wiley Periodicals, Inc.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Carlsen, M. (Intern)
Pages: 1149-1158
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Computational Chemistry
Volume: 35
Issue number: 15
ISSN (Print): 0192-8651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.428 SNIP 1.297 CiteScore 3.51
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.417 SNIP 1.451 CiteScore 3.81
BFI (2014): BFI-level 1
second‐order derivatives, Hessian, internal coordinates, operators, molecular potentials

DOIs: 10.1002/jcc.23609
Source: FindIt
Source-ID: 266904896
Publication: Research - peer-review › Journal article – Annual report year: 2014

Med computeren på jagt efter gode former i strømninger

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Nørtoft, P. (Intern)
Publication date: 1 Mar 2013

Publication information
Type: Ph.d. Cup 2013
Source/Publisher: Information / iBureauet
Main Research Area: Technical/natural sciences
Electronic versions:
Peter_N_rtoft.pdf
Links:
http://phdcup.dk/

Bibliographical note
Article for the national Ph.d. Cup 2013.

Relations
Press / Media items:
A Convex Variational Model for Restoring Blurred Images with Multiplicative Noise

In this paper, a new variational model for restoring blurred images with multiplicative noise is proposed. Based on the statistical property of the noise, a quadratic penalty function technique is utilized in order to obtain a strictly convex model under a mild condition, which guarantees the uniqueness of the solution and the stabilization of the algorithm. For solving the new convex variational model, a primal-dual algorithm is proposed, and its convergence is studied. The paper ends with a report on numerical tests for the simultaneous deblurring and denoising of images subject to multiplicative noise. A comparison with other methods is provided as well.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Hong Kong Baptist University
Authors: Dong, Y. (Intern), Tieyong Zeng (Ekstern)
Pages: 1598-1625
Publication date: 2013
Main Research Area: Technical/natural sciences

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Journal: S I A M Journal on Imaging Sciences
Volume: 6
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ISSN (Print): 1936-4954
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.5 SJR 1.824 SNIP 1.789
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.812 SNIP 2.258 CiteScore 3.64
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.481 SNIP 2.478 CiteScore 3.28
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.863 SNIP 3.523 CiteScore 5.05
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.174 SNIP 3.985 CiteScore 4.26
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.899 SNIP 1.467 CiteScore 2.17
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 2
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Original language: English
Convexity, Deblurring, Multiplicative noise, Primal-dual algorithm, Total variation regularization, Variational model

Electronic versions:
120870621.pdf
DOIs:
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Bibliographical note
A Dantzig-Wolfe Decomposition Algorithm for Economic MPC of Distributed Energy Systems

In economic model predictive control of distributed energy systems, the constrained optimal control problem can be expressed as a linear program with a block-angular structure. In this paper, we present an efficient Dantzig-Wolfe decomposition algorithm specifically tailored to problems of this type. Simulations show that a MATLAB implementation of the algorithm is significantly faster than several state-of-the-art linear programming solvers and that it scales in a favorable way.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering, DONG Energy A/S
Authors: Sokoler, L. E. (Intern), Standardi, L. (Intern), Edlund, K. (Ekstern), Jørgensen, J. B. (Intern)
Number of pages: 6
Publication date: 2013

Host publication information
Title of host publication: Proceedings of the 18th Nordic Process Control Workshop
Main Research Area: Technical/natural sciences
Conference: 18th Nordic Process Control Workshop, Oulu, Finland, 22/08/2013 - 22/08/2013
Source-ID: u::8476
Publication: Research - peer-review › Article in proceedings – Annual report year: 2013

A Decomposition Algorithm for Optimal Control of Distributed Energy System

In economic model predictive control of distributed energy systems, the constrained optimal control problem can be expressed as a linear program with a block-angular structure. In this paper, we present an efficient Dantzig-Wolfe decomposition algorithm specifically tailored to problems of this type. Simulations show that a MATLAB implementation of the algorithm is significantly faster than several state-of-the-art linear programming solvers and that it scales in a favorable way.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering, DONG Energy A/S
Authors: Sokoler, L. E. (Intern), Edlund, K. (Ekstern), Standardi, L. (Intern), Jørgensen, J. B. (Intern)
Number of pages: 6
Publication date: 2013

Host publication information
Title of host publication: 2013 4th IEEE PES Innovative Smart Grid Technologies Europe (ISGT Europe)
Publisher: IEEE
ISBN (Print): 978-1-4799-2984-9
Main Research Area: Technical/natural sciences
Conference: 2013 4th IEEE PES Innovative Smart Grid Technologies Europe, Lyngby, Denmark, 06/10/2013 - 06/10/2013
DOIs: 10.1109/ISGTEurope.2013.6695248
Source-ID: u::8881
Publication: Research - peer-review › Article in proceedings – Annual report year: 2013

A Fast Condensing Method for Solution of Linear-Quadratic Control Problems

In both Active-Set (AS) and Interior-Point (IP) algorithms for Model Predictive Control (MPC), sub-problems in the form of linear-quadratic (LQ) control problems need to be solved at each iteration. The solution of these sub-problems is usually the main computational effort. In this paper we consider a condensing (or state elimination) method to solve an extended version of the LQ control problem, and we show how to exploit the structure of this problem to both factorize the dense Hessian matrix and solve the system. Furthermore, we present two efficient implementations. The first implementation is formally identical to the Riccati recursion based solver and has a computational complexity that is linear in the control horizon length and cubic in the number of states. The second implementation has a computational complexity that is quadratic in the control horizon length as well as the number of states. When the state dimension is high, this implementation is faster than the Riccati recursion based implementation.
A free boundary problem for a reaction-diffusion system with nonlinear memory

We consider a integro-partial differential equation with a free boundary which appears in the theory of the nuclear dynamics. First, local existence and uniqueness are obtained by using the contraction mapping theorem. Then, the behavior of the free boundary and the blow-up criteria are obtained. Finally, we examine the long-time behavior of the global solution. We show that the solution is global and fast if the initial data are small.
A Grey-Box Model for Spray Drying Plants

Multi-stage spray drying is an important and widely used unit operation in the production of food powders. In this paper we develop and present a dynamic model of the complete drying process in a multi-stage spray dryer. The dryer is divided into three stages: The spray stage and two fluid bed stages. Each stage is assumed ideally mixed and described by mass- and energy balances. The model is able to predict the temperature, the residual moisture and the particle size in each stage. Process constraints are also proposed to predict deposits due to stickiness of the powder. The model predictions are compared to datasets gathered at GEA Process Engineering’s test facility. The identified grey-box model parameters are identified from data and the resulting model fits the data well. The complexity of the model has been selected such that it is suitable for development of real-time optimization algorithms in an economic optimizing MPC framework.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Department of Electrical Engineering, Automation and Control, Center for Energy Resources Engineering, GEA Process Engineering A/S
Authors: Petersen, L. N. (Intern), Poulsen, N. K. (Intern), Niemann, H. H. (Intern), Utzen, C. (Ekstern), Jørgensen, J. B. (Intern)
Pages: 559-564
Publication date: 2013

Host publication information
Title of host publication: Proceedings of the 10th IFAC International Symposium on Dynamics and Control of Process Systems
Publisher: Elsevier Science
Article number: FrM2T2.3
ISBN (Print): 9781629937267
Main Research Area: Technical/natural sciences
DOIs:
10.3182/20131218-3-in-2045.00118
Source: dtu
Source-ID: u::10297
Publication: Research - peer-review › Article in proceedings – Annual report year: 2013
An Implementation of the Frequency Matching Method

During the last decade multiple-point statistics has become increasingly popular as a tool for incorporating complex prior information when solving inverse problems in geosciences. A variety of methods have been proposed but often the implementation of these is not straightforward. One of these methods is the recently proposed Frequency Matching method to compute the maximum a posteriori model of an inverse problem where multiple-point statistics, learned from a training image, is used to formulate a closed form expression for an a priori probability density function. This paper discusses aspects of the implementation of the Frequency Matching method and the techniques adopted to make it computationally feasible also for large-scale inverse problems. The source code is publicly available at GitHub and this paper also provides an example of how to apply the Frequency Matching method to a linear inverse problem.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, CERE – Center for Energy Resources Engineering
Authors: Lange, K. (Intern), Frydendall, J. (Intern), Hansen, T. M. (Intern), Zunino, A. (Intern), Mosegaard, K. (Intern)
Number of pages: 45
Publication date: 2013

Publication Information
Place of publication: Kgs. Lyngby
Publisher: Technical University of Denmark (DTU)
Original language: English

Series: DTU Compute-Technical Report-2013
Number: 09
ISSN: 1601-2321
Main Research Area: Technical/natural sciences
Multiple-points statistics, Training image, A priori information, Maximum a posteriori model
Electronic versions:
tr13_09_Lange_K.pdf
Publication: Research › Report – Annual report year: 2013

Anwendung der "Uncertainty Quantification" bei eisenbahndynamischen Problemen

The paper describes the results of the application of "Uncertainty Quantification" methods in railway vehicle dynamics. The system parameters are given by probability distributions. The results of the application of the Monte-Carlo and generalized Polynomial Chaos methods to a simple bogie model will be discussed.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Bigoni, D. (Intern), Engsig-Karup, A. P. (Intern), True, H. (Intern)
Pages: 152-158
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Z E Vrail - Glasers Annalen
Volume: 137
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Ratings:
Scopus rating (2016): SJR 0.1 SNIP 0.137
Scopus rating (2015): SJR 0.101 SNIP 0.008
Scopus rating (2014): SJR 0.1 SNIP 0.123
Scopus rating (2013): SJR 0.159 SNIP 0
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SJR 0.101 SNIP 0.041
ISI indexed (2012): ISI indexed no
Scopus rating (2011): SJR 0.173 SNIP 0.223
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 0.15 SNIP 0.108
A Riccati Based Homogeneous and Self-Dual Interior-Point Method for Linear Economic Model Predictive Control

