Resch · Bönisch · Benkert · Furui · Seo · Bez (Eds.)
High Performance Computing on Vector Systems

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Editors

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Proceedings of the High Performance Computing Center
Stuttgart, March 2005

With 128 Figures, 81 in Color, and 31 Tables

Springer

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Front cover figure: Image of two dimensional magnetohydrodynamics simulation where current density has decayed from an Orszag-Tang vortex to form cross-like structures

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Library of Congress Control Number: 2006924568

Mathematics Subject Classification (2000): 65-06, 68U20, 65C20

ISBN-10 3-540-29124-5 Springer Berlin Heidelberg New York
ISBN-13 978-3-540-29124-4 Springer Berlin Heidelberg New York

Springer is a part of Springer Science+Business Media

springer.com

Printed in Germany

Typeset by the editors using a Springer TEX macro package
Production and data conversion: LE-TEX Jelonek, Schmidt & Vöckler GbR, Leipzig
Cover design: *design & production* GmbH, Heidelberg

Printed on acid-free paper 46/3142/YL - 5 4 3 2 1 0

Preface

In March 2005 about 40 scientists from Europe, Japan and the US came together the second time to discuss ways to achieve sustained performance on supercomputers in the range of Teraflops. The workshop held at the High Performance Computing Center Stuttgart (HLRS) was the second of this kind. The first one had been held in May 2004. At both workshops hardware and software issues were presented and applications were discussed that have the potential to scale and achieve a very high level of sustained performance.

The workshops are part of a collaboration formed to bring to life a concept that was developed in 2000 at HLRS and called the "Teraflop Workbench". The purpose of the collaboration into which HLRS and NEC entered in 2004 was to turn this concept into a real tool for scientists and engineers. Two main goals were set out by both partners:

- To show for a variety of applications from different fields that a sustained level of performance in the range of several Teraflops is possible.
- To show that different platforms (vector based systems, cluster systems) can be coupled to create a hybrid supercomputer system from which applications can harness an even higher level of sustained performance.

In 2004 both partners signed an agreement for the "Teraflop Workbench Project" that provides hardware and software resources worth about 6 MEuro (about 7 Million $ US) to users and in addition provides the funding for 6 scientists for 5 years. These scientists are working together with application developers and users to tune their applications. Furthermore, this working group looks into existing algorithms in order to identify bottlenecks with respect to modern architectures. Wherever necessary these algorithms are improved, optimized, or even new algorithms are developed.

The Teraflop Workbench Project is unique in three ways:

First, the project does not look at a specific architecture. The partners have accepted that there is not a single architecture that is able to provide an outstanding price/performance ratio. Therefore, the Teraflop Workbench is a hybrid architecture. It is mainly composed of three hardware components

- A large vector supercomputer system. The NEC SX-8/576M72 has 72 nodes and 576 vector processors. Each processor has a peak performance of 22 GFLOP/s which results in a peak overall performance of the system of 12.67 TFLOP/s. The sustained performance is about 9 TFLOP/s for Linpack and about 3–6 TFLOP/s for applications. Some of the results are shown in this book. The system is equipped with 9.2 TB of main memory and hence allows to run very large simulation cases.
- A large cluster of PCs. The 200 node system comes with 2 processors per node and a total peak performance of about 2.4 TFLOP/s. The system is perfectly suitable for a variety of applications in physics and chemistry.
- Two shared memory front end systems for offloading development work but also for providing large shared memory for pre-processing jobs. The two systems are equipped with 32 Itanium (Madison) processors and provide a peak performance of about 0.19 TFLOP/s each. They come with 0.256 TB and 0.512 TB of shared memory respectively which should be large enough even for larger pre-processing jobs. They are furthermore used for applications that rely on large shared memory such as some of the ISV codes used in automobile industry.

Second, the collaboration takes an unconventional approach towards data management. While mostly the focus is on management of data the Teraflop Workbench Project considers data to be the central issue in the whole simulation workflow. Hence, a file system is at the core of the whole workbench. All three hardware architectures connect directly to this file system. Ideally the user only once has to transfer basic input information from his desk to the workbench. After that data reside inside the central file system and are only modified either for pre-processing, simulation or visualization.

Third, the Teraflop Workbench Project does not look at a single application or a small number of well defined problems. Very often extreme fine-tuning is employed to achieve some level of performance for a single application. This is reasonable wherever a single application can be found that is of overwhelming importance for a centre. For a general purpose supercomputing centre like the HLRS this is not possible. The Teraflop Workbench Project therefore sets out to tackle as many fields and as many applications as possible. This is also reflected in the contents of this book. The reader will find a variety of application fields that range from astrophysics to industrial combustion processes and from molecular dynamics to turbulent flows. In total the project supports about 20 projects of which most are presented here.

In the following the book presents key contributions about architectures and software but many more papers were collected that describe how applications can benefit from the architecture of the Teraflop Workbench Project. Typically sustained performance levels are given although the algorithms and the concrete problems of every field still are at the core of each contribution.

