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.
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.
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.

General information
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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. (Intern), Madsen, H. (Intern), Jørgensen, J. B. (Intern)
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Main Research Area: Technical/natural sciences
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2014

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.
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 HP-MPC) 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.

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.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing
Authors: Gade-Nielsen, N. F. (Intern), Dammann, B. (Intern), Jørgensen, J. B. (Intern)
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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
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, TICRA
Authors: Borries, O. P. (Intern), Sørensen, H. H. B. (Intern), Dammann, B. (Intern), Jørgensen, E. (Intern), Meincke, P. (Intern), Sorensen, S. B. (Ekstern), Hansen, P. C. (Intern)
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BFI conference series: European Conference on Antennas and Propagation (5010932)
Main Research Area: Technical/natural sciences
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DOIs:
10.1109/EuCAP.2014.6901738
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.
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.
A High-Order WENO Finite Difference Water Wave Model for Interactive Ship-Wave Simulation

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling, Scientific Computing, Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Engsig-Karup, A. P. (Intern), Lindberg, O. (Intern), Glimberg, S. L. (Intern), Dammann, B. (Intern), Bingham, H. B. (Intern), Madsen, P. A. (Intern)
Number of pages: 2
Publication date: 2012
Main Research Area: Technical/natural sciences
Source: dtu
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Publication: Research - peer-review › Paper – Annual report year: 2012

High Resolution Orientation Distribution Function
A new method for reconstructing a High Resolution Orientation Distribution Function (HRODF) from X-ray diffraction data is presented. It is shown that the method is capable of accommodating very localized features, e.g. sharp peaks from recrystallized grains on a background of a texture component from the deformed material. The underlying mathematical formalism supports all crystallographic space groups and reduces the problem to solving a (large) set of linear equations. An implementation on multi-core CPUs and Graphical Processing Units (GPUs) is discussed along with an example on simulated data.

General information
State: Published
Organisations: Metal Structures in Four Dimensions, Materials Research Division, Risø National Laboratory for Sustainable Energy, Scientific Computing, Department of Informatics and Mathematical Modeling, Institute of Computational Mathematics and Mathematical Geophysics
Authors: Schmidt, S. (Intern), Gade-Nielsen, N. F. (Intern), Høstergaard, M. (Ekstern), Dammann, B. (Intern), Kazantsev, I. G. (Ekstern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.28 SJR 0.186 SNIP 0.306
BFI (2015): BFI-level 1
Scopus rating (2015): SNIP 0.337 SJR 0.217 CiteScore 0.29
BFI (2014): BFI-level 1
Scopus rating (2014): SNIP 0.448 SJR 0.269 CiteScore 0.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Iterative Methods for MPC on Graphical Processing Units

The high floating point performance and memory bandwidth of Graphical Processing Units (GPUs) makes them ideal for a large number of computations which often arises in scientific computing, such as matrix operations. GPUs achieve this performance by utilizing massive parallelism, which requires reevaluating existing algorithms with respect to this new architecture. This is of particular interest to large-scale constrained optimization problems with real-time requirements. The aim of this study is to investigate different methods for solving large-scale optimization problems with focus on their applicability for GPUs. We examine published techniques for iterative methods in interior points methods (IPMs) by applying them to simple test cases, such as a system of masses connected by springs. Iterative methods allows us deal with the ill-conditioning occurring in the later iterations of the IPM as well as to avoid the use of dense matrices, which may be too large for the limited memory capacity of current graphics cards.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Scientific Computing, Department of Informatics and Mathematical Modeling
MPC Toolbox with GPU Accelerated Optimization Algorithms

The introduction of Graphical Processing Units (GPUs) in scientific computing has shown great promise in many different fields. While GPUs are capable of very high floating point performance and memory bandwidth, its massively parallel architecture requires algorithms to be reimplemented to suit the different architecture. Interior point method can be used to solve convex optimization problems. These problems often arise in fields such as in Model Predictive Control (MPC), which may have real-time requirements for the solution time. This paper presents a case study in which we utilize GPUs for a Linear Programming Interior Point Method to solve a test case where a series of power plants must be controlled to minimize the cost of power production. We demonstrate that using GPUs for solving MPC problems can provide a speedup in solution time.

