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.

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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Scopus rating (2016): CiteScore 2.45 SJR 1.903 SNIP 1.682
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.932 SNIP 2.017 CiteScore 2.43
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.986 SNIP 2.165 CiteScore 2.72
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.74 SNIP 1.77 CiteScore 2.19
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.618 SNIP 1.582 CiteScore 2.23
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.65 SNIP 1.768
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.092 SNIP 1.883
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.668 SNIP 1.624
Scopus rating (2007): SJR 1.782 SNIP 1.897
Web of Science (2007): Indexed yes
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Scopus rating (2005): SJR 2.318 SNIP 2.19
Scopus rating (2004): SJR 1.958 SNIP 1.728
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.843 SNIP 2.032
Scopus rating (2001): SJR 2.423 SNIP 1.807
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.

Validation of vortex code viscous models using lidar wake measurements and CFD
The newly implemented vortex code Omnivor coupled to the aero-servo-elastic tool hawc2 is described in this paper. Vortex wake improvements by the implementation of viscous effects are considered. Different viscous models are
implemented and compared with each other. Turbulent flow fields with sheared inflow are used to compare the vortex code performance with CFD and lidar measurements. Laminar CFD computations are used to evaluate the performance of the viscous models. Consistent results between the vortex code and CFD tool are obtained up to three diameters downstream. The modelling of viscous boundaries appear more important than the modelling of viscosity in the wake. External turbulence and shear appear sufficient but their full potential flow modelling would be preferred.

General information
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Organisations: Department of Wind Energy, Aeroelastic Design, Department of Applied Mathematics and Computer Science
Authors: Branlard, E. (Intern), Machefaux, E. (Intern), Gaunaa, M. (Intern), Sørensen, H. H. B. (Intern), Troldborg, N. (Intern)
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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.

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Authors: Sørensen, H. H. B. (Intern)
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Main Research Area: Technical/natural sciences

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Scopus rating (2016): CiteScore 1.19 SJR 0.306 SNIP 0.841
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.339 SNIP 0.933 CiteScore 1.2
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.423 SNIP 1.241 CiteScore 1.36
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 0.386 SNIP 1.246 CiteScore 1.34
ISI indexed (2013): ISI indexed yes
Auto-tuning Dense Vector and Matrix-vector Operations for Fermi GPUs

In this paper, we consider the automatic performance tuning of dense vector and matrix-vector operations on GPUs. Such operations form the backbone of level 1 and level 2 routines in the Basic Linear Algebra Subroutines (BLAS) library and are therefore of great importance in many scientific applications. As examples, we develop single-precision CUDA kernels for the Euclidian norm (SNRM2) and the matrix-vector multiplication (SGEMV). The target hardware is the most recent Nvidia Tesla 20-series (Fermi architecture). We show that auto-tuning can be successfully applied to achieve high performance for dense vector and matrix-vector operations by appropriately utilizing the fine-grained parallelism of the GPU. Our tuned kernels display between 25-100% better performance than the current CUBLAS 3.2 library.

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Organisations: Department of Informatics and Mathematical Modeling, Scientific Computing
Authors: Sørensen, H. H. B. (Intern)
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Series: Lecture Notes in Computer Science
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Main Research Area: Technical/natural sciences
High-Performance Matrix-Vector Multiplication on the GPU

In this paper, we develop a high-performance GPU kernel for one of the most popular dense linear algebra operations, the matrix-vector multiplication. The target hardware is the most recent Nvidia Tesla 20-series (Fermi architecture), which is designed from the ground up for scientific computing. We show that it is essentially a matter of fully utilizing the fine-grained parallelism of the many-core GPU in order to achieve high-performance for dense matrix-vector multiplication. We show that auto-tuning can be successfully employed to the GPU kernel so that it performs well for all matrix shapes and sizes.

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Organisations: Department of Informatics and Mathematical Modeling, Scientific Computing
Authors: Sørensen, H. H. B. (Intern)
Pages: 377-386
Publication date: 2012

Accelerating Dense Linear Algebra on the GPU

GPUs have already become an integral part of high performance scientific computing, since they offer dedicated parallel hardware that can potentially accelerate the execution of many scientific applications. In this talk, I will consider the automatic performance acceleration of dense vector and matrix-vector operations on GPUs. Such operations form the backbone of level 1 and level 2 routines in the Basic Linear Algebra Subroutines (BLAS) library and are therefore of great importance in many scientific applications. The target hardware is the most recent NVIDIA Tesla 20-series (Fermi architecture). Most of the techniques I discuss for accelerating dense linear algebra are applicable to memory-bound GPU algorithms in general.

