

FRAUNHOFER INSTITUTE FOR ALGORITHMS AND SCIENTIFIC COMPUTING SCAI

SHORTER TIME TO SOLUTION WITH SAMG



aux_matrix=>wrk(l:naux); list=>wrk(naux+1:naux+nlist) ...
y perform coarsening, level by level, for MPI: organize overlap for finest level matrix
create_levels: do mg_level=2, mg_max_level
create_levels: do mg_level=2, mg_max_level
call samg_driver_strong(mg_level-1, SAMG_MPI_COMM, SAMG_NUM_THREADS ...)]
y MPI collective error handling, terminate the samg setup ?
call samg_mpi err handling(SAMG_MPI_COMM_samg_erroade)

NUMERICAL SIMULATION IN INDUSTRY

The role and importance of numerical simulation for industry is immense. It is continually increasing, as computing-based simulation approaches enter an increasing number of industrial sectors, and become mission-critical components in industrial processes.

A major bottleneck: the linear solver

As the complexity of industrial numerical modelling increases – in line with the need for increased resolution of physical phenomena to meet customer expectations – there is a corresponding growth in the size and complexity of the linear sparse matrix systems that need to be solved as a core function of most simulation software. Beyond a certain size, however, classical solvers are inappropriate for handling such systems as their efficiency degenerates with increasing model size.

The remedy offered by Fraunhofer SCAI

A drastic improvement of the solver performance is a prerequisite for the practicability of numerical simulation for complex phenomena. This requires the development of highly efficient linear solvers and/or the efficient exploitation of modern parallel hardware. Fraunhofer SCAI takes care of both aspects by combining optimal numerical algorithms with the potential of parallel systems.





FRAUNHOFER'S SOLVER LIBRARY SAMG

Fraunhofer SCAI has developed a state-of-the-art solver library, SAMG, with a focus on industrial use. SAMG is kept at the forefront of technology through continuous further development. In contrast to classical linear solvers, SAMG solvers are optimal in the sense that the computational time of using SAMG depends only linearly on the number of unknowns. Depending on the application and problem size, SAMG solvers reduce the computational time by 1-2 orders of magnitude or even more, compared with standard linear solvers.

Why is SAMG so efficient?

SAMG is based on highly efficient algebraic multigrid (AMG) technology: Instead of only operating on a given linear system of equations, SAMG combines numerical information from a series of increasingly coarse systems of equations in order to solve the given linear system much more rapidly. The necessary hierarchy is constructed automatically and the hierarchical process is completely invisible to the SAMG user. The algebraic multigrid technology was originally developed jointly by scientists from Fraunhofer and the University of Colorado Boulder, USA.

1 Example of an algebraically constructed hierarchy of levels

2 Principle of data transfer from coarse to fine levels (interpolation)

3 Schematic view of an AMG process





SAMG, A MATURE SOLVER LIBARY

SAMG can easily be incorporated into existing numerical simulation software. The features which make SAMG attractive are:

- **Generality**: Apart from certain requirements on matrix properties, SAMG is largely independent of the nature of a given linear problem.
- Efficiency: SAMG is fast and parallelized (for both cluster and multicore computers).
- **Robustness**: For a given type of application, SAMG is not sensitive to variations in matrix properties.
- Portability: SAMG supports all major serial and parallel platforms.
- **State-of-the-art**: SAMG is continuously further developed to include all industrially relevant new algorithms.

Parallel computing

The standard SAMG library is optimized for serial and multi-core computers. For compute clusters, two different distributed computing versions of the library are available, SAMGp and XSAMG. In this brochure, for simplicity, we generally refer to SAMG as a shortcut for the suite of libraries, serial as well as parallel.

We offer

- licensing of the SAMG solver library (serial and parallel)
- tailoring of SAMG to specific requirements and applications
- consulting and support for numerical solvers
- performance improvement of industrial simulators

Our target groups

Our software can be exploited by partners and customers involved in simulation software development in various application areas, including

- fluid mechanics
- oil reservoir simulation
- heat conduction
- groundwater simulationelectrochemical process simulation
- structural mechanicsfoundry technology
- circuit simulation



Algebraic Multigrid Methods for Systems

Serial and parallel (OpenMP)



Cluster parallel (Hybrid MPI/OpenMP)



Auto-parallel SAMG for Clusters

Autoparallel (Hybrid MPI/OpenMP)





XSAMG – AUTOPARALLEL SAMG FOR CLUSTERS

While SAMG supports serial and multi-core computations, SAMGp supports distributed computing on clusters of multi-core compute nodes. In contrast to SAMGp, the new XSAMG library exploits the parallelism offered by multiple nodes of a compute cluster by automatically distributing data across different nodes.

Because of this automatism, the calling user program itself does not have to be prepared for distributed computing at all. That is, XSAMG lifts a user's single-node application beyond the performance limits of a single node by making the linear solver phase "cluster aware". In this way, solution times are drastically reduced without the need for a user to be concerned about the complicated underlying parallel cluster software infrastructure. XSAMG offers the standard way of exploiting multiple cores ("multi-threading"), plus the use of multiple compute cluster nodes.