Numerical Methods for Solution of the Extended Linear Quadratic Control Problem

In this paper we present the extended linear quadratic control problem, its efficient solution, and a discussion of how it arises in the numerical solution of nonlinear model predictive control problems. The extended linear quadratic control problem is the optimal control problem corresponding to the Karush-Kuhn-Tucker system that constitute the majority of computational work in constrained nonlinear and linear model predictive control problems solved by efficient MPC-tailored interior-point and active-set algorithms. We state various methods of solving the extended linear quadratic control problem and discuss instances in which it arises. The methods discussed in the paper have been implemented in efficient C code for both CPUs and GPUs for a number of test examples.
Parallel Programming using OpenCL on Modern Architectures

This report is intended as a quick introduction to the OpenCL framework and the aim is to facilitate a smooth transfer into the use OpenCL C for developers with previous GPGPU experience. The purpose of OpenCL is to allow for developers to use all compute resources available on a heterogeneous hardware platform. As well as being an introduction to OpenCL, the report also presents an overview of AMD GPU hardware, covering both the VLIW5/4 architectures and the upcoming Graphics-Core-Next architecture which is to form the basis of AMDs future generation GPUs that are to be as capable at compute as they are at graphics. To conclude the presentation of OpenCL as a language for compute, a matrix-matrix multiplication example is devised and optimized for the VLIW4, Tesla and Fermi architectures. The performance is measured as a function of both matrix and work-group size and results are discussed. Where applicable, the equivalent CUDA implementation is tested for comparison.

General information
State: Published
Organisations: Department of Informatics and Mathematical Modeling, Scientific Computing
Authors: Nielsen, A. S. (Ekstern), Engsig-Karup, A. P. (Intern), Dammann, B. (Intern)
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tr12_05.pdf
Publication: Research › Report – Annual report year: 2012

Parallel Sparse Matrix - Vector Product: Pure MPI and hybrid MPI-OpenMP Implementation

This technical report contains a case study of a sparse matrix-vector product routine, implemented for parallel execution on a compute cluster with both pure MPI and hybrid MPI-OpenMP solutions. C++ classes for sparse data types were developed and the report shows how these class can be used, as well as performance results for different cases, i.e. different types of sparse matrices.

General information
State: Published
Organisations: Department of Mechanical Engineering, Solid Mechanics, Department of Informatics and Mathematical Modeling, Scientific Computing
Authors: Alexandersen, J. (Intern), Lazarov, B. S. (Intern), Dammann, B. (Intern)
Number of pages: 61
Publication date: 2012

Publication information
Place of publication: Kgs. Lyngby
Development of an efficient GPU-accelerated model for fully nonlinear water waves

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Image Analysis and Computer Graphics, Technical University of Denmark
Authors: Madsen, M. G. (Ekstern), Engsig-Karup, A. P. (Intern), Dammann, B. (Intern), Frisvad, J. R. (Intern)
Publication date: 2010
Event: Abstract from Scientific Computing with CUDA, Roskilde University, Denmark,
Main Research Area: Technical/natural sciences
Electronic versions:
MadsenEtAl.pdf
Source: orbit
Source-ID: 269058
Publication: Research › Conference abstract for conference – Annual report year: 2010

Matematikken i computerens verden - computeren i matematikkens tjeneste

General information
State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling
Authors: Dammann, B. (Intern), Hansen, P. C. (Intern)
Number of pages: 288
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Editors: Hansen, C. B., Hansen, P. C., Hansen, V. L., Andersen, M. M.
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Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 246000
Publication: Education › Book chapter – Annual report year: 2009

Toward a scalable flexible-order model for 3D nonlinear water waves
For marine and coastal applications, current work are directed toward the development of a scalable numerical 3D model for fully nonlinear potential water waves over arbitrary depths. The model is high-order accurate, robust and efficient for large-scale problems, and support will be included for flexibility in the description of structures by the use of curvilinear boundary-fitted meshes. The mathematical equations for potential waves in the physical domain is transformed through $\sigma$-mapping(s) to a time-invariant boundary-fitted domain which then becomes a basis for an efficient solution strategy on a time-invariant mesh. The 3D numerical model is based on a finite difference method as in the original works \cite{LiFleming1997,BinghamZhang2007}. Full details and other aspects of an improved 3D solution can be found in \cite{EBL08}. The new and improved approach for three-dimensional problems employs a GMRES solver with multigrid preconditioning to achieve optimal scaling of the overall solution effort, i.e., directly with $n$ the total number of grid points. Grid independent iteration count and optimal scaling has been demonstrated to be independent of the mesh and the physics. A robust method is achieved through a special treatment of the boundary conditions along solid boundaries using a fictitious a ghost point technique, and is necessary for a robust multigrid preconditioning strategy. The solution strategy is found to be both robust for general nonlinear wave problems, with no need for additional smoothing or filtering.
over that imposed naturally by the finite difference scheme. By the adjusting the numerical discretization parameters, the accuracy in dispersion and flow kinematics (accuracy) together with the solution effort (efficiency) can be optimized for the model to be nearly competitive with dedicated models based on simplified equations, e.g. Boussinesq-type equations. At the symposium, we will present examples demonstrating the fundamental properties of the numerical model (OceanWave3D) together with the latests achievements.