As an opening paper NEC provides a scientifically very interesting technical contribution about the most recent system of the NEC SX family the SX-8. All of the projects described in this book either use the SX-8 system of HLRS as the simulation facility or provide comparisons of applications on the SX-8 and other systems. The paper can hence be seen as an introduction of the underlying hardware that is used by various projects.

In their paper about vector processors and micro processors Peter Lammers from the HLRS, Gerhard Wellein, Thomas Zeiser, and Georg Hager from the Computing Centre, and Michael Breuer from the chair for fluid mechanics at the University of Erlangen, Germany, look at two competing basic processor architectures from an application point of view. The authors compare the NEC SX-8 system with the SGI Altix architecture. The comparison is not only about the processor but involves the overall architecture. Results are presented for two applications that are developed at the department of fluid mechanics. One is a finite volume based direct numerical simulation code while the other is based on the Lattice Boltzmann method and is again used in direct numerical simulation. Both codes rely heavily on memory bandwidth and as expected the vector system provides superior performance. Two points are, however, very notable. First, the absolute performance for both codes is rather high with one of them reaching even 6 TFLOP/s. Second, the performance advantage of the vector based system has to be put into relation with the costs which gives an interesting result.

A similar but more extensive comparison of architectures can be found in the next contribution. Jonathan Carter and Leonid Oliker from Lawrence Berkeley National Laboratory, USA have done a lot of work in the field of architecture evaluation. In their paper they describe recent results on the evaluation of modern parallel vector architectures like the Cray X1, the Earth Simulator and the NEC SX-8 and compare them to state of the art microprocessors like the Intel Itanium the AMD Opteron and the IBM Power processor. For their simulation of magnetohydrodynamics they also use a Lattice Boltzmann based method. Again it is not surprising that vector systems outperform microprocessors in single processor performance. What is striking is the large difference which combined with cost arguments changes the picture dramatically.

Together these first three papers give an impression of what the situation in supercomputing currently is with respect to hardware architectures and with respect to the level of performance that can be expected. What follows are three contributions that discuss general issues in simulation – one is about sparse matrix treatment, a second is about first-principles simulation while the third tackles the problem of transition and turbulence in wall-bounded shear flow. All three problems are of extreme importance for simulation and require a huge level of performance.

Toshiyuki Imamura from the University of Electro-Communications in Tokyo, Susumu Yamada from the Japan Atomic Energy Research Institute (JAERI) in Tokyo, and Masahiko Machida from Core Research for Evolutional Science and Technology (CREST) in Saitama, Japan tackle the problem of condensation of fermions to investigate the possibility of special physical properties like superfluidity. They employ a trapped Hubbard model and end up with a large sparse matrix. By introducing a new preconditioned conjugate gradient method they are able to improve the performance over traditional Lanzcos algorithms by a factor of 1.5. In turn they are able to achieve a sustained performance of 16.14 TFLOP/s on the earth simulator solving a 120-billion-dimensional matrix.

In a very interesting and well founded paper Yoshiyuki Miyamoto from the Fundamental and Environmental research Laboratories of NEC Corporation describes simulations of ultra-fast phenomena in carbon nanotubes. The author employs a new approach based on the time-dependent densitiy functional theory (TDDFT), where the real-time propagation of the Kohn-Sham wave functions of electrons are treated by integrating the time-evolution parameter. This technique is combined with a classical molecular dynamics simulation in order to make visible very fast phenomena in condensed matters.

With Philipp Schlatter, Steffen Stolz, and Leonhard Kleiser from the ETH Zürich, Switzerland we again change subject and focus even more on the application side. The authors give an overview of numerical simulation of transition and turbulence in wall-bounded shear flows. This is one of the most challenging problems for simulation requiring a level of performance that is currently beyond our reach. The authors describe the state of the art in the field and discuss Large Eddy Simulation (LES) and Subgrid-Scale models (SGS) and their usage for direct numerical simulation.

The following papers present projects tackled as part of the Teraflop Workbench Project.

Malte Neumann and Ekkehard Ramm from the Institute of Structural Mechanics in Stuttgart, Germany, Ulrich Küttler and Wolfgang A. Wall from the Chair for Computational Mechanics in Munich, Germany, and Sunil Reddy Tiyyagura from the HLRS present findings for the computational efficiency of parallel unstructured finite element simulations. The paper tackles some of the problems that come with unstructured meshes. An optimized method for the finite element integration is presented. It is interesting to see that the authors have employed methods to increase the performance of the code on vector systems and can show that also microprocessor architectures can benefit from these optimizations. This supports previous findings that cache optimized programming and vector processor optimized programming very often lead to similar results.