CRIEPI – Central Research Institute of Electric Power Industry

CRIEPI is doing research and development related to energy and the environment for the solution of various problems in electricity utilities and society. SAMG has been used for many years in the Fluid Dynamics Sector of the Civil Engineering Research Laboratory. Only recently, XSAMG has been introduced to speed up fluid dynamics simulation by means of the autoparallelism of XSAMG. In particular, aerodynamic features of huge ground-mounted photovoltaic panels are computed by CRIEPI's serial in-house LES simulation code, powered by XSAMG.

Congratulations on the success of XSAMG. It was amazing that our serial flow analysis code was easily powered by MPI-parallel matrix solutions, thanks to the newly developed XSAMG.

Yuzuru Eguchi and Takahiro Murakami – Civil Engineering Research Laboratory, CRIEPI, Abiko, Japan



1 Numerical grid for photovoltaic panels (over 10,000,000 elements)

2 Velocity profile on horizontal plane for oblique wind



SIMULATION OF CASTING AND INJECTION MOLDING

Since its foundation in 1988, MAGMA GmbH has been a pacesetter in defining new directions for the foundry industry. MAGMA has developed MAGMASOFT[®], a comprehensive simulation tool used for the production of castings worldwide. Its simulation capabilities provide users with a better understanding of key processes such as mold filling, solidification, mechanical properties, thermal stresses and distortion.

Challenge

Customers of MAGMA want to run bigger and more accurate simulations, meaning finer meshes and, as a result, larger systems of equations. Hence, MAGMASOFT needs robust and scalable solvers. Ideally, the execution time of the solver should be only proportional to the problem size, a requirement which is not met by classical solvers. SAMG was identified as potentially being the ideal solver for MAGMASOFT.

Benefit for Magma and their customers

MAGMA decided to employ SAMG to accelerate their simulators. Customers now achieve acceleration factors between 2 and 10 compared to standard solvers. Hence, MAGMA's customers can run more simulations per day, facilitating an improved optimization of their castings and casting processes.

1 Predicted sand density distribution during production of an organically bound sand core for use in the casting of a turbocharger housing

2 Distortion of a structural die-cast aluminium component after ejection from the die. Colors indicate the deviation from the desired component geometry

We are pleased with the cooperation with the Fraunhofer Institute SCAI, since they have experts who understand our needs. Working with SCAI is a win-win situation. SCAI helps us tackle our challenges and we help SCAI to improve their solver technology.

Marc Schneider – MAGMA GmbH, Aachen, Germany







MODELING IN OIL RESERVOIR SIMULATION

The primary purpose of reservoir simulation is the accurate description of multiphase flow in porous, highly heterogeneous and fractured media with very complex geometries. The numerical difficulties of these systems may be subject to dramatic changes due to abrupt flow variations induced by the high-heterogeneity and complex well operations during the simulation process.

The numerical challenge

Reservoir models have been growing in complexity (regarding geometry, discretization and physical models including, for instance, thermal and chemical influences in addition to geomechanics), heterogeneity, and size, causing these systems to become increasingly difficult to solve. Using classical linear methods to solve the underlying linear equations is no longer practical.

1 Oil platform

2 Exemplary illustration of different wells and surface facilities of an off-shore field

3 Visualization of streamline-based simulation of a reservoir: Colors indicate which regions are affected by different well bores





STREAMLINE-BASED APPROACH

With its streamline-based reservoir flow simulator, 3DSL, Streamsim Technolgies has set the industrial standard in streamline-based simulation. 3DSL provides insight into how geology, fluid properties, and wells interact to affect recovery.

We have been using SAMG as primary solver in our simulator for many years now. The extraordinary speed of our software is – to a large extent – due to the high efficiency of SAMG. We highly appreciate the long-lasting and fruitful cooperation with the SAMG group.



Marco Thiele - Streamsim Technologies Inc., San Francisco, USA

FULLY IMPLICIT APPROACH

Computer Modelling Group (CMG) is one of the leading providers of commercial reservoir simulators for fully implicit modeling featuring, in particular, black oil, compositional and thermal simulations. Due to the complexity of the models considered at CMG, SAMG had to be extended and, in particular, special model properties had to be exploited. Only then could the potential of SAMG be fully exploited.

Fraunhofer has developed special approaches for robust and efficient application of SAMG in our commercial simulators. We are very happy with the performance and are looking forward to incorporating SAMG as a work horse into our products.

Dave Collins - CMG Ltd., Calgary, Canada



1 Vertical permeability of an irregularly shaped reservoir for an oil, water and gas production simulation



NUMERICAL SIMULATION AT VOLKSWAGEN

Design processes at Volkswagen are strongly supported by numerical simulation. In particular, Computational Fluid Dynamics (CFD) is used to simulate flow-related aspects in order to reduce the design cycle time for developing new car models as well as to improve the quality of new designs. Heat conduction and radiation is another area where Volkswagen makes heavy use of numerical simulation.

Improving performance

In order to ensure highest accuracy of simulation, today's model sizes have become so large that the computational time for individual simulations – if run on standard computers with standard numerical solvers – is no longer acceptable.

