

Preface

The book is divided into four parts: Parallel Algorithms for Matrix Computations, Parallel Optimization, Management of Parallel Programming Models and Data, and Parallel Scientific Computing in Industrial Applications.

The first part of the book includes chapters on parallel matrix computations. The chapter by R. Granat, I. Jonsson, and B. Kågström, “RECSY and SCASY Library Software: Recursive Blocked and Parallel Algorithms for Sylvester-type Matrix Equations with Some Applications”, gives an overview of state-of-the-art high-performance computing (HPC) algorithms and software for solving various standard and generalized Sylvester-type matrix equations. Computer-aided control system design (CACSD) is a great source of applications for matrix equations including different eigenvalue and subspace problems and for condition estimation. The parallelization is invoked at two levels: *globally* in a distributed memory paradigm, and *locally* on shared memory or multicore nodes as part of the distributed memory environment.

In the chapter by A. Jakušev, R. Čiegis, I. Laukaitytė, and V. Trofimov, “Parallelization of Linear Algebra Algorithms Using ParSol Library of Mathematical Objects”, the mathematical objects library ParSol is described and evaluated. It is applied to implement the finite difference scheme to solve numerically a system of PDEs describing a nonlinear interaction of two counter-propagating laser waves.

The chapter by R.L. Muddle, J.W. Boyle, M.D. Mihajlović, and M. Heil, “The Development of an Object-Oriented Parallel Block Preconditioning Framework”, is devoted to the analysis of block preconditioners that are applicable to problems that have different types of degree of freedom. The authors discuss the development of an object-oriented parallel block preconditioning framework within OOMPH-LIB, the object-oriented, multi-physics, finite-element library, available as open-source software. The performance of this framework is demonstrated for problems from non-linear elasticity, fluid mechanics, and fluid-structure interaction.

In the chapter by C. Denis, R. Couturier, and F. Jézéquel, “A Sparse Linear System Solver Used in a Distributed and Heterogenous Grid Computing Environment”, the GREMLINS (GRid Efficient Linear Systems) solver of systems of linear

equations is developed. The algorithm is based on multisplitting techniques, and a new balancing algorithm is presented.

The chapter by A.G. Sunderland, “Parallel Diagonalization Performance on High-Performance Computers”, analyzes the performance of parallel eigensolvers from numerical libraries such as ScaLAPACK on the latest parallel architectures using data sets derived from large-scale scientific applications.

The book continues with the second part focused on parallel optimization. In the chapter by J. Žilinskas, “Parallel Global Optimization in Multidimensional Scaling”, global optimization methods are outlined, and global optimization algorithms for multidimensional scaling are reviewed with particular emphasis on parallel computing. Global optimization algorithms are computationally intensive, and solution time crucially depends on the dimensionality of a problem. Parallel computing enables solution of larger problems.

The chapter by K. Woodsend and J. Gondzio, “High-Performance Parallel Support Vector Machine Training”, shows how the training process of support vector machines can be reformulated to become suitable for high-performance parallel computing. Data is pre-processed in parallel to generate an approximate low-rank Cholesky decomposition. An optimization solver then exploits the problem’s structure to perform many linear algebra operations in parallel, with relatively low data transfer between processors, resulting in excellent parallel efficiency for very-large-scale problems.

The chapter by R. Paulavičius and J. Žilinskas, “Parallel Branch and Bound Algorithm with Combination of Lipschitz Bounds over Multidimensional Simplices for Multicore Computers”, presents parallelization of a branch and bound algorithm for global Lipschitz minimization with a combination of extreme (infinite and first) and Euclidean norms over a multidimensional simplex. OpenMP is used to implement the parallel version of the algorithm for multicore computers. The efficiency of the parallel algorithm is studied using an extensive set of multidimensional test functions for global optimization.

The chapter by S. Ivanikovas, E. Filatovas, and J. Žilinskas, “Experimental Investigation of Local Searches for Optimization of Grillage-Type Foundations”, presents a multistart approach for optimal pile placement in grillage-type foundations. Various algorithms for local optimization are applied, and their performance is experimentally investigated and compared. Parallel computations is used to speed up experimental investigation.