In this paper, we develop an efficient interior-point method (IPM) for the linear programs arising in economic model predictive control of linear systems. The novelty of our algorithm is that it combines a homogeneous and self-dual model, and a specialized Riccati iteration procedure. We test the algorithm in a conceptual study of power systems management. Simulations show that in comparison to state of the art software implementation of IPMs, our method is significantly faster and scales in a favourable way.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering, DONG Energy A/S
Authors: Sokoler, L. E. (Intern), Frison, G. (Intern), Edlund, K. (Ekstern), Skajaa, A. (Intern), Jørgensen, J. B. (Intern)
Pages: 592-598
Publication date: 2013

Host publication information
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Publisher: IEEE
ISBN (Print): 978-1-4799-1557-6
Main Research Area: Technical/natural sciences
DOIs: 10.1109/CCA.2013.6662814
Source: dtu
Source-ID: u::8520
Publication: Research - peer-review › Article in proceedings – Annual report year: 2013

A sparse scattering model for nanoparticles on rough substrates

We present and validate an efficient forward scattering model for nanoparticles on rough contaminated substrates.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Karamehmedovic, M. (Intern), Hansen, P. (Ekstern), Wriedt, T. (Ekstern)
Pages: 10
Publication date: 2013

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Title of host publication: META’13 Sharjah - United Arab Emirates : The 4th International Conference on Metamaterials, Photonic Crystals and Plasmonics
Main Research Area: Technical/natural sciences
Conference: 4th International Conference on Metamaterials, Photonic Crystals and Plasmonics, META’13, Sharjah, United Arab Emirates, 18/03/2013 - 18/03/2013
Source: dtu
Source-ID: u::8748
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2013

Atomic scattering from an adsorbed monolayer solid with a helium beam that penetrates to the substrate

Diffraction and one-phonon inelastic scattering of a thermal energy helium atomic beam are evaluated in the situation that the target monolayer lattice is so dilated that the atomic beam penetrates to the interlayer region between the monolayer and the substrate. The scattering is simulated by propagating a wavepacket and including the effect of a feedback of the
inelastic wave onto the diffracted wave, which represents a coherent re-absorption of the created phonons. Parameters are chosen to be representative of an observed p(1 × 1) commensurate monolayer solid of H2/NaCl(001) and a conjectured p(1 × 1) commensurate monolayer solid of H2/KCl(001). For the latter, there are cases where part of the incident beam is trapped in the interlayer region for times exceeding 50 ps, depending on the spacing between the monolayer and the substrate and on the angle of incidence. The feedback effect is large for cases of strong transient trapping. © 2013 American Institute of Physics.
A Tuning Procedure for ARX-based MPC

We present an optimization based tuning procedure with certain robustness properties for an offset free Model Predictive Controller (MPC). The MPC is designed for univariate processes that can be represented by an ARX model. The advantage of ARX model representations is that standard system identification techniques using convex optimization can be used for identification of such models from input-output data. The stochastic model of the ARX model identified from input-output data is modified with an ARMA model designed as part of the MPC-design procedure to ensure offset-free control. The ARMAX model description resulting from the extension can be realized as a state space model in innovation form. The MPC is designed and implemented based on this state space model in innovation form. Expressions for the closed-loop dynamics of the unconstrained system is used to derive the sensitivity function of this system. The closed-loop expressions are also used to numerically evaluate absolute integral performance measures. Due to the closed-loop expressions, these evaluations can be performed relatively quickly. Consequently, the tuning may be performed by numerical minimization of the integrated absolute error subject to the a constraint on the maximum of the sensitivity function. The latter constraint provides a robustness measure that is essential for the procedure.

General information

State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Chemical and Biochemical Engineering, Computer Aided Process Engineering Center, Center for Energy Resources Engineering, Scientific Computing
Authors: Olesen, D. (Intern), Huusom, J. K. (Intern), Jørgensen, J. B. (Intern)
Pages: 188-193
Publication date: 2013
A Tuning Procedure for ARX-based MPC of Multivariate Processes

We present an optimization based tuning procedure with certain robustness properties for an offset free Model Predictive Controller (MPC). The MPC is designed for multivariate processes that can be represented by an ARX model. The stochastic model of the ARX model identified from input-output data is modified with an ARMA model designed as part of the MPC-design procedure to ensure offset-free control. The MPC is designed and implemented based on a state space model in innovation form. Expressions for the closed-loop dynamics of the unconstrained system is used to derive the sensitivity function of this system. The closed-loop expressions are also used to numerically evaluate absolute integral performance measures. Due to the closed-loop expressions these evaluations can be done relative quickly. Consequently, the tuning may be performed by numerical minimization of the integrated absolute error subject to a constraint on the maximum of the sensitivity function. The latter constraint provides a robustness measure that is essential for the procedure. The method is demonstrated for two simulated examples: A Wood-Berry distillation column example and a cement mill example.

Auto-tuning of level 1 and level 2 BLAS for GPUs

The use of high-performance libraries for dense linear algebra operations is of great importance in many numerical scientific applications. The most common operations form the backbone of the Basic Linear Algebra Subroutines (BLAS) library. In this paper, we consider the performance and auto-tuning of level 1 and level 2 BLAS routines on graphical processing units. As examples, we develop single-precision Compute Unified Device Architecture kernels for three of the most popular operations, the Euclidian norm (SNRM2), the matrix–vector multiplication (SGEMV), and the triangular solution (STRSV). The target hardware is the most recent Nvidia (Santa Clara, CA, USA) Tesla 20-series (Fermi architecture), which is designed from the ground up for high-performance computing. We show that it is essentially a matter of fully utilizing the fine-grained parallelism of the many-core graphical processing unit to achieve high performance for level 1 and level 2 BLAS operations. We show that auto-tuning can be successfully employed to kernels for these operations so that they perform well for all input sizes.
A Warm-Started Homogeneous and Self-Dual Interior-Point Method for Linear Economic Model Predictive Control

In this paper, we present a warm-started homogenous and self-dual interior-point method (IPM) for the linear programs arising in economic model predictive control (MPC) of linear systems. To exploit the structure in the optimization problems, our algorithm utilizes a Riccati iteration procedure which is adapted to the non-standard system solved in homogenous and self-dual IPMs, and specifically tailored to economic MPC. Fast convergence is further achieved by means of a recent warm-starting strategy for homogenous and self-dual IPMs that has not previously been applied to MPC. We implement
our algorithm in MATLAB and its performance is analyzed based on a smart grid power management case study. Closed loop simulations show that 1) our algorithm is significantly faster than state-of-the-art IPMs based on sparse linear algebra routines, and 2) warm-starting reduces the number of iterations by approximately 15-35%.

Computational Efficiency of Economic MPC for Power Systems Operation

In this work, we propose an Economic Model Predictive Control (MPC) strategy to operate power systems that consist of independent power units. The controller balances the power supply and demand, minimizing production costs. The control problem is formulated as a linear program that is solved by a computationally efficient implementation of the Dantzig-Wolfe decomposition. To make the controller suitable for real-time applications, we investigate a suboptimal MPC scheme, introducing an early termination strategy to the Dantzig-Wolfe algorithm. Simulations demonstrate that the early termination technique substantially reduces the computation time.

Connecting image sparsity and sampling in iterative reconstruction for limited angle X-ray CT

In this work, we propose an Economic Model Predictive Control (MPC) strategy to operate power systems that consist of independent power units. The controller balances the power supply and demand, minimizing production costs. The control problem is formulated as a linear program that is solved by a computationally efficient implementation of the Dantzig-Wolfe decomposition. To make the controller suitable for real-time applications, we investigate a suboptimal MPC scheme, introducing an early termination strategy to the Dantzig-Wolfe algorithm. Simulations demonstrate that the early termination technique substantially reduces the computation time.
Construction of smooth compactly supported windows generating dual pairs of Gabor frames

Let \( g \) be any real-valued, bounded and compactly supported function, whose integer-translates \( \{ T_{kg} \}_{k \in \mathbb{Z}} \) form a partition of unity. Based on a new construction of dual windows associated with Gabor frames generated by \( g \), we present a method to explicitly construct dual pairs of Gabor frames. This new method of construction is based on a family of polynomials which is closely related to the Daubechies polynomials, used in the construction of compactly supported wavelets. For any \( k \in \mathbb{N} \cup \{ \infty \} \) we consider the Meyer scaling functions and use these to construct compactly supported windows \( g \in C^k(\mathbb{R}) \) associated with a family of smooth compactly supported dual windows. For any \( n \in \mathbb{N} \) the pair of dual windows \( g, h_n \in C^k(\mathbb{R}) \) have compact support in the interval \([-2/3, 2/3]\) and share the property of being constant on half the length of their support. We therefore obtain arbitrary smoothness of the dual pair of windows \( g, h_n \) without increasing their support.
Decentralized Large-Scale Power Balancing
A power balancing strategy based on Douglas-Rachford splitting is proposed as a control method for largescale integration of flexible consumers in a Smart Grid. The total power consumption is controlled through a negotiation procedure between all units and a coordinating system level. The balancing problem is formulated as a centralized large-scale optimization problem but is then decomposed into smaller subproblems that are solved locally by each unit connected to an aggregator. For large-scale systems the method is faster than solving the full problem and can be distributed to include an arbitrary number of units.

Decomposition and Projection Methods for Distributed Robustness Analysis of Interconnected Uncertain Systems
We consider a class of convex feasibility problems where the constraints that describe the feasible set are loosely coupled. These problems arise in robust stability analysis of large, weakly interconnected uncertain systems. To facilitate distributed implementation of robust stability analysis of such systems, we describe two algorithms based on decomposition and simultaneous projections. The first algorithm is a nonlinear variant of Cimmino's mean projection algorithm, but by taking the structure of the constraints into account, we can obtain a faster rate of convergence. The second algorithm is devised by applying the alternating direction method of multipliers to a convex minimization reformulation of the convex feasibility problem. Numerical results are then used to show that both algorithms require far less iterations than the accelerated nonlinear Cimmino algorithm.
Designing Scientific Software for Heterogeneous Computing: With application to large-scale water wave simulations

The main objective with the present study has been to investigate parallel numerical algorithms with the purpose of running efficiently and scalably on modern many-core heterogeneous hardware. In order to obtain good efficiency and scalability on modern multi- and many-core architectures, algorithms and data structures must be designed to utilize the underlying parallel architecture. The architectural changes in hardware design within the last decade, from single to multi and many-core architectures, require software developers to identify and properly implement methods that both exploit concurrency and maintain numerical efficiency.

