

## **Final Project Report**

DOE grant DE-FC02-01ER25476: Terascale Optimal PDE Simulations (TOPS)  
Old Dominion University (2001 to 2004)  
PIs: David E. Keyes and Alex Pothen

Scientific Discovery through Advanced Computing (SciDAC) is a five year program launched in 2001 by the Department of Energy (DOE) in order to develop the scientific computing software and hardware infrastructure required to advance DOE research programs. The Terascale Optimal PDE Solvers (TOPS) component of SciDAC is an Integrated Software Infrastructure Center (ISIC) that focuses on developing optimal or near-optimal schemes for partial differential equations (PDE) simulations and closely related tasks.

TOPS started officially in October 2001 and for the first three years Old Dominion University (ODU) was lead institution. In October 2004 Columbia University (CU) replaced ODU as the lead institution.

The TOPS members from ODU focused on various aspects of the linear and nonlinear solver infrastructure required by the PDE simulation codes, working directly with SciDAC teams from the Fusion Energy Sciences (FES) program. Specifically, we collaborated with the Center for Extended Magnetohydrodynamic Modeling (CEMM) and with the Center for Magnetic Reconnection Studies (CMRS).

The goal of the FES program is to develop improved physics models of various components of a fusion based power device, the core of this research being the simulation of magnetohydrodynamics (MHD). The simulation of MHD is particularly challenging because of its multiscale nature.

MHD represents the dynamics of a conducting fluid (plasma) and is governed by a system of partial differential equations that include the Navier-Stokes equations, which describe the fluid dynamics, Maxwell's equations, which describe the electric and magnetic fields, and Ohm's law, which couples the Navier-Stokes and Maxwell equations.

An MHD simulation code usually studies the time evolution of primitive variables such as the velocity or the magnetic field, the time dependent nature of the simulation opening the possibility for various approaches: explicit, semi-implicit, and implicit. At present many MHD simulation codes are implemented using explicit or semi-implicit approaches, which basically involve only linear solves within each time step. The goal of TOPS was to introduce more robust implicit solutions. Due to the nonlinear nature of the MHD equations the implicit approach requires nonlinear solves within each time step, the linear solves becoming iterations within the nonlinear solves. This added level of complexity comes with

more stability, a major advantage of a fully implicit solution being the possibility to take significantly larger steps during the time integration.

As part of our collaboration with CEMM we worked directly with a team of fusion physicists from the Princeton Plasma Physics Laboratory (PPPL), led by Steve Jardin. Their MHD simulation code, called M3D, is semi-implicit, therefore it requires linear solves but no nonlinear solves. M3D has various Poisson-like linear operators that need to be solved at every time step. At the beginning of our collaboration the code was already implemented on top of PETSc, a major solver package in TOPS.

The M3D code was based on a domain decomposition preconditioned Krylov iteration. Due to the lack of symmetry the Krylov iteration method used was GMRES. The domain decomposition preconditioning was one level additive Schwarz with ILU on subdomains. While our long term goal is to replace their semi-implicit approach by a fully implicit one, we contributed with improvements to their current semi-implicit code. Among these was the use of multilevel preconditioning, which provides optimal scaling. This was done through the multigrid preconditioner available in Hypre, another major solver package available in TOPS, which interfaces with PETSc. At the same time we also provided them direct solver functionality for their linear solves (as opposed to the iterative Krylov approach). Although direct solvers don't scale well, they may be required for more accurate solutions in some regimes. The direct solver functionality came through SuperLU, also a major solver package in TOPS and also with an interface to PETSc.

The collaboration with CMRS was different. While with CEMM we contributed with improvements to their existing, relatively sophisticated, semi-implicit code, with CMRS we decided to begin with simple models, but with a fully implicit approach.

Our CMRS collaborators were Amitava Bhattacharjee and Kai Germaschewski, originally at University of Iowa, then at University of New Hampshire. The two dimensional magnetic reconnection model we received from them is described by four coupled MHD equations, using a formulation that is based on stream functions rather than on primitive variables. In this formulation the major primitive variable unknowns, the velocity and the magnetic field, are replaced by a set of unknowns that include two potentials (stream functions), in order to enforce two divergence free conditions on the velocity and the magnetic fields (