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Organisations: Department of Informatics and Mathematical Modeling, Scientific Computing
Authors: Sørensen, H. H. B. (Intern)
Publication date: 2011
Fast high-performance modeling tools for many-core architectures

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Publication date: 2011
Event: Poster session presented at Model Based Control, Technical University of Denmark.
Main Research Area: Technical/natural sciences
GPU, Scientific computing, model based control
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http://gpulab.imm.dtu.dk/
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Publication: Research › Poster – Annual report year: 2011

Tuning of BLAS level 1 and 2

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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling
Authors: Sørensen, H. H. B. (Intern)
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Development of Desktop Computing Applications and Engineering Tools on GPUs

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Authors: Sørensen, H. H. B. (Intern), Glimberg, S. L. (Intern), Hansen, T. J. (Intern), Frisvad, J. R. (Intern), Engsig-Karup, A. P. (Intern)
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Main Research Area: Technical/natural sciences
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Source: orbit
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Performance auto-tuning of rectangular matrix-vector multiplication: how to outperform CUBLAS

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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling
Authors: Sørensen, H. H. B. (Intern)
Publication date: 2010

Publication information
A hybrid method for the parallel computation of Green's functions
Quantum transport models for nanodevices using the non-equilibrium Green's function method require the repeated calculation of the block tridiagonal part of the Green's and lesser Green's function matrices. This problem is related to the calculation of the inverse of a sparse matrix. Because of the large number of times this calculation needs to be performed, this is computationally very expensive even on supercomputers. The classical approach is based on recurrence formulas which cannot be efficiently parallelized. This practically prevents the solution of large problems with hundreds of thousands of atoms. We propose new recurrences for a general class of sparse matrices to calculate Green's and lesser Green's function matrices which extend formulas derived by Takahashi and others. We show that these recurrences may lead to a dramatically reduced computational cost because they only require computing a small number of entries of the inverse matrix. Then, we propose a parallelization strategy for block tridiagonal matrices which involves a combination of Schur complement calculations and cyclic reduction. It achieves good scalability even on problems of modest size.

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Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, Stanford University, University of Copenhagen, Aarhus University
Authors: Petersen, D. E. (Ekstern), Li, S. (Ekstern), Stokbro, K. (Ekstern), Sørensen, H. H. B. (Intern), Hansen, P. C. (Intern), Skelboe, S. (Ekstern), Darve, E. (Ekstern)
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.166 SNIP 2.193 CiteScore 3.12
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.227 SNIP 2.45 CiteScore 3.3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.161 SNIP 2.052 CiteScore 2.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.06 SNIP 2.194 CiteScore 2.99
ISI indexed (2011): ISI indexed yes
Efficient wave-function matching approach for quantum transport calculations

The wave-function matching (WFM) technique has recently been developed for the calculation of electronic transport in quantum two-probe systems. In terms of efficiency it is comparable to the widely used Green's function approach. The WFM formalism presented so far requires the evaluation of all the propagating and evanescent bulk modes of the left and right electrodes in order to obtain the correct coupling between device and electrode regions. In this paper we will describe a modified WFM approach that allows for the exclusion of the vast majority of the evanescent modes in all parts of the calculation. This approach makes it feasible to apply iterative techniques to efficiently determine the few required bulk modes, which allows for a significant reduction of the computational expense of the WFM method. We illustrate the efficiency of the method on a carbon nanotube field-effect-transistor device displaying band-to-band tunneling and modeled within the semiempirical extended Hückel theory framework.
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.16
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.933 SNIP 0.94 CiteScore 2.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.667 SNIP 1.262 CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.785 SNIP 1.339 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.206 SNIP 1.394 CiteScore 3.57
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.382 SNIP 1.438 CiteScore 3.61
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.417 SNIP 1.451
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.109 SNIP 1.474
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.982 SNIP 1.524
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.923 SNIP 1.546
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.796 SNIP 1.56
Web of Science (2006): Indexed yes
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Scopus rating (2003): SJR 2.75 SNIP 1.536
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Scopus rating (2001): SJR 2.946 SNIP 1.635
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Computational aspects of electronic transport in nanoscale devices