Graphical Processing Units (GPUs) have proven to be very effective units for computing the solution of scientific problems described by partial differential equations (PDEs). GPUs have today become standard devices in portable, desktop, and supercomputers, which makes parallel software design applicable, but also a challenge for scientific software developers at all levels. We have developed a generic C++ library for fast prototyping of large-scale PDEs solvers based on flexible-order finite difference approximations on structured regular grids. The library is designed with a high abstraction interface to improve developer productivity. The library is based on modern template-based design concepts as described in Glimberg, Engsig-Karup, Nielsen & Dammann (2013). The library utilizes heterogeneous CPU/GPU environments in order to maximize computational throughput by favoring data locality and low-storage algorithms, which are becoming more and more important as the number of concurrent cores per processor increases.

We demonstrate in a proof-of-concept the advantages of the library by assembling a generic nonlinear free surface water wave solver based on unified potential flow theory, for fast simulation of large-scale phenomena, such as long distance wave propagation over varying depths or within large coastal regions. Simulations that are valuable within maritime engineering because of the adjustable properties that follow from the flexible-order implementation. We extend the novel work on an efficient and robust iterative parallel solution strategy proposed by Engsig-Karup, Madsen & Glimberg (2011), for the bottleneck problem of solving a _-transformed Laplace problem in three dimensions at every time integration step. A geometric multigrid preconditioned defect correction scheme is used to attain high-order accurate solutions with fast convergence and scalable work effort. To minimize data storage and enhance performance, the numerical method is based on matrix-free finite difference approximations, implemented to run efficiently on many-core GPUs. Also, single-precision calculations are found to be attractive for reducing transfers and enhancing performance for both pure single and mixed-precision calculations without compromising robustness. A structured multi-block approach is presented that decomposes the problem into several subdomains, supporting flexible block structures to match the physical domain. For data communication across processor nodes, messages are sent using MPI to repeatedly update boundary information between adjacent coupled subdomains. The impact on convergence and performance scalability using the proposed hybrid CUDA-MPI strategy will be presented. A survey of the convergence and performance properties of the preconditioned defect correction method is carried out with special focus on large-scale multi-GPU simulations. Results indicate that a limited number of multigrid restrictions are required, and that it is strongly coupled to the wave resolutions. These results are encouraging for the heterogeneous multi-GPU systems as they reduce the communication overhead significantly and prevent both global coarse grid corrections and inefficient processor utilization at the coarsest levels.

We find that spatial domain decomposition scales well for large problems sizes, but for problems of limited sizes, the maximum attainable speedup is reached for a low number of processors, as it leads to an unfavorable communication to compute ratio. To circumvent this, we have considered a recently proposed parallel-in-time algorithm referred to as Parareal. In an attempt to introduce algorithmic concurrency in the time discretization. Parareal may be perceived as a two-level multigrid method in time, where the numerical solution is first sequentially advanced via course integration and then updated simultaneously on multiple GPUs in a predictor-corrector fashion. A parameter study is performed to establish proper choices for maximizing speedup and parallel efficiency. The Parareal algorithm is found to be sensitive to a number of numerical and physical parameters, making practical speedup a matter of parameter tuning. Results are presented to confirm that it is possible to attain reasonable speedups, independently of the spatial problem size.

To improve application range, curvilinear grid transformations are introduced to allow representation of complex boundary geometries. The curvilinear transformations increase the complexity of the implementation of the model equations. A number of free surface water wave cases have been demonstrated with boundary-fitted geometries, where the combination of a flexible geometry representation and a fast numerical solver can be a valuable engineering tool for large-scale simulation of real maritime scenarios.

The present study touches some of the many possibilities that modern heterogeneous computing can bring if careful and parallel-aware design decisions are made. Though several free surface examples are outlined, we are yet to demonstrate results from a real large-scale engineering case.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Glimberg, S. L. (Intern), Engsig-Karup, A. P. (Intern), Dammann, B. (Ekstern)
Development of a GPU-accelerated MIKE 21 Solver for Water Wave Dynamics
With encouragement by the company DHI are the aim of this B.Sc. thesis1 to investigate, whether if it is possible to accelerate the simulation speed of DHIs commercial product MIKE 21 HD, by formulating a parallel solution scheme and implementing it to be executed on a CUDA-enabled GPU (massive parallel hardware).

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Technical University of Denmark, DHI Denmark
Authors: Ackermann, P. E. (Ekstern), Pedersen, P. J. D. (Ekstern), Engsig-Karup, A. P. (Intern), Clausen, T. (Ekstern), Grooss, J. (Intern)
Pages: 129-130
Publication date: 2013

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Series: Lecture Notes in Computer Science
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Main Research Area: Technical/natural sciences
Conference: Facing the Multicore-Challenge III, Stuttgart, Germany, 19/09/2012 - 19/09/2012
Electronic versions:
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DOIs:
10.1007/978-3-642-35893-7_15

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Poster presentation.
Publication: Research › peer-review › Article in proceedings – Annual report year: 2013

Development of software components for heterogeneous many-core architectures

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Technical University of Denmark
Authors: Glimberg, S. L. (Intern), Engsig-Karup, A. P. (Intern), Nielsen, A. S. (Ekstern), Dammann, B. (Ekstern)
Pages: 73–104
Publication date: 2013

Host publication information
Title of host publication: Designing Scientific Applications on GPUs
Publisher: Taylor & Francis
Dual Decomposition for Large-Scale Power Balancing

Dual decomposition is applied to power balancing of flexible thermal storage units. The centralized large-scale problem is decomposed into smaller subproblems and solved locally by each unit in the Smart Grid. Convergence is achieved by coordinating the units' consumption through a negotiation procedure with the dual variables.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Halvgaard, R. (Intern), Jørgensen, J. B. (Intern), Vandenberghe, L. (Intern)
Number of pages: 2
Publication date: 2013

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Main Research Area: Technical/natural sciences
Conference: 18th Nordic Process Control Workshop, Oulu, Finland, 22/08/2013 - 22/08/2013
Decomposition methods, Decentralized Control, Model Predictive Control, Smart Grid, Smart power applications
Electronic versions:
prod11377507846395.Halvgaard_Dual_Decomposition_for_Large_Scale_Power_Balancing.pdf

Bibliographical note
Extended abstract presented as poster.
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2013

Early Termination of Dantzig-Wolfe Algorithm for Economic MPC

In this paper we apply the Economic Model Predictive Control (MPC) for balancing the power supply and demand in the future power systems in the most economic way. The control problem is formulated as a linear program, having a block-angular structure solved by the implementation of the Dantzig-Wolfe decomposition. For real-time applications we introduce an early termination technique. Simulations demonstrate that the algorithm developed operates efficiently a power system, reducing significantly computational time.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Center for Energy Resources Engineering
Authors: Standardi, L. (Intern), Sokoler, L. E. (Intern), Poulsen, N. K. (Intern), Jørgensen, J. B. (Intern)
Number of pages: 6
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Economic Model Predictive Control, Linear Programming, Distributed Optimization, Power Systems
Electronic versions:
NPCW_laus_Full_Paper.pdf
Source: dtu
Source-ID: u::8625
Publication: Research - peer-review › Article in proceedings – Annual report year: 2013

Efficient Hybrid-Spectral Model for Fully Nonlinear Numerical Wave Tank

A new hybrid-spectral solution strategy is proposed for the simulation of the fully nonlinear free surface equations based on potential flow theory. A Fourier collocation method is adopted horizontally for the discretization of the free surface equations. This is combined with a modal Chebyshev Tau method in the vertical for the discretization of the Laplace
equation in the fluid domain, which yields a sparse and spectrally accurate Dirichlet-to-Neumann operator. The Laplace problem is solved with an efficient Defect Correction method preconditioned with a spectral discretization of the linearised wave problem, ensuring fast convergence and optimal scaling with the problem size. Preliminary results for very nonlinear waves show expected convergence rates and a clear advantage of using spectral schemes.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Ecole Centrale de Nantes
Authors: Christiansen, T. (Intern), Bingham, H. B. (Intern), Engsig-Karup, A. P. (Intern), Ducrozet, G. (Ekstern), Ferrant, P. (Ekstern)
Number of pages: 10
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BFI conference series: International Conference on Ocean, Offshore and Arctic Engineering (5010067)
Main Research Area: Technical/natural sciences
Conference: 32nd International Conference on Ocean, Offshore and Arctic Engineering (OMAE 2013), Nantes, France, 09/06/2013 - 09/06/2013
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Source: FindIt
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2014

Efficient Implementation of the Riccati Recursion for Solving Linear-Quadratic Control Problems
In both Active-Set (AS) and Interior-Point (IP) algorithms for Model Predictive Control (MPC), sub-problems in the form of linear-quadratic (LQ) control problems need to be solved at each iteration. The solution of these sub-problems is typically the main computational effort at each iteration. In this paper, we compare a number of solvers for an extended formulation of the LQ control problem: a Riccati recursion based solver can be considered the best choice for the general problem with dense matrices. Furthermore, we present a novel version of the Riccati solver, that makes use of the Cholesky factorization of the Pn matrices to reduce the number of flops. When combined with regularization and mixed precision, this algorithm can solve large instances of the LQ control problem up to 3 times faster than the classical Riccati solver.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Center for Energy Resources Engineering
Authors: Frison, G. (Intern), Jørgensen, J. B. (Intern)
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Publisher: IEEE
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Main Research Area: Technical/natural sciences
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2013