The third part of the book covers management issues of parallel programs and data. In the chapter by D. Henty and A. Gray, “Comparison of the UK National Supercomputer Services: HPCx and HECToR”, an overview of the two current UK national HPC services, HPCx and HECToR, are given. Such results are particularly interesting, as these two machines will now be operating together for some time and users have a choice as to which machine best suits their requirements. Results of extensive experiments are presented.

In the chapter by I.T. Todorov, I.J. Bush, and A.R. Porter, “DL_POLY_3 I/O: Analysis, Alternatives, and Future Strategies”, it is noted that an important bottleneck in the scalability and efficiency of any molecular dynamics software is the I/O

speed and reliability as data has to be dumped and stored for postmortem analysis. This becomes increasingly more important when simulations scale to many thousands of processors and system sizes increase to many millions of particles. This study outlines the problems associated with I/O when performing large classic MD runs and shows that it is necessary to use parallel I/O methods when studying large systems.

The chapter by M. Piotrowski, “Mixed Mode Programming on HPCx”, presents several benchmark codes based on iterative Jacobi relaxation algorithms: a pure MPI version and three mixed mode (MPI + OpenMP) versions. Their performance is studied and analyzed on mixed architecture – cluster of shared memory nodes. The results show that none of the mixed mode versions managed to outperform the pure MPI, mainly due to longer MPI point-to-point communication times.

The chapter by A. Grothey, J. Hogg, K. Woodsend, M. Colombo, and J. Gondzio, “A Structure Conveying Parallelizable Modeling Language for Mathematical Programming”, presents an idea of using a modeling language for the definition of mathematical programming problems with block constructs for description of structure that may make parallel model generation of large problems possible. The proposed structured modeling language is based on the popular modeling language AMPL and implemented as a pre-/postprocessor to AMPL. Solvers based on block linear algebra exploiting interior point methods and decomposition solvers can therefore directly exploit the structure of the problem.

The chapter by R. Smits, M. Kramer, B. Stappers, and A. Faulkner, “Computational Requirements for Pulsar Searches with the Square Kilometer Array”, is devoted to the analysis of computational requirements for beam forming and data analysis, assuming the SKA Design Studies’ design for the SKA, which consists of 15-meter dishes and an aperture array. It is shown that the maximum data rate from a pulsar survey using the 1-km core becomes about $2.7 \cdot 10^{13}$ bytes per second and requires a computation power of about $2.6 \cdot 10^{17}$ ops for a deep real-time analysis.

The final and largest part of the book covers applications of parallel computing. In the chapter by R. Čiegis, F. Gaspar, and C. Rodrigo, “Parallel Multiblock Multigrid Algorithms for Poroelastic Models”, the application of a parallel multigrid method for the two-dimensional poroelastic model is investigated. A domain is partitioned into structured blocks, and this geometrical structure is used to develop a parallel version of the multigrid algorithm. The convergence for different smoothers is investigated, and it is shown that the box alternating line Vanka-type smoother is robust and efficient.

The chapter by V. Starikovičius, R. Čiegis, O. Iliev, and Z. Lakdawala, “A Parallel Solver for the 3D Simulation of Flows Through Oil Filters”, presents a parallel solver for the 3D simulation of flows through oil filters. The Navier–Stokes–Brinkmann system of equations is used to describe the coupled laminar flow of incompressible isothermal oil through open cavities and cavities with filtering porous media. Two parallel algorithms are developed on the basis of the sequential numerical algorithm. The performance of implementations of both algorithms is studied on clusters of multicore computers.

The chapter by S. Eastwood, P. Tucker, and H. Xia, “High-Performance Computing in Jet Aerodynamics”, is devoted to the analysis of methods for reduction of the noise generated by the propulsive jet of an aircraft engine. The use of high-performance computing facilities is essential, allowing detailed flow studies to be carried out that help to disentangle the effects of numerics from flow physics. The scalability and efficiency of the presented parallel algorithms are investigated.

The chapter by G. Jankevičiūtė and R. Čiegis, “Parallel Numerical Solver for the Simulation of the Heat Conduction in Electrical Cables”, is devoted to the modeling of the heat conduction in electrical cables. Efficient parallel numerical algorithms are developed to simulate the heat transfer in cable bundles. They are implemented using MPI and targeted for distributed memory computers, including clusters of PCs.