To make realistic simulations at Volkswagen practicable, modern parallel computers are employed with thousands of processors running in parallel. In addition, Volkswagen uses the highly efficient solver modules from the SAMG library. Both software and hardware scalability complement each other resulting in the highly efficient performance of simulations at VW. 1 Numerical flow simulation around a complete vehicle

The application of the SAMG technology has crucially helped us to make our CFD simulations scalable for large parallel clusters In heat conduction SAMG enabled certain simulations which were virtually impossible before We rely on the robustness and efficiency of Fraunhofer's SAMG software in improving the performance of our simulation processes.

Octavian Frederich

Eric Pattyn

Jan Blickwede

VW AG, Wolfsburg, Germany



STRUCTURAL INTEGRITY OF ELECTRICAL DEVICES

Fujitsu Laboratories of Europe (FLE) is the European arm of the Fujitsu Laboratories Ltd. FLE is researching the use of the FrontISTR solver to simulate substrate problems with the aim of analyzing the structural integrity of electrical devices (e.g., printed wiring boards, PWBs).

Challenge

FrontISTR is a state-of-the-art FEM-based structural analysis code for industrial CAD models. Most of FLE's models are huge (40 million elements or more) and have a geometry which is thin, long or flat. Typically, conventional solvers like ILU-preconditioned CG are extremely inefficient. FLE was researching ways to drastically accelerate the FrontISTR simulator.

Evaluating SAMG for substrate problems

The joint evaluation of SAMG has shown that the straightforward application of standard AMG is not going to be efficient. However, after having introduced some new, application-specific extensions, SAMG became orders of magnitude faster than conventional solvers.

1 Different copper layers with different wiring patterns

Our applications are very large, 40 million elements or more for realistic PWB simulations. Our joint research has shown SAMG to have the potential to reduce simulation times from days to minutes. This is a breakthrough result for us since it is a pre-requisite for using such simulation software on a daily basis.



Peter Chow - Fujitsu Laboratories of Europe, London, UK



ELECTROCHEMICAL PROCESSES

Electrochemical processes play an increasingly important role in the production of industrial parts: electronics (plating on wafers and PCBs), aeronautics (turbine blades with micro-cooling channels, molds), medicine (needles, implants), automotive design and production (trim components, engine parts, injection systems), etc. On the other side of the spectrum is corrosion, also an electrochemical process – be it an undesired one – which especially impacts the oil & gas and offshore industry.

Leading simulation software

Elsyca provides world-leading CAE simulation software and engineering services for corrosion engineering and corrosion resistant design, cathodic protection and AC mitigation, as well as for surface finishing and electro-chemical manufacturing. By combining computer simulation and practical engineering skills, Elsyca is capable of modeling, simulating and optimizing the complete range of electrochemical processes.

1 Chrome wheel

2 Finite element mesh for simulating electro-chemical chromium plating of wheels

3 Mesh for simulating electro-chemical machining of a diesel injection system



We have been using SAMG for many years now and are very satisfied. For classical electrochemical models, SAMG reduces the total simulation time by factors of 2.5 - 5. SAMG is capable of solving the most complex simulations such as the electrochemical machining of diesel injection systems.



Leslie Bortels - Elsyca, Wijgmaal, Belgium



GROUNDWATER SIMULATION

FEFLOW is a leading software package for the finite-element modeling of fluid flow, mass and heat transport processes in porous and fractured media. It is used by consulting firms, research institutes, universities and government organizations all over the world. FEFLOW is developed by DHI-WASY GmbH.

Applications

FEFLOW has been using SAMG as solver for many years now. SAMG has been optimized for the special requirements of FEFLOW, in particular, relating to the efficient treatment of transient simulations. The scope of applications ranges from simple local-scale to very complex, largescale simulations. Quite recently, certain FEFLOW applications reached a model size for which SAMG was the enabling component. 1 Simulation of a borehole heat exchanger (BHE) array

2 Modeling underground storage of liquidized gas in cave

3 Nuclear waste repository simulation in a complex geologic formation

4 Fingering convection due to sinking of heavy constituent



We are very happy with the newest release of SAMG. Recently we simulated huge fluid flow and transport models with up to 30 million variables. Without SAMG as our solver engine, it would have been impossible to solve such problems in a practicable time.

Hans-Jörg Diersch and Fabien Cornaton – DHI-WASY Berlin, Germany



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Sale of licenses



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EDITORIAL NOTES

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DEDICATION TO THE FUTURE

The Fraunhofer Institute for Algorithms and Scientific Computing SCAI conducts research in the field of computer simulations for product and process development, and is a prominent corporate partner in the industrial and science sectors.

SCAI designs and optimizes industrial applications, implements custom solutions for production and logistics, and offers calculations on high-performance computers. Our services are based on industrial engineering, combined with state-of-the-art methods from applied mathematics and information technology.

SCAI especially excels in coupled simulation of different physical disciplines, and develops software for visualization of calculation results. In bioinformatics, SCAI offers workflow-oriented and integrated IT infrastructures for information extraction. SCAI has accumulated specialized expertise in both structured storing and administration of data and research results, and in the organization of projects.

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