Exercise effects in a virtual type 1 diabetes patient: Using stochastic differential equations for model extension
The use of virtual patients for in silico testing of control algorithms for an artificial pancreas is growing. It is an easy, fast and low-cost alternative to pre-clinical testing. To simulate the everyday life of a type 1 diabetes (T1D) patient a simulator must be able to take into account physical activity. Exercise constitutes a substantial challenge to closed-loop control of T1D. The effects are many and depend on intensity and duration and may be delayed by several hours. In this study, we use a model for the glucoregulatory system based on the minimal model and a previously published extension incorporating exercise effects on insulin and glucose dynamics. Our model is constructed as a stochastic state space model consisting of a set of stochastic differential equations (SDEs). In a stochastic state space model, the residual error
is split into random measurement error and misspecification noise. The latter of the two can be used to pinpoint model
deficiencies or unknown influential factors during the development of the model. The model is thus built on the basis of
physiological knowledge of the system combined with information from observed data. Model parameters are estimated on
clinical data from a study including exercise bouts of 20 minutes performed on 12 T1D patients treated with continuous
subcutaneous insulin infusion. The predictive abilities of the model are investigated. In conclusion, this study illustrates the
advantages of using SDEs in the development of an extended glucoregulatory model including effects of exercise suited
for in silico testing.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Center for Energy Resources Engineering,
Scientific Computing, Dynamical Systems, Copenhagen University Hospital
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H. (Intern)
Number of pages: 1
Pages: A-78
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Conference: 6th International Conference on Advanced Technologies & Treatments for Diabetes (ATTD 2013), Paris,
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.335 SNIP 1.152 CiteScore 1.44
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.223 SNIP 1.035 CiteScore 1.52
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.315 SNIP 1.14 CiteScore 2.09
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.153 SNIP 1.058 CiteScore 2.74
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.962 SNIP 1.103 CiteScore 2.5
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.029 SNIP 1.1 CiteScore 2.17
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.997 SNIP 1.187
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.936 SNIP 0.97
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.727 SNIP 0.889
Scopus rating (2007): SJR 0.6 SNIP 0.789
Scopus rating (2006): SJR 0.817 SNIP 0.891
Extracting knowledge from protein structure geometry

Protein structure prediction techniques proceed in two steps, namely the generation of many structural models for the protein of interest, followed by an evaluation of all these models to identify those that are native-like. In theory, the second step is easy, as native structures correspond to minima of their free energy surfaces. It is well known however that the situation is more complicated as the current force fields used for molecular simulations fail to recognize native states from misfolded structures. In an attempt to solve this problem, we follow an alternate approach and derive a new potential from geometric knowledge extracted from native and misfolded conformers of protein structures. This new potential, Metric Protein Potential (MPP), has two main features that are key to its success. Firstly, it is composite in that it includes local and nonlocal geometric information on proteins. At the short range level, it captures and quantifies the mapping between the sequences and structures of short (7-mer) fragments of protein backbones through the introduction of a new local energy term. The local energy term is then augmented with a nonlocal residue-based pairwise potential, and a solvent potential. Secondly, it is optimized to yield a maximized correlation between the energy of a structural model and its root mean square (RMS) to the native structure of the corresponding protein. We have shown that MPP yields high correlation values between RMS and energy and that it is able to retrieve the native structure of a protein from a set of high-resolution decoys.
Fast hydrodynamics on heterogenous many-core hardware

General information
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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Technical University of Denmark
Authors: Engsig-Karup, A. P. (Intern), Glimberg, S. L. (Intern), Nielsen, A. S. (Ekstern), Lindberg, O. (Intern)
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Main Research Area: Technical/natural sciences
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Source: dtu
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Publication: Research - peer-review › Book chapter – Annual report year: 2013

First-order convex feasibility algorithms for x-ray CT
Purpose: Iterative image reconstruction (IIR) algorithms in computed tomography (CT) are based on algorithms for solving a particular optimization problem. Design of the IIR algorithm, therefore, is aided by knowledge of the solution to the optimization problem on which it is based. Often times, however, it is impractical to achieve accurate solution to the optimization of interest, which complicates design of IIR algorithms. This issue is particularly acute for CT with a limited
angular-range scan, which leads to poorly conditioned system matrices and difficult to solve optimization problems. In this paper, we develop IIR algorithms which solve a certain type of optimization called convex feasibility. The convex feasibility approach can provide alternatives to unconstrained optimization approaches and at the same time allow for rapidly convergent algorithms for their solution—thereby facilitating the IIR algorithm design process.

Methods: An accelerated version of the Chambolle–Pock (CP) algorithm is adapted to various convex feasibility problems of potential interest to IIR in CT. One of the proposed problems is seen to be equivalent to least-squares minimization, and two other problems provide alternatives to penalized, least-squares minimization.

Results: The accelerated CP algorithms are demonstrated on a simulation of circular fan-beam CT with a limited scanning arc of 144°. The CP algorithms are seen in the empirical results to converge to the solution of their respective convex feasibility problems.

Conclusions: Formulation of convex feasibility problems can provide a useful alternative to unconstrained optimization when designing IIR algorithms for CT. The approach is amenable to recent methods for accelerating first-order algorithms which may be particularly useful for CT with limited angular-range scanning. The present paper demonstrates the methodology, and future work will illustrate its utility in actual CT application.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, University of Chicago
Authors: Sidky, E. Y. (Ekstern), Jørgensen, J. H. (Intern), Pan, X. (Ekstern)
Number of pages: 15
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Main Research Area: Technical/natural sciences

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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.227 SNIP 1.299 CiteScore 2.46
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.307 SNIP 1.553 CiteScore 2.63
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.523 SNIP 1.631 CiteScore 2.79
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.766 SNIP 1.767 CiteScore 3.17
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.42 SNIP 1.669 CiteScore 3.08
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.353 SNIP 1.627 CiteScore 3.03
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.617 SNIP 1.744
Hybrid-Spectral Model for Fully Nonlinear Numerical Wave Tank

General information
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Christiansen, T. R. B. (Intern), Engsig-Karup, A. P. (Intern), Bingham, H. B. (Intern)
Number of pages: 3
Pages: 37-40
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Conference: 28th International Workshop on Water Waves and Floating Bodies (IWWFB 2013), Marseille, France, 07/04/2013 - 07/04/2013
Electronic versions:
iwwfb28_10.pdf
Source: dtu
Source-ID: u::8562
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2013

Inclusion estimation from a single electrostatic boundary measurement: Paper
We present a numerical method for the detection and estimation of perfectly conducting inclusions in conducting homogeneous host media in . The estimation is based on the evaluation of an indicator function that depends on a single pair of Cauchy data (electric potential and current) given at the boundary of the medium. The indicator function is derived using Green’s third identity with the fundamental solution for the Dirichlet Laplacian on the unit disc. Using a truncated Taylor expansion, the indicator function is expressed in terms of an integral over a perturbed inclusion boundary, resulting in a natural physical interpretation. The method is implemented numerically, tested on different example problems and compared to a decomposition approach based on the method of fundamental solutions. The method shows promising results and seems robust to noisy, low sampling-frequency data.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Karamehmedovic, M. (Intern), Knudsen, K. (Intern)
Number of pages: 18
Pages: 025005
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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.84 SJR 1.502 SNIP 1.386
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.389 SNIP 1.411 CiteScore 1.82
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.257 SNIP 1.346 CiteScore 1.63
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.19 SNIP 1.566 CiteScore 2.13
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.239 SNIP 1.838 CiteScore 2.15
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.127 SNIP 1.6 CiteScore 1.9
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.365 SNIP 1.587
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.33 SNIP 1.759
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.211 SNIP 1.884
Scopus rating (2007): SJR 1 SNIP 1.984
Scopus rating (2006): SJR 0.893 SNIP 1.763
Scopus rating (2005): SJR 1.129 SNIP 1.954
Scopus rating (2004): SJR 0.795 SNIP 1.615
Scopus rating (2003): SJR 0.723 SNIP 1.389
Scopus rating (2002): SJR 1.114 SNIP 1.457
Scopus rating (2001): SJR 0.987 SNIP 1.502
Scopus rating (2000): SJR 0.896 SNIP 1.52
Scopus rating (1999): SJR 0.815 SNIP 1.347
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Source: dtu
Source-ID: n:oai:DTIC-ART:iop/377305786::24681
Introduction to Continuous Optimization

Optimization, or mathematical programming, is a fundamental subject within decision science and operations research, in which mathematical decision models are constructed, analyzed, and solved.

The book’s focus lies on providing a basis for the analysis of optimization models and of candidate optimal solutions for continuous optimization models. The main part of the mathematical material therefore concerns the analysis and linear algebra that underlie the workings of convexity and duality, and necessary/sufficient local/global optimality conditions for continuous optimization problems. Natural algorithms are then developed from these optimality conditions, and their most important convergence characteristics are analyzed. The book answers many more questions of the form “Why?” and “Why not?” than “How?”. We use only elementary mathematics in the development of the book, yet are rigorous throughout.

The book provides lecture, exercise and reading material for a first course on continuous optimization and mathematical programming, geared towards third-year students, and has already been used as such for nearly ten years. The preface to the second edition describes the main changes made since the first, 2005, edition.

The book can be used in mathematical optimization courses at any mathematics, engineering, economics, and business schools. It is a perfect starting book for anyone who wishes to develop his/her understanding of the subject of optimization, before actually applying it.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Andreasson, N. (Ekstern), Evgrafov, A. (Intern), Patriksson, M. (Ekstern), Gustavsson, E. (Ekstern), Önnheim, M. (Ekstern)
Number of pages: 484
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Inverse Problems in Geosciences: Modelling the Rock Properties of an Oil Reservoir

Even the most optimistic forecasts predict that Danish oil production will decrease by 80% in the period between 2006 and 2040, and only a strong innovative technological effort can change that. Due to the geological structures of the subsurface in the Danish part of the North Sea, Denmark is currently missing out on approximately 70% of the oil, which is left behind, trapped in unreachable parts of the reservoirs.

An increase in the oil recovery rate can be achieved by better planning and optimisation of oil production. Both require an improved description of the rock properties of the subsurface of the reservoirs. Hence the focus of this work has been on acquiring models of spatial parameters describing rock properties of the subsurface using geostatistical a priori knowledge and available geophysical data. Such models are solutions to often severely under-determined, inverse problems.