**General information**

State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Coastal, Maritime and Structural Engineering, Department of Mechanical Engineering
Authors: Engsig-Karup, A. P. (Intern), Ducrozet, G. (Intern), Bingham, H. B. (Intern), Dammann, B. (Intern)
Publication date: 2009
Main Research Area: Technical/natural sciences
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Source: orbit
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2009

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An Introduction to Programming using MATLAB

Basic introduction to computing programming using MATLAB as first programming language.

**General information**

State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling
Authors: Rojas Larrazabal, M. D. L. C. (Intern), Dammann, B. (Intern)
Publication date: 2008

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Publication: Education › Compendium/lecture notes – Annual report year: 2008

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Estimation of non-linear continuous time models for the heat exchange dynamics of building integrated photovoltaic modules

This paper focuses on a method for linear or non-linear continuous time modelling of physical systems using discrete time data. This approach facilitates a more appropriate modelling of more realistic non-linear systems. Particularly concerning advanced building components, convective and radiative heat interchanges are non-linear effects and represent significant contributions in a variety of components such as photovoltaic integrated facades or roofs and those using these effects as passive cooling strategies, etc. Since models are approximations of the physical system and data is encumbered with measurement errors it is also argued that it is important to consider stochastic models. More specifically this paper advocates for using continuous-discrete stochastic state space models in the form of non-linear partially observed stochastic differential equations (SDE’s)-with measurement noise for modelling dynamic systems in continuous time using discrete time data. First of all the proposed method provides a method for modelling non-linear systems with partially observed states. The approach allows parameters to be estimated from experimental data in a prediction error (PE) setting, which gives less biased and more reproducible results in the presence of significant process noise than the more commonly used output error (OE) setting. To facilitate the use of continuous-discrete stochastic state space models, a PE estimation scheme that features maximum likelihood (ML) and maximum a posteriori (MAP) estimation is presented along with a software implementation. As a case study, the modelling of the thermal characteristics of a building integrated PV component is considered. The EC-JRC Ispra has made experimental data available. Both linear and non-linear models are identified. It is shown that a description of the non-linear heat transfer is essential. The resulting model is a non-linear first order stochastic differential equation for the heat transfer of the PV component.

**General information**

State: Published
Organisations: Mathematical Statistics, Department of Informatics and Mathematical Modeling, Scientific Computing
Authors: Jimenez, M. (Ekstern), Madsen, H. (Intern), Bloem, J. (Ekstern), Dammann, B. (Intern)
Pages: 157-167
Publication date: 2008
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Journal: Energy and Buildings
A matlab framework for estimation of NLME models using stochastic differential equations

General information
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Organisations: Mathematical Statistics, Department of Informatics and Mathematical Modeling, Scientific Computing, Department of Chemical and Biochemical Engineering
Authors: Mortensen, S. B. (Intern), Klim, S. (Intern), Dammann, B. (Intern), Kristensen, N. R. (Intern), Madsen, H. (Intern), Overgaard, R. V. (Intern)
Pages: 623-642
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  Web of Science (2017): Indexed Yes
  BFI (2016): BFI-level 1
  Scopus rating (2016): CiteScore 1.8 SJR 0.696 SNIP 0.801
  BFI (2015): BFI-level 1
  Scopus rating (2015): SJR 0.709 SNIP 0.953 CiteScore 1.77
  BFI (2014): BFI-level 1
  Scopus rating (2014): SJR 0.696 SNIP 0.851 CiteScore 1.82
  BFI (2013): BFI-level 1
  Scopus rating (2013): SJR 0.561 SNIP 0.802 CiteScore 1.7
  ISI indexed (2013): ISI indexed yes
  BFI (2012): BFI-level 1
  Scopus rating (2012): SJR 0.974 SNIP 1.179 CiteScore 2.07
  ISI indexed (2012): ISI indexed yes
  BFI (2011): BFI-level 1
  Scopus rating (2011): SJR 0.955 SNIP 1.109 CiteScore 2.2
  ISI indexed (2011): ISI indexed yes
  Web of Science (2011): Indexed yes
  BFI (2010): BFI-level 1
  Scopus rating (2010): SJR 0.884 SNIP 0.79
  Web of Science (2010): Indexed yes
  BFI (2009): BFI-level 1
  Scopus rating (2009): SJR 1.072 SNIP 1.226
  BFI (2008): BFI-level 1
  Scopus rating (2008): SJR 1.024 SNIP 0.993
  Scopus rating (2007): SJR 0.579 SNIP 0.938
  Web of Science (2007): Indexed yes
  Scopus rating (2006): SJR 0.452 SNIP 0.758
  Scopus rating (2005): SJR 0.577 SNIP 1.109
3D Topology optimization of Stokes flow problems