This thesis is concerned with the modeling of electronic properties of nano-scale devices. In particular the computational aspects of calculating the transmission and current-voltage characteristics of Landauer-Büttiker two-probe systems are in focus. To begin with, the main existing methods are described in detail and benchmarked. These are the Green’s function method and the wave function matching method. The methods are subsequently combined in a hybrid scheme in order to benefit from a common formalism. The most time demanding stages of common electronic transport calculations are identified. For systems of more than about a hundred atoms, two specific tasks stand out; the evaluation of self-energy matrices to describe the coupling between the electrodes and the device, and the solution of the central region Schrödinger equation either by matrix inverse of by solving a system of linear equations. In this work the objective is to develop new efficient algorithms for these tasks in order to model nano-scale systems of larger size in the future. The starting point of the new methods is the combined formalism of the Green’s function and wave function matching methods. The first new algorithm described is for the calculation of the block tridiagonal matrix inverse of a block tridiagonal matrix in O(N) operations. This algorithm also leads to an optimal evaluation of the frequently used Caroli transmission formula. A modified wave function matching scheme is then developed which allows for a significant reduction in the cost of the self-energy matrix calculations when combined with an iterative eigensolver. Finally, such an iterative eigensolver is developed and implemented based of a shift-and-invert Krylov subspace approach. The method is applied to a selection of nano-scale systems and speed-ups of up to an order of magnitude are achieved.
Block Tridiagonal Matrix Inversion and Fast Transmission Calculations

**General information**

State: Published
Organisations: Scientific Computing, Department of Informatics and Mathematical Modeling, University of Copenhagen
Authors: Petersen, D. E. (Ekstern), Sørensen, H. H. B. (Intern), Hansen, P. C. (Intern), Skelboe, S. (Ekstern), Stokbro, K. (Ekstern)
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ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.161 SNIP 2.052 CiteScore 2.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.06 SNIP 2.194 CiteScore 2.99
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.185 SNIP 2.096
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.439 SNIP 2.219
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.247 SNIP 2.03
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.377 SNIP 2.379
Web of Science (2007): Indexed yes
Krylov subspace method for evaluating the self-energy matrices in electron transport calculations

We present a Krylov subspace method for evaluating the self-energy matrices used in the Green's function formulation of electron transport in nanoscale devices. A procedure based on the Arnoldi method is employed to obtain solutions of the quadratic eigenvalue problem associated with the infinite layered systems of the electrodes. One complex and two real shift-and-invert transformations are adopted to select interior eigenpairs with complex eigenvalues on or in the vicinity of the unit circle that correspond to the propagating and evanescent modes of most influence in electron transport calculations. Numerical tests within a density functional theory framework are provided to validate the accuracy and robustness of the proposed method, which in most cases is an order of magnitude faster than conventional methods.
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Scopus rating (2012): SJR 3.206 SNIP 1.394 CiteScore 3.57
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.382 SNIP 1.438 CiteScore 3.61
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.417 SNIP 1.451
Web of Science (2010): Indexed yes
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Scopus rating (2009): SJR 3.109 SNIP 1.474
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.982 SNIP 1.524
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.923 SNIP 1.546
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.796 SNIP 1.56
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.763 SNIP 1.607
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.742 SNIP 1.606
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.75 SNIP 1.536
Web of Science (2003): Indexed yes
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Scopus rating (2001): SJR 2.946 SNIP 1.635
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Scopus rating (2000): SJR 2.986 SNIP 1.631
Web of Science (2000): Indexed yes
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Projects:

Parallelization of vortex methods
Parallelization of vortex methods using GPU, openMP, MPI, AVX vectorization.

Department of Wind Energy
Aeroelastic Design

Department of Applied Mathematics and Computer Science
Period: 01/12/2013 → 01/04/2015
Number of participants: 2
Project participant:
Branlard, Emmanuel Simon Pierre (Intern)
Sørensen, Hans Henrik Brandenborg (Intern)

Scientific Computing and Parallel Algorithms in Computational Nano science

Department of Informatics and Mathematical Modeling
Period: 15/04/2005 → 02/07/2008
Number of participants: 7
Phd Student:
Sørensen, Hans Henrik Brandenborg (Intern)
Supervisor:
Skelboe, Stig (Ekstern)
Stokbro, Kurt (Intern)
Main Supervisor:
Hansen, Per Christian (Intern)
Examiner:
Sørensen, Mads Peter (Intern)
Darve, Eric (Ekstern)
Wacker, Andreas (Ekstern)

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