The chapter by A. Deveikis, “Orthogonalization Procedure for Antisymmetrization of J -shell States”, presents an efficient procedure for construction of the anti-symmetric basis of j -shell states with isospin. The approach is based on an efficient algorithm for construction of the idempotent matrix eigenvectors, and it reduces to an orthogonalization procedure. The presented algorithm is much faster than the diagonalization routine `rs()` from the EISPACK library.

In the chapter by G.A. Siamas, X. Jiang, and L.C. Wrobel, “Parallel Direct Numerical Simulation of an Annular Gas–Liquid Two-Phase Jet with Swirl”, the flow characteristics of an annular swirling liquid jet in a gas medium is examined by direct solution of the compressible Navier–Stokes equations. A mathematical formulation is developed that is capable of representing the two-phase flow system while the volume of fluid method has been adapted to account for the gas compressibility. Fully 3D parallel direct numerical simulation (DNS) is performed utilizing 512 processors, and parallelization of the code was based on domain decomposition.

In the chapter by I. Laukaitytė, R. Čiegis, M. Lichtner, and M. Radziunas, “Parallel Numerical Algorithm for the Traveling Wave Model”, a parallel algorithm for the simulation of the dynamics of high-power semiconductor lasers is presented. The model equations describing the multisection broad-area semiconductor lasers are solved by the finite difference scheme constructed on staggered grids. The algorithm is implemented by using the ParSol tool of parallel linear algebra objects.

The chapter by X. Guo, M. Pinna, and A.V. Zvelindovsky, “Parallel Algorithm for Cell Dynamics Simulation of Soft Nano-Structured Matter”, presents a parallel algorithm for large-scale cell dynamics simulation. With the efficient strategy of domain decomposition and the fast method of neighboring points location, simulations of large-scale systems have been successfully performed.

The chapter by Ž. Dapkūnas and J. Kulys, “Docking and Molecular Dynamics Simulation of Complexes of High and Low Reactive Substrates with Peroxidases”, presents docking and parallel molecular dynamics simulations of two peroxidases (*ARP* and *HRP*) and two compounds (*LUM* and *IMP*). The study of docking simulations gives a clue to the reason of different reactivity of *LUM* and similar reactivity of *IMP* toward two peroxidases. In the case of *IMP*, $-\text{OH}$ group is near $\text{Fe}=\text{O}$ in both peroxidases, and hydrogen bond formation between $-\text{OH}$ and $\text{Fe}=\text{O}$ is

possible. In the case of *LUM*, N-H is near Fe=O in *ARP* and the hydrogen formation is possible, but it is farther in *HRP* and hydrogen bond with Fe=O is not formed.

The works were presented at the bilateral workshop of British and Lithuanian scientists “High Performance Scientific Computing” held in Druskininkai, Lithuania, 5–8 February 2008. The workshop was supported by the British Council through the INYS program.

The British Council’s International Networking for Young Scientists program (INYS) brings together young researchers from the UK and other countries to make new contacts and promote the creative exchange of ideas through short conferences. Mobility for young researchers facilitates the extended laboratory in which all researchers now operate: it is a powerful source of new ideas and a strong force for creativity. Through the INYS program, the British Council helps to develop high-quality collaborations in science and technology between the UK and other countries and shows the UK as a leading partner for achievement in world science, now and in the future. The INYS program is unique in that it brings together scientists in any priority research area and helps develop working relationships. It aims to encourage young researchers to be mobile and expand their knowledge. The INYS supported workshop “High Performance Scientific Computing” was organized by the University of Edinburgh, UK, and Vilnius Gediminas Technical University, Lithuania. The meeting was coordinated by Professor R. Čiegis and Dr. J. Žilinskas from Vilnius Gediminas Technical University and Dr. D. Henty from The University of Edinburgh. The homepage of the workshop is available at <http://techmat.vgtu.lt/~inga/inys2008/>.

Twenty-four talks were selected from thirty-two submissions from young UK and Lithuanian researchers. Professor B. Kågström from Umeå University, Sweden, and Dr. I. Todorov from Daresbury Laboratory, UK, gave invited lectures. Review lectures were also given by the coordinators of the workshop.

This book contains review papers and revised contributed papers presented at the workshop. All twenty-three papers have been reviewed. We are very thankful to the reviewers for their recommendations and comments.

We hope that this book will serve as a valuable reference document for the scientific community and will contribute to the future cooperation between the participants of the workshop.

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Parallel Scientific Computing and Optimization

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