We have proposed a method for efficient and accurate interpolation of rock properties from seismic data. It is based on a recently published paper on interpolation of rock properties that breaks with the dominating influence of spatial coordinates in traditional interpolation methods. The thesis contains work involving a test case study of the method demonstrating how the interpolation in attribute space ensures the geological structures of the computed models and how the method can be further improved by an orthogonal transformation of the attribute space.

We have formulated a closed form expression of an a priori probability density function that quantifies the statistical probability of models describing the rock properties of a reservoir. This can be used to evaluate the probability that a model adhere to prior knowledge by having specific multiple-point statistics, for instance, learned from a training image. Existing methods efficiently sample an a priori probability density function to create a set of acceptable models; but they
cannot evaluate the probability of a model.

We have developed and implemented the Frequency Matching method that uses the closed form expression of the a priori probability density function to formulate an inverse problem and compute the maximum a posteriori solution to it. Other methods for computing models that simultaneously fit data observations and honour a priori knowledge are not capable of computing the maximum a posteriori solution. Instead they either sample the posterior probability density function or they sample the a priori probability density function to optimise the likelihood function.

This thesis consists of a summary report and seven research papers submitted, reviewed and/or published in the period 2010 - 2013.

Isogeometric shape optimization in fluid mechanics
The subject of this work is numerical shape optimization in fluid mechanics, based on isogeometric analysis. The generic goal is to design the shape of a 2-dimensional flow domain to minimize some prescribed objective while satisfying given geometric constraints. As part of the design problem, the steady-state, incompressible Navier-Stokes equations, governing a laminar flow in the domain, must be solved. Based on isogeometric analysis, we use B-splines as the basis for both the design optimization and the flow analysis, thereby unifying the models for geometry and analysis, and, at the same time, facilitating a compact representation of complex geometries and smooth approximations of the flow fields. To drive the shape optimization, we use a gradient-based approach, and to avoid inappropriate parametrizations during optimization, we regularize the optimization problem by adding to the objective function a measure of the quality of the boundary parametrization. A detailed description of the methodology is given, and three different numerical examples are considered, through which we investigate the effects of the regularization, of the number of geometric design variables, and of variations in the analysis resolution, initial design and Reynolds number, and thereby demonstrate the robustness of the methodology.
Model-Based Closed-Loop Glucose Control in Type 1 Diabetes: The DiaCon Experience

Background:
To improve type 1 diabetes mellitus (T1DM) management, we developed a model predictive control (MPC) algorithm for closed-loop (CL) glucose control based on a linear second-order deterministic-stochastic model. The deterministic part of the model is specified by three patient-specific parameters: insulin sensitivity factor, insulin action time, and basal insulin infusion rate. The stochastic part is identical for all patients but identified from data from a single patient. Results of the first clinical feasibility test of the algorithm are presented.

Methods:
We conducted two randomized crossover studies. Study 1 compared CL with open-loop (OL) control. Study 2 compared glucose control after CL initiation in the euglycemic (CL-Eu) and hyperglycemic (CL-Hyper) ranges, respectively. Patients
were studied from 22:00–07:00 on two separate nights.

Results:
Each study included six T1DM patients (hemoglobin A1c 7.2% ± 0.4%). In study 1, hypoglycemic events (plasma glucose < 54 mg/dl) occurred on two OL and one CL nights. Average glucose from 22:00–07:00 was 90 mg/dl [74–146 mg/dl; median (interquartile range)] during OL and 108 mg/dl [101–128 mg/dl] during CL (determined by continuous glucose monitoring). However, median time spent in the range 70–144 mg/dl was 67.9% (3.0–73.3%) during OL and 80.8% (70.5–89.7%) during CL. In study 2, there was one episode of hypoglycemia with plasma glucose <54 mg/dl in a CL-Eu night. Mean glucose from 22:00–07:00 and time spent in the range 70–144 mg/dl were 121 mg/dl (117–133 mg/dl) and 69.0% (30.7–77.9%) in CL-Eu and 149 mg/dl (140–193 mg/dl) and 48.2% (34.9–72.5%) in CL-Hyper, respectively.

Conclusions:
This study suggests that our novel MPC algorithm can safely and effectively control glucose overnight, also when CL control is initiated during hyperglycemia.
Model Identification Using Stochastic Differential Equation Grey-Box Models in Diabetes

BACKGROUND:
The acceptance of virtual preclinical testing of control algorithms is growing and thus also the need for robust and reliable models. Models based on ordinary differential equations (ODEs) can rarely be validated with standard statistical tools. Stochastic differential equations (SDEs) offer the possibility of building models that can be validated statistically and that are capable of predicting not only a realistic trajectory, but also the uncertainty of the prediction. In an SDE, the prediction error is split into two noise terms. This separation ensures that the errors are uncorrelated and provides the possibility to pinpoint model deficiencies.

METHODS:
An identifiable model of the glucoregulatory system in a type 1 diabetes mellitus (T1DM) patient is used as the basis for development of a stochastic-differential-equation-based grey-box model (SDE-GB). The parameters are estimated on clinical data from four T1DM patients. The optimal SDE-GB is determined from likelihood-ratio tests. Finally, parameter tracking is used to track the variation in the "time to peak of meal response" parameter.

RESULTS:
We found that the transformation of the ODE model into an SDE-GB resulted in a significant improvement in the prediction and uncorrelated errors. Tracking of the "peak time of meal absorption" parameter showed that the absorption rate varied according to meal type.

CONCLUSION:
This study shows the potential of using SDE-GBs in diabetes modeling. Improved model predictions were obtained due to the separation of the prediction error. SDE-GBs offer a solid framework for using statistical tools for model validation and model development.
MPC for Wind Power Gradients - Utilizing Forecasts, Rotor Inertia, and Central Energy Storage

We consider the control of a wind power plant, possibly consisting of many individual wind turbines. The goal is to maximize the energy delivered to the power grid under very strict grid requirements to power quality. We define an extremely low power output gradient and demonstrate how decentralized energy storage in the turbines’ inertia combined with a central storage unit or deferrable consumers can be utilized to achieve this goal at a minimum cost. We propose a variation on model predictive control to incorporate predictions of wind speed. Due to the aerodynamics of the turbines the model contains nonconvex terms. To handle this nonconvexity, we propose a sequential convex optimization method, which typically converges in fewer than 10 iterations. We demonstrate our method in simulations with various wind scenarios and prices for energy storage. These simulations show substantial improvements in terms of limiting the power ramp rates (disturbance rejection) at the cost of very little power. This capability is critical to help balance and stabilize the future power grid with a large penetration of intermittent renewable energy sources.

New Hybrid Variational Recovery Model for Blurred Images with Multiplicative Noise

A new hybrid variational model for recovering blurred images in the presence of multiplicative noise is proposed. Inspired by previous work on multiplicative noise removal, an I-divergence technique is used to build a strictly convex model under a condition that ensures the uniqueness of the solution and the stability of the algorithm. A split-Bregman algorithm is adopted to solve the constrained minimisation problem in the new hybrid model efficiently. Numerical tests for simultaneous deblurring and denoising of the images subject to multiplicative noise are then reported. Comparison with other methods clearly demonstrates the good performance of our new approach.
Newton-type method for the variational discretization of topology optimization problems

We present a locally quadratically convergent optimization algorithm for solving topology optimization problems. The distinguishing feature of the algorithm is to treat the design as a smooth function of the state and not vice versa as in the traditional nested approach to topology optimization, which we achieve by inverting a part of perturbed optimality conditions for the problem. In this way, the computational bottleneck is conveniently shifted from evaluating the merit function to a direction finding subproblem. The latter involves solving certain linearized PDEs, and the computational effort is similar to that of finding a gradient of the merit function in the traditional nested approach. We illustrate the performance of the algorithm on benchmark topology optimized problems in fluid mechanics.

Nonconvex optimization for improved exploitation of gradient sparsity in CT image reconstruction

We present a globally convexified optimization algorithm for solving CT image reconstruction problems. The distinguishing feature of the algorithm is to treat the design as a smooth function of the state and not vice versa as in the traditional nested approach to topology optimization, which we achieve by inverting a part of perturbed optimality conditions for the problem. In this way, the computational bottleneck is conveniently shifted from evaluating the merit function to a direction finding subproblem. The latter involves solving certain linearized PDEs, and the computational effort is similar to that of finding a gradient of the merit function in the traditional nested approach. We illustrate the performance of the algorithm on benchmark topology optimized problems in fluid mechanics.
Nonlinear Model Predictive Control for Oil Reservoirs Management

The current world average recovery factor from oil fields is widely agreed to be about 30-35%. An increase of 10% point of this recovery factor would bring about 500 billion of oil barrels, sufficient to meet 16 years of current global production. To realize this potential production increase, the research community is working on improving current feedback model-based optimal control technologies. The topic of this thesis is production optimization for water flooding in the secondary phase of oil recovery. We developed numerical methods for nonlinear model predictive control (NMPC) of an oil field. The controller consists of:

- A model based optimizer for maximizing some predicted financial measure of the reservoir (e.g. the net present value).
- A parameter and state estimator.
- Use of the moving horizon principle for data assimilation and implementation of the computed control input.

The optimizer uses gradient-based optimization and the required gradients are computed by the adjoint method. We propose the use of efficient high order implicit time integration methods for the solution of the forward and the adjoint equations of the dynamical model. The Ensemble Kalman filter is used for data assimilation. Further, we studied the use of robust control strategies in both open-loop, i.e. without measurement feedback, and closed-loop, i.e. with measurement feedback, configurations.

This thesis has three main original contributions:

The first contribution in this thesis is to improve the computationally expensive gradient computation by using high-order ESDIRK (Explicit Singly Diagonally Implicit Runge-Kutta) temporal integration methods and continuous adjoints. The high order integration scheme allows larger time steps and therefore faster solution times. We compare gradient computation by the continuous adjoint method to the discrete adjoint method and the finite-difference method. We demonstrate that the optimization algorithm can be accelerated by using the continuous time adjoint equations. This is the first time in the literature that the higher order continuous adjoint and higher order discrete adjoint methods have been investigated for oil production optimization.