The role of supercomputing in industrial combustion modeling is described in an industrial paper by Natalia-Currle Linde, Uwe Küster, Michael Resch, and Benedetto Risio which is a collaboration of HLRS and RECOM Services – a small enterprise at Stuttgart, Germany. The quality of simulation in the optimum design and steering of high performance furnaces of power plants has reached a level at which it can compete with physical experiments. Such simulations require not only an extremely high level of performance but also the ability to do parameter studies. In order to relieve the user from the burden of submitting a set of jobs the authors have developed a framework that supports the user. The Science Experimental Grid Laboratory (SEGL) allows to define complex workflows which can be executed in a Grid environment like the Teraflop Workbench. It furthermore supports the dynamic generation of parameter sets which is crucial for optimization.

Helicopter simulations are presented by Thorsten Schwarz, Walid Khier, and Jochen Raddatz from the Institute of Aerodynamics and Flow Technology of the German Aerospace Center (DLR) at Braunschweig, Germany. The authors use a structured Reynolds-averaged Navier-Stokes solver to compute the flow field around a complete helicopter. Performance results are given both for the NEC SX-6 and the new NEC SX-8 architecture.

Hybrid simulations of aeroacoustics are described by Qinyin Zhang, Phong Bui, Wageeh A. El-Askary, Matthias Meinke, and Wolfgang Schröder from the Department of Aerodynamics of the RWTH Aachen, Germany. Aeroacoustics is a field that is getting important for aerospace industries. Modern engines of airplanes are so silent that the noise created from aeroacoustic turbulences has often become a more critical source of sound. The simulation of such phenomena is split into two parts. In a first part the acoustic source regions are resolved using a large eddy simulation method. In the second step the acoustic field is computed on a coarser grid. First results of the coupled approach are presented for relatively simple geometries. Simulations are carried out on 10 processors but will require much higher performance for more complex problems.

Albert Ruprecht from the Institute of Fluid Mechanics and Hydraulic Machinery of the University of Stuttgart, Germany, shows simulation of a water turbine. The optimization of these turbines is crucial to extract the potential of water power plants when producing electricity. The author uses a parallel Navier-Stokes solver and provides some interesting results.

A topic that is unusual for vector architectures is atomistic simulation. Franz Gähler from the Institute of Theoretical and Applied Sciences of the University of Stuttgart, Germany, and Katharina Benkert from the HLRS describe a comparison of an ab initio code and a classical molecular dynamics code for different hardware architectures. It turns out that the ab initio simulations perform excellently on vector machines. Again it is, however, worth to look at the ratio of performance on vector and microprocessor systems. The molecular dynamics code in its existing version is better suited for large clusters of microprocessor systems. In their contribution the authors describe how they want to improve the code to increase the performance also for vector based systems.

Martin Bernreuther from the Institute of Parallel and Distributed Systems and Jadran Vrabec from the Institute of Thermodynamics and Thermal Process Engineering of the University of Stuttgart, Germany, in their paper tackle the problem of molecular simulation of fluids with short range potentials. The authors develop a simulation framework for molecular dynamics simulations that specifically targets the field of thermodynamics and process engineering. The concept of the framework is described in detail together with algorithmic and parallelization aspects. Some first results for a smaller cluster are shown.

An unusual application for vector based systems is astrophysics. Konstantinos Kifonidis, Robert Buras, Andreas Marek, and Thomas Janka from the Max-Planck-Institute for Astrophysics at Garching, Germany, give an overview of the problems and the current status of supernova modeling. Furthermore they describe their own code development with a focus on the aspects of neutrino transports. First benchmark results are reported for an SGI Altix system as well as for the NEC SX-8. The performance results are interesting but so far only a small number of processors is used.

With the next paper we return to classical computational fluid dynamics. Kamen N. Beronov, Franz Durst, and Nagihan Özyilmaz from the Chair for Fluid Mechanics of the University of Erlangen, Germany, together with Peter Lammers from HLRS present a study on wall-bounded flows. The authors first present the state of the art in the field and compare different approaches. They then argue for a Lattice Boltzmann approach providing also first performance results.

A further and last example in the same field is described in the paper of Andreas Babucke, Jens Linn, Markus Kloker, and Ulrich Rist from the Institute of Aerodynamics and Gasdynamics of the University of Stuttgart, Germany. A new code for direct numerical simulations solving the complete compressible 3-D Navier-Stokes equations is presented. For the parallelization a hybrid approach is chosen reflecting the hybrid nature of clusters of shared memory machines like the NEC SX-8 but also multiprocessor node clusters. First performance measurements show a sustained performance of about 60% on 40 processors of the SX-8. Further improvements of scalability have to be expected.

The papers presented in this book provide on the one hand a state of the art in hardware architecture and performance benchmarking. They furthermore lay out the wide range of fields in which sustained performance can be achieved if appropriate algorithms and excellent programming skills are put together. As the first of books in this series to describe the Teraflop Workbench Project the collection provides a lot of papers presenting new approaches and strategies to achieve high sustained performance. In the next volume we will see many more results and further improvements.

Stuttgart, January 2006

M. Resch
W. Bez

Contents

Future Architectures in Supercomputing

Performance and Applications on Vector Systems

Applications I: Finite Element Method

Applications II: Fluid Dynamics

Applications III: Particle Methods

Applications IV: Turbulence Simulation

List of Contributors