The present talk is concerned with the application of topology optimization to creeping flow problems in 3D. This research is driven by the fact that topology optimization has proven very successful as a tool in academic and industrial design problems. Success stories are reported from such diverse fields as solid mechanics and optics and is due to the method's flexibility in the (rough) parametrization of the design, see [1] and the reference therein for an overview. Borrvall and Petersson [2] is the seminal reference for topology optimization in fluid flow problems. They considered design of energy efficient devices for 2D Stokes flow. Creeping flow problems are described by the Stokes equations which model very viscous fluids at macro scales or ordinary fluids at very small scales. The latter gives the motivation for topology optimization problems based on the Stokes equations being a model for the fluid behavior in a micro fluidic device. Such a device has finite size and a large degree of freedom for the design of geometry. Physically Stokes flow is an exotic inertia free flow. This, however, complicates mixing by passive devices. Passive devices, that is, devices without moving parts, are often of practical interest since they are easily manufacturable and maintenance free. In order to tackle such a challenging problem a robust method is needed which we approach by this contribution. The finite size of a micro fluidic device calls for 3D modelling of the equations, in particular when the design geometry is non-trivial as typically seen in topology design. The presentation elaborates on effects caused by 3D fluid modelling on the design. Numerical examples relevant for optimal micro fluidic mixer design are shown where the design is planar - compliant with micro fabrication techniques - and where the designs are 3D. Moreover, preliminary results show that a formulation of an optimization problem that maximizes mixing with a constraint on the pressure drop across the device gives promising results. To measure the mixing a step temperature profile is convected through the design and the resulting temperature profile at the outlet boundary is measured. The closer the outlet temperature profile is to the average inlet temperature the better mixing occurs in the device. For this problem the $P_e\gg1$ such that mixing by pure diffusion is not an option. Instead, the optimizer suggests a design that stretches the hot-cold interface, which is encouraging since "stretching and folding" is known to be key ingredients in efficient mixing. The modelling is performed using a finite element based solver, with analytically derived sensitivities that drives a gradient based optimization algorithm. Secondly, this talk also has its focus on the parallel implementation of the solution procedures, using OpenMP [3] on medium to large SMP computers. The necessary setup to achieve a good performance is described in detail. Further, issues such as scalability and portability are discussed. [1] M.P. Bendse and O. Sigmund. Topology optimization - theory, methods and applications, 2nd Edition, Springer 2003. [2] T. Borrvall, J. Petersson. Topology optimization of fluids in Stokes flow. Int. J. Num. Meth. Fluids, Vol. 41, 77-107, 2003. DOI:10.1002/fld.426 [3] The OpenMP Application Program Interface, http://www.openmp.org/

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Authors: Gersborg-Hansen, A. (Intern), Dammann, B. (Intern)
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Parallel solution of systems of linear equations generated by COMSOL 3.2 using the Sun Performance Library
This note investigates the use of the Sun Performance Library for parallel solution of a system of linear equations generated by COMSOL 3.2. In many engineering disciplines this is a computational bottleneck for large problems which are often met in research practice. Most researches are primarily concerned with developing a proper (COMSOL) model
rather than developing efficient linear algebra solvers which motivates this investigation of the efficiency of the coupling COMSOL + SPL. The technicalities of making such a coupling is described in detail along with a measure of the speedup for a testproblem run in 2D and 3D. Moreover this note quantifies the performance of COMSOL running on a Sparc ULTRA III processor. The study shows that for small problems such as debugging tasks, teaching exercises etc. the Sun computer is not competitive compared with a standard PC.