The second contribution of this thesis is the application of the Robust Optimization strategy in both open-loop (i.e. without measurement feedback) and closed-loop (i.e. with measurement feedback). In the oil industry, Robust Optimization has been suggested to compensate for inherent geological uncertainties in an oil field. In robust optimization of an oil reservoir, the water injection and production borehole pressures are computed such that the predicted net present value of an ensemble of permeability field realizations is maximized. In our study, the permeability field is the uncertain parameters. We compare the performance of the RO strategy to a certainty equivalent optimization strategy, based on the ensemble mean of the permeability field realizations as its permeability field, and to a reactive strategy. In open-loop, for the case studied, the reactive strategy performed better than the open-loop RO strategy. These observations are nontrivial, as previous literature suggests that the open-loop RO strategy performs better than the reactive strategy. Simulations indicate that the inferior performance of the open-loop RO strategy compared to the reactive strategy is due to the inability of the RO strategy to efficiently encompass ensembles with very different and conflicting optimal control trajectories. Hence, we propose a modified RO strategy that allow shut in of uneconomical wells. The modified RO strategy performs significantly better than the other open-loop strategies and the reactive strategy. Finally, this is the first time in literature that the RO optimization has been investigated in closed-loop. Surprisingly, for the case studied, the closed-loop certainty equivalent strategy yields a higher NPV than the closed-loop RO strategy. The uncertainty reduction of the permeability field estimate due to data assimilation explains the good performance of the closed-loop certainty equivalent optimization strategy. Consequently, in closed-loop, the increased computational effort of the RO strategy compared to the certainty equivalent strategy is not justified for the particular case studied in this paper.

The third contribution of this thesis is a mean-variance method for risk mitigation in production optimization of oil reservoirs. We introduce a return-risk bicriterior objective function for the profit-risk tradeoff. With this objective function we link the optimization problem in production optimization to the Markowitz portfolio optimization problem in finance or to the robust design problem in topology optimization. In this study we focus on open-loop configuration, i.e. without measurement feedback. We demonstrate that a return-risk bi-criterion objective function is a valuable tool for the profit-risk tradeoff. If combined with the previous contribution, this result trigger the necessity of comparing the closed-loop CE
strategy with the closed-loop MV strategy.

The thesis consists of a summary report and a collection of five research papers written during the period May 2010 to August 2013. Three papers are published in conference proceedings, one paper is published in Computational Geosciences journal and another paper is submitted to Journal of Petroleum Science and Engineering.

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Oblique projections and standard-form transformations for discrete inverse problems
This tutorial paper considers a specific computational tool for the numerical solution of discrete inverse problems, known as the standard-form transformation, by which we can treat general Tikhonov regularization problems efficiently. In the tradition of B. N. Datta's expositions of numerical linear algebra, we use the close relationship between oblique projections, pseudoinverses, and matrix computations to derive a simple geometric motivation and algebraic formulation of the standard-form transformation.

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Parallel Implementation of Riccati Recursion for Solving Linear-Quadratic Control Problems

In both Active-Set (AS) and Interior-Point (IP) algorithms for Model Predictive Control (MPC), sub-problems in the form of linear-quadratic (LQ) control problems need to be solved at each iteration. The solution of these sub-problems is usually the main computational effort. In this paper an alternative version of the Riccati recursion solver for LQ control problems is presented. The performance of both the classical and the alternative version is analyzed from a theoretical as well as a numerical point of view, and the alternative version is found to be approximately 50% faster than the classical one, for systems with many states. A number of parallel implementations of the alternative version has been proposed and tested.

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Power Management for Energy Systems
In this thesis, we consider the control of two different industrial applications that belong at either end of the electricity grid; a power consumer in the form of a commercial refrigeration system, and wind turbines for power production. Our primary studies deal with economic model predictive control of a commercial multi-zone refrigeration system, consisting of several
cooling units that share a common compressor, and is used to cool multiple areas or rooms, e.g., in supermarkets. Substantial amounts of energy are consumed in refrigeration systems worldwide and there is a strong motivation for introducing more energy efficient as well as cost reducing control techniques. At the same time, the power grid is evolving from a centralized system with rather controllable production in the conventional power plants to a much more decentralized network of many independent power generators and a large penetration of renewable, fossil-free energy sources such as solar and wind power. To facilitate such intermittent power producers, we must not only control the production of electricity, but also the consumption, in an efficient and exible manner. By enabling the use of thermal energy storage in supermarkets, we open up for exible power consumption schemes with the possibility of reducing operational costs and we develop and demonstrate prototype control technology that creates completely new business opportunities for selling regulating power to the grid. Moreover, this enables a larger penetration of wind energy in the power production and increases the potential market size for wind power generators and other renewable energy sources. Thus, we aim at promoting the use of environmentally sustainable power production technologies while creating new business opportunities for both power consumers and producers of renewable energy.

The second application, wind turbines, takes us to the production side of the power grid. The key concern here is to improve the quality and integrability of power delivered to the grid from large parks of wind turbines. Our goal is to reduce the fluctuating nature of the power output and to meet tightened demands from the grid by enabling a more intelligent control at both the individual turbine level, at the park controller level, and in cooperation with exible power consumers or other means of energy storage. The possible interaction and synergies of the two applications are obvious reasons to consider both in this thesis, and as we will see, the similarities in our formulations of the dierent control problems allow us to apply almost identical techniques despite the lack of immediate similarity.

For control of the commercial refrigeration application as well as the wind turbine application, we propose an economic optimizing model predictive controller, economic MPC. MPC is a feedback control technique that is characterized by its explicit handling of constrained control problems in which a model is used to predict the future behavior of a system along with forecasts of future disturbances. At each time step the values of the control inputs are computed by solving an open-loop nite time optimal control problem over a dened prediction horizon. Only the rst step in this optimal open-loop sequence is implemented as a control command. Feedback is obtained by solving the open-loop problem repeatedly, in a receding horizon fashion, as new predictions become available.

Our investigations are primarily concerned with: 1) modeling of the applications to suit the chosen control framework; 2) formulating the MPC controller laws to overcome challenges introduced by the industrial applications, and deening economic objectives that reect the real physics of the systems as well as our control objectives; 3) solving the involved, non-trivial optimization problems eciently in real-time; 4) demonstrating the feasibility and potential of the proposed methods by extensive simulation and comparison with existing control methods and evaluation of data from systems in actual operation.

We present contributions on:

- Economic MPC for commercial refrigeration systems, including
  - Linear economic MPC formulations that utilize the exibility in refrigeration systems to counteract ucations in the balance between power consumption and production.
  - Economic MPC with probabilistic constraints, ensuring a robust performance and constraint satisfaction in spite of inaccurate system models and forecasts.
  - Nonlinear economic MPC, reecting the nonconvexity in the realistic description of temperature dependent efficiencies in the refrigeration cycle.
  - Nonlinear economic MPC for uncertain predictions and the implementation of very simple predictors that use entirely historical data of, e.g., electricity prices and outdoor temperatures.

- Economic MPC for wind turbines, including
  - Optimal steady-state calculation for wind farms.
  - Nonlinear economic MPC for individual turbines.
  - Change of variables and convex formulations of economic MPC for individual turbines.

Tractable optimization methods for the MPC problems, including

- Sequential convex programming (SCP) for specic nonconvex problems originating from our studies of commercial refrigeration as well as from our studies concerning wind power.
- Successful demonstration of the SCP approach on three dierent problems the commercial refrigeration system with linear dynamics and constraints and a nonconvex objective, the individual wind turbine with nonlinear dynamics and constraints, and the static optimization of the wind farm with a black-box model.

The major contribution is the formulation of these problems and the demonstrations to show that the SCP method can be used for their solution.

We demonstrate, i.a., substantial cost savings, on the order of 30 %, compared to a standard thermostat-based supermarket refrigeration system and show how our methods exhibit sophisticated demand response to real-time variations in electricity prices. Violations of the temperature ranges can be kept at a very low frequency of occurence inspite of the presence of uncertainty. For the power output from wind turbines, ramp rates, as low a 3 % of the rated power per minute, can be effectively ensured with the use of energy storage and we show how the active use of rotor inertia as an additional energy storage can reduce the needed storage capacity by up to 30 % without reducing the power output.

**General information**

- **State:** Published
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Practical Implementations of Advanced Process Control for Linear Systems

This paper describes some practical problems encountered, when implementing Advanced Process Control, APC, schemes on linear processes. The implemented APC controllers discussed will be LQR, Riccati MPC and Condensed...
MPC controllers illustrated by simulation of the Four Tank Process and a linearised CSTR. Advantages and disadvantages of these controllers will be discussed. All three controller types show a set of common undesirable characteristics, which must be accounted for. At the end of the evaluation horizon the “optimal” solution has an unstable characteristic, which can be suppressed by selecting different control and evaluation horizon. Depending on the number of degrees of freedom, offset-free control of the number of controlled variables can be achieved by integration of the innovation errors and introduction of noise models. If the measured or unmeasured disturbances increase, offset-free control cannot be achieved without violation of process constraints. A target calculation function can be used to calculate the optimal achievable target for the process. The use of hard and soft constraints for process input constraints in the MPC controllers, ensures feasible solutions. The computational load as function of controllers type, Model dimension and constraint type will be discussed. Finally the special requirements set by processes including a pure integration dynamics will be illustrated by a linearised CSTR process. The simulated results presented, will later on be implemented on and demonstrated on pilot plant equipment on the department of Chemical Engineering DTU Lyngby.

Practical Implementations of Advanced Process Control for Linear Systems

Most advanced process control systems are based on Model Predictive Control (MPC). In this paper we discuss three critical issues for the practical implementation of linear MPC for process control applications. The first issue is related to offset free control and disturbance models; the second issue is related to the use of soft output constraints in MPC; and the third issue is related to the computationally efficient solution of the quadratic program in the dynamic regulator of the MPC. We have implemented MPC in .Net using C# and the MPCMath library. The implemented MPC is based on the target-regulator structure. It enables offset-free control; it can be computed efficiently on-line using several optimization algorithms; and accommodates soft constraint for the outputs and for shaping the set-point tracking penalty function. We report selected observations using this implementation and discuss their practical implications for process control. If the control and evaluation intervals are chosen too short, the predicted behaviour of the controllers may have unstable characteristics. Depending on the degrees of freedom, offset-free control of a number of the controlled variables can be achieved by introduction of noise models and integration of the innovation errors. If the disturbances increase, offset-free control cannot be achieved without violation of process constraints. A target calculation function is used to calculate the optimal achievable target for the process. The use of soft constraints for process output constraints in the MPC controllers, ensures feasible solutions. The computational load as function of controllers type, model dimension and constraint type are shown.
tomography (CT) is nontrivial, because both full sampling in the discrete-to-discrete imaging model and the reduction in sampling admitted by sparsity-exploiting methods are ill-defined. The present article proposes definitions of full sampling by introducing four sufficient-sampling conditions (SSCs). The SSCs are based on the condition number of the system matrix of a linear imaging model and address invertibility and stability. In the example application of breast CT, the SSCs are used as reference points of full sampling for quantifying the undersampling admitted by reconstruction through TV-minimization. In numerical simulations, factors affecting admissible undersampling are studied. Differences between few-view and few-detector bin reconstruction as well as a relation between object sparsity and admitted undersampling are quantified.

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Real-Time Simulation of Ship-Structure and Ship-Ship Interaction

This paper gives the status of the development of a ship-hydrodynamic model for real-time ship-wave calculation and ship-structure and ship-ship interaction in a full mission marine simulator. The hydrodynamic model is based on potential flow theory, linear or non-linear free surface boundary condition and higher-order accurate numerical approximations. The equations presented facilitate both Neumann-Kelvin and double-body linearizations. The body boundary condition on the ship hull is approximated by a static and dynamic moving pressure distribution. The pressure distribution method is used, because it is simple, easy to implement and computationally efficient. Multiple many-core graphical processing units (GPUs) are used for parallel execution and the model is implemented using a combination of C/C++, CUDA and MPI. Two ship hydrodynamic cases are presented: Kriso Container Carrier at steady forward speed and lock entrance of a TEU 12.000 Container Carrier. These calculations reveal that the pressure distribution model is a too simple approximation of the body boundary condition and that it has the limitations of a flat-ship approximation. It is necessary to investigate more accurate approximations of the body boundary condition, which does not compromise the overall computational efficiency.

Sensitivity Analysis of the Critical Speed in Railway Vehicle Dynamics

We present an approach to global sensitivity analysis aiming at the reduction of its computational cost without compromising the results. The method is based on sampling methods, cubature rules, High-Dimensional Model Representation and Total Sensitivity Indices. The approach has a general applicability in many engineering fields and does not require the knowledge of the particular solver of the dynamical system. This analysis can be used as part of the virtual homologation procedure and to help engineers during the design phase of complex systems. The method is applied to a half car with a two-axle Cooperrider bogie, in order to study the sensitivity of the critical speed with respect to suspension parameters. The importance of a certain suspension component is expressed by the variance in critical speed that is ascribable to it. This proves to be useful in the identification of parameters for which the exactness of their values is critically important.
SIPPI: A Matlab toolbox for sampling the solution to inverse problems with complex prior information: Part 1—Methodology

From a probabilistic point-of-view, the solution to an inverse problem can be seen as a combination of independent states of information quantified by probability density functions. Typically, these states of information are provided by a set of observed data and some a priori information on the solution. The combined states of information (i.e. the solution to the inverse problem) is a probability density function typically referred to as the a posteriori probability density function. We present a generic toolbox for Matlab and Gnu Octave called SIPPI that implements a number of methods for solving such probabilistically formulated inverse problems by sampling the a posteriori probability density function. In order to describe the a priori probability density function, we consider both simple Gaussian models and more complex (and realistic) a priori models based on higher order statistics. These a priori models can be used with both linear and non-linear inverse problems. For linear inverse Gaussian problems we make use of least-squares and kriging-based methods to describe the a posteriori probability density function directly. For general non-linear (i.e. non-Gaussian) inverse problems, we make use of the extended Metropolis algorithm to sample the a posteriori probability density function. Together with the extended Metropolis algorithm, we use sequential Gibbs sampling that allow computationally efficient sampling of complex a priori models. The toolbox can be applied to any inverse problem as long as a way of solving the forward problem is provided. Here we demonstrate the methods and algorithms available in SIPPI. An application of SIPPI, to a tomographic cross borehole inverse problems, is presented in a second part of this paper.
SIPPI: A Matlab toolbox for sampling the solution to inverse problems with complex prior information: Part 2—Application to crosshole GPR tomography

We present an application of the SIPPI Matlab toolbox, to obtain a sample from the a posteriori probability density function for the classical tomographic inversion problem. We consider a number of different forward models, linear and non-linear, such as ray based forward models that rely on the high frequency approximation of the wave-equation and 'fat' ray based forward models relying on finite frequency theory. In order to sample the a posteriori probability density function we make use of both least squares based inversion, for linear Gaussian inverse problems, and the extended Metropolis sampler, for non-linear non-Gaussian inverse problems. To illustrate the applicability of the SIPPI toolbox to a tomographic field data set we use a cross-borehole traveltime data set from Arrenæs, Denmark. Both the computer code and the data are released in the public domain using open source and open data licenses. The code has been developed to facilitate inversion of 2D and 3D travel time tomographic data using a wide range of possible a priori models and choices of forward models.

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Sizing of Microparticles from Angular Scattering Ratio
This technical note deals with light scattering measurements for sizing of micrometer-scale particles in a suspension.

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Authors: Hjorth, P. G. (Intern), Karamehmedovic, M. (Intern)
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Solar/electric heating systems for the future energy system
The project “Solar/electric heating systems in the future energy system” was carried out in the period 2008-2013. The project partners were DTU Byg, DTU Informatics (now DTU Compute), DMI, ENFOR A/S and COWI A/S. The companies Ajva ApS, Ohmatex ApS and Innogie ApS worked together with the project partners in two connected projects in order to develop solar/electric heating systems for laboratory tests. The project was financed by the Danish Agency for Science, Technology and Innovation under the Danish Council for Strategic Research in the program Sustainable Energy and Environment. The DSF number of the project is 2104-07-0021/09-063201/DSF. This report is the final report of the project. The aim of the project is to elucidate how individual heating units for single family houses are best designed in order to fit into the future energy system. The units are based on solar energy, electrical heating elements/heat pump, advanced heat storage tanks and advanced control systems.
Heat is produced by solar collectors in sunny periods and by electrical heating elements/heat pump. The electrical heating elements/heat pump will be in operation in periods where the heat demand cannot be covered by solar energy. The aim is to use the auxiliary heating units when the electricity price is low, e.g. due to large electricity production by wind turbines.
The unit is equipped with an advanced control system where the control of the auxiliary heating is based on forecasts of the electricity price, the heat demand and the solar energy production. Consequently, the control is based on weather forecasts.
Three differently designed heating units are tested in a laboratory test facility. The systems are compared on the basis of:
- energy consumption for the auxiliary heating
- energy cost for the auxiliary heating
- net utilized solar energy

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Sparse Image Reconstruction in Computed Tomography

In recent years, increased focus on the potentially harmful effects of x-ray computed tomography (CT) scans, such as radiation-induced cancer, has motivated research on new low-dose imaging techniques. Sparse image reconstruction methods, as studied for instance in the field of compressed sensing (CS), have shown significant empirical potential for this purpose. For example, total variation regularized image reconstruction has been shown in some cases to allow reducing x-ray exposure by a factor of 10 or more, while maintaining or even improving image quality compared to conventional reconstruction methods.

However, the potential in CT has mainly been demonstrated in individual proof-of-concept studies, from which it is hard to distill general conditions for when sparse reconstruction methods perform well. As a result, there is a fundamental lack of understanding of the effectiveness and limitations of sparse reconstruction methods in CT, in particular in a quantitative sense. For example, relations between image properties such as contrast, structure and sparsity, tolerable noise levels, sufficient sampling levels, the choice of sparse reconstruction formulation and the achievable image quality remain unclear. This is a problem of high practical concern, because the large scale of CT problems makes detailed exploration of the parameter space very time-consuming. Due to the limited quantitative understanding, sparse reconstruction has not yet become the method of choice in practical CT applications.

This thesis takes a systematic approach toward establishing quantitative understanding of conditions for sparse reconstruction to work well in CT. A general framework for analyzing sparse reconstruction methods in CT is introduced and two sets of computational tools are proposed:

1. An optimization algorithm framework enabling easy derivation of algorithms for sparse reconstruction problems, and
2. Tools for characterizing sparse reconstruction in CT, i.e., establishing relations between parameters governing reconstruction quality.

The flexibility of the optimization algorithm framework is demonstrated by constructing convergent optimization algorithms for a range of sparse reconstruction problems of interest to CT. The practical usefulness of the framework is shown through case studies of the effectiveness of specific sparse reconstruction problems in tomographic reconstruction.

The characterization methods proposed in the thesis focus on the role of image sparsity for the level of sampling required for accurate CT reconstruction. While a relation between sparsity and sampling is motivated by CS, no theoretical guarantees of accurate sparse reconstruction are known for CT. In simulation studies, a sparsity-sampling relation is established in CT. This enables quantification of the undersampling allowed by sparse reconstruction methods.

Both the prototyping framework and the characterization methods add to the understanding of sparse reconstruction methods in CT and serve as initial contributions to a general set of computational characterization tools. Thus, the thesis contributions help advance sparse reconstruction methods toward routine use in...
Stochastic Wave Dynamics and Uncertainty Quantification

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Authors: Engsig-Karup, A. P. (Intern), Bigoni, D. (Intern), Glimberg, S. L. (Intern)
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The Homogeneous Interior-Point Algorithm: Nonsymmetric Cones, Warmstarting, and Applications
The overall topic of this thesis is convex conic optimization, a sub-field of mathematical optimization that attacks optimization problem with a certain geometric structure. These problems allow for modelling of an extremely wide range of real-world problems, but the availability of solution algorithms for these problems is still limited.

The goal of this thesis is to investigate and shed light on two computational aspects of homogeneous interior-point algorithms for convex conic optimization:
The first part studies the possibility of devising a homogeneous interior-point method aimed at solving problems involving constraints that require nonsymmetric cones in their formulation. The second part studies the possibility of warmstarting the homogeneous interior-point algorithm for conic problems. The main outcome of the first part is the introduction of a completely new homogeneous interior-point algorithm designed to solve nonsymmetric convex conic optimization problems. The algorithm is presented in detail and then analyzed. We prove its convergence and complexity. From a theoretical viewpoint, it is fully competitive with other algorithms and from a practical viewpoint, we show that it holds lots of potential, in several cases being superior to other solution methods.

The main outcome of the second part of the thesis is two new warmstarting schemes for the homogeneous interior-point algorithm for conic problems. Again, we first motivate and present the schemes and then analyze them. It is proved that they, under certain circumstances, result in an improved worst-case complexity as compared to a normal coldstart. We then move on to present an extensive series of computational results substantiating the practical usefulness of these warmstarting schemes. These experiments include standard benchmarking problem test sets as well as an application from smart energy systems.

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The Potential of Economic Model Predictive Control for Spray Drying Plants
In 2015 the milk quota system in the European Union will be completely liberalized. As a result, analysts expect production of skimmed and whole milk powder to increase by 5-6% while its price will decline by about 6-7%. Multi-stage spray drying is the prime process for the production of food powders. The process is highly energy consuming and capacity depends
among other factors on correct control of the dryer. Consequently efficient control and optimization of the spray drying process has become increasingly important to accommodate the future market challenges.

The goal of the presentation is to present our results regarding modeling of the process and how the efficiency and profitability can be lifted by introducing an economic optimizing MPC scheme.

Firstly, we develop a first-principle engineering model that can be used to simulate spray drying processes with high accuracy. The model can be adjusted to describe drying of various products and describes the complete drying process of a multi-stage spray dryer. The dryer is divided into three stages, the spray stage and two uid bed stages. Each stage is assumed ideally mixed and described by mass- and energy balances. The model is able to predict outlet temperatures, the residual moisture and particle size of the product. We also give a novel approach to predict deposits due to stickiness of the powder. The model predictions are compared to datasets gathered at GEA Process Engineering's test facility. The identified model parameters are identified from data and the resulting model fits the data well.

Secondly, the effect of disturbances, ambient air humidity and solids content in the feed, is studied by simulation. We show that conventional control is insufficient at controlling the product quality as well as driving the plant to the most economic conditions. Furthermore, we show that the efficiency can be increased by correct adjustment of heat and inlet airflow at each stage.

The recent focus in research has shifted from reference tracking MPC to optimization of economic objective functions. We will discuss how this optimization can be performed by advanced process control techniques, such as Economic Model Predictive Control (E-MPC). We suggest adding an E-MPC based supervisory control layer on top of the contemporary PI-controllers. The strong interconnection between drying stages and process constraints are well suited for MPC.

**General information**
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Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Dynamical Systems, Department of Electrical Engineering, Automation and Control, Center for Energy Resources Engineering, GEA Process Engineering A/S
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Towards real time simulation of ship-ship interaction - Part II: double body flow linearization and GPU implementation

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Viscoelastic Modelling of Road Deflections for use with the Traffic Speed Deflectometer
This Ph.D. study is at its core about how asphalt and road structures responds to dynamic loads.
Existing models for the deflections under a moving load using beam equations are revisited and it is concluded they leave room for improvement for the particular setup and problem at hand. Then a different approach is set up to model visco-elastic deflections starting from the physically based framework of continuum mechanics by using Finite Element Methods (FEM) combined with the Laplace transform.
It is shown that this approach coincides with a more standard time-stepping FEM setup in the case of a generalized Maxwell model.
Validations by comparison to ViscoRoute simulations are also made.
This justifies the use of the Laplace FEM for generating simulated data using a Huet-Sayegh model for the visco-elastic behaviour of asphalt.
These simulated data, along with measured data, are then used to suggest an approach for a computationally simpler synthetic model capturing essential behaviour of deflection bassins under a moving wheel.
Additionally the setup allows for simulated comparisons of the cases of loadings emulating the use of a Falling Weight Deflectometer with loadings emulating a moving wheel as in the case of using a Traffic Speed Deflectometer. The flexibility of the method also allows for looking into cases excluded by imposing simplifying assumptions such as the structure imagined to be an infinite halfspace.

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Warmstarting the homogeneous and self-dual interior point method for linear and conic quadratic problems
We present two strategies for warmstarting primal-dual interior point methods for the homogeneous self-dual model when applied to mixed linear and quadratic conic optimization problems. Common to both strategies is their use of only the final (optimal) iterate of the initial problem and their negligible computational cost. This is a major advantage when compared to previously suggested strategies that require a pool of iterates from the solution process of the initial problem.
Consequently our strategies are better suited for users who use optimization algorithms as black-box routines which usually only output the final solution. Our two strategies differ in that one assumes knowledge only of the final primal solution while the other assumes the availability of both primal and dual solutions. We analyze the strategies and deduce conditions under which they result in improved theoretical worst-case complexity. We present extensive computational results showing work reductions when warmstarting compared to coldstarting in the range 30–75% depending on the problem class and magnitude of the problem perturbation. The computational experiments thus substantiate that the warmstarting strategies are useful in practice.

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Waterflooding optimization in uncertain geological scenarios

In conventional waterflooding of an oil field, feedback based optimal control technologies may enable higher oil recovery than with a conventional reactive strategy in which producers are closed based on water breakthrough. To compensate for the inherent geological uncertainties in an oil field, robust optimization has been suggested to improve and robustify optimal control strategies. In robust optimization of an oil reservoir, the water injection and production borehole pressures (bhp) are computed such that the predicted net present value (NPV) of an ensemble of permeability field realizations is maximized. In this paper, we both consider an open-loop optimization scenario, with no feedback, and a closed-loop optimization scenario. The closed-loop scenario is implemented in a moving horizon manner and feedback is obtained using an ensemble Kalman filter for estimation of the permeability field from the production data. For open-loop implementations, previous test case studies presented in the literature, show that a traditional robust optimization strategy (RO) gives a higher expected NPV with lower NPV standard deviation than a conventional reactive strategy. We present and study a test case where the opposite happen: The reactive strategy gives a higher expected NPV with a lower NPV standard deviation than the RO strategy. To improve the RO strategy, we propose a modified robust optimization strategy (modified RO) that can shut in uneconomical producer wells. This strategy inherits the features of both the reactive and the RO strategy. Simulations reveal that the modified RO strategy results in operations with larger returns and less risk than the reactive strategy, the RO strategy, and the certainty equivalent strategy. The returns are measured by the expected NPV and the risk is measured by the standard deviation of the NPV. In closed-loop optimization, we investigate and compare the performance of the RO strategy, the reactive strategy, and the certainty equivalent strategy. The certainty equivalent strategy is preferable in the closed-loop situation as it requires significantly less computational resources than the robust optimization strategy. Feedback reduces the uncertainty and this is the reason for the similar performance of the two strategies.
Robust optimization, Ensemble Kalman filter, Oil reservoir, Production optimization, Automatic history matching

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Model Predictive Control Algorithms for Pen and Pump Insulin Administration

Despite recent developments within diabetes management such as rapid-acting insulin, continuous glucose monitors (CGM) and insulin pumps, tight blood glucose control still remains a challenge. A fully automated closed-loop controller, also known as an artificial pancreas (AP), has the potential to ease the life and reduce the risk of acute and chronic diabetic complications. However, the noise associated to CGMs, the long insulin action time for continuous subcutaneous infusion of insulin (CSII) pumps, and the high intra- and inter-patient variability significantly limits the performance of current closed-loop controllers.

In this thesis, we present different control strategies based on Model Predictive Control (MPC) for an artificial pancreas. We use Nonlinear Model Predictive Control (NMPC) in order to determine the optimal insulin and blood glucose profiles. The optimal control problem (OCP) is solved using a multiple-shooting based algorithm. We use an explicit Runge-Kutta method (DOPRI45) with an adaptive stepsize for numerical integration and sensitivity computation. The OCP is solved using a Quasi-Newton sequential quadratic programming (SQP) with a linesearch and a BFGS update for the Hessian of the Lagrangian. In addition, we apply a Continuous-Discrete Extended Kalman Filter (CDEKF) in order to simulate cases where the meal size is uncertain, or even unannounced.

We also propose a novel control strategy based on linear MPC for overnight stabilization of blood glucose. The model parameters are personalized using a priori available patient information. We consider an autoregressive integrated moving average with exogenous input (ARIMAX) model. We summarize and the results of the overnight clinical studies conducted at Hvidovre Hospital. Based on these results, we propose improvements for the stochastic part of our controller model. We state and compare three different stochastic model structures. The first one is the ARIMAX structure that has been used for the clinical studies. The second one is an autoregressive moving average with exogenous input (ARMAX) model. The third one is an adaptive ARMAX model in which we estimate the parameters of the stochastic part using a Recursive Least Square (RLS) method. We test the controller in a virtual clinic of 100 patients. This virtual clinic is based on the Hovorka model. We consider the case where only half of the bolus is administrated at mealtime, and the case where the insulin sensitivity increases during the night.

This thesis consists of a summary report, glucose and insulin profiles of the clinical studies and research papers submitted, peer-reviewed and/or published in the period September 2009 - September 2012.
Continuous-Discrete Time Prediction-Error Identification Relevant for Linear Model Predictive Control

A prediction-error method tailored for model-based predictive control is presented. The prediction-error method studied is based on predictions using the Kalman filter and Kalman predictors for a linear discrete-time stochastic state space model. The linear discrete-time stochastic state space model is realized from a continuous-discrete-time linear stochastic system specified using transfer functions with time-delays. It is argued that the prediction-error criterion should be selected such that it is compatible with the objective function of the predictive controller in which the model is to be applied. The suitability of the proposed prediction error method for predictive control is demonstrated for dual composition control of a simulated binary distillation column.