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Organisations: Solid Mechanics, Department of Mathematics, Scientific Computing, Department of Informatics and Mathematical Modeling, Technical University of Denmark
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**Topology optimization of mass distribution problems in Stokes flow**
We consider topology optimization of mass distribution problems in 2D and 3D Stokes flow with the aim of designing devices that meet target outflow rates. For the purpose of validation, the designs have been post processed using the image processing tools available in FEMLAB. In turn, this has enabled an evaluation of the design with a body fitted mesh in a standard analysis software relevant in engineering practice prior to design manufacturing. This work investigates the proper choice of a maximum penalization value during the optimization process that ensures that the target outflow rates are met in the validation test.

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Organisations: Solid Mechanics, Department of Mechanical Engineering, Department of Informatics and Mathematical Modeling, Uppsala University
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**An Ensemble of Vesicles in Two Dimensions**

**General information**
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Organisations: Department of Chemistry
Authors: Dammann, B. (Intern), Ipsen, J. H. (Intern)
Pages: 99-104
Publication date: 1997
Main Research Area: Technical/natural sciences

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Effect of Vacancies and Surfactants on the Dynamics of Ordering Processes in Multi-component Systems

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Organisations: Department of Chemistry
Authors: Gilhoej, H. (Ekstern), Laradji, M. (Ekstern), Dammann, B. (Intern), Jeppesen, C. (Ekstern), Mouritsen, O. G. (Intern), Toxvaerd, S. (Ekstern), Zuckermann, M. J. (Ekstern)
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Projects:

High Performance Computational Methods for Low-Noise Supercontinuum Lasers for Optical Coherence Tomography Systems
Department of Applied Mathematics and Computer Science
Period: 01/10/2015 → 01/01/2019
Number of participants: 4
Phd Student:
Mieritz, Andreas Falkenstrøm (Intern)
Supervisor:
Dammann, Bernd (Intern)
Engsig-Karup, Allan Peter (Intern)
Main Supervisor:
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Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Large-Scale Algorithms for Nano-Scale atomistic Simulations
Department of Applied Mathematics and Computer Science
Period: 01/01/2014 → 17/03/2014
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Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Scientific GPU Computing for Dynamical Optimization
Department of Applied Mathematics and Computer Science
Number of participants: 6
Phd Student: Gade-Nielsen, Nicolai Fog (Intern)
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Imnsland, Lars (Ekstern)
Knudsen, Jørgen K. H. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Scientific GPU Computing for PDE Solvers
Department of Informatics and Mathematical Modeling
Period: 01/05/2010 → 12/12/2013
Number of participants: 6
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Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Model studies of random surfaces, interfaces, and microemulsions
Department of Chemistry
Period: 01/12/1992 → 14/01/1997
Number of participants: 3
Phd Student: Dammann, Bernd (Intern)
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Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstipendium
Project: PhD

MEMPHYS -- Membrane and Statistical Physics Group
Principal Areas of Research: Statistical mechanics and thermodynamics, computer simulation techniques, phase transitions and critical phenomena, calorimetry, fluorescence spectroscopy, electron-spin resonance spectroscopy, biomembrane physics and chemistry, physical chemistry of surfaces and interfaces, soft matter, materials science. Phase transitions in solids and fluids, Monte Carlo methods, liquid crystals, overlayers on solid surfaces, domain--growth kinetics, grain growth and grain boundaries, interfaces and melting, solidification, fractals and pattern formation, transport
phenomena, ceramic high-temperature superconductors, polymers, random surfaces, lipid monolayers and bilayers, biological membranes, lipid membranes and liposomes incorporated with cholesterol, proteins, polypeptides, drugs and insecticides, phospholipase action. Visiting scientists in 1999: Prof. Martin J. Zuckermann (McGill) Prof. Robert Cantor Dr. James Polson (McGill) Dr. Thomas Heimburg (MPI, Goettingen) During the period the project has received financial support from the following sources: The Danish Natural Science Research Council The Danish Technical Science Research Council The Danish Medical Research Council Canadian Institute for Advanced Research Carlsberg Foundation The Danish Research Academy The Hasselblad Foundation

Department of Chemistry

Department of Chemistry

Period: 01/07/1985 → 31/12/2000
Number of participants: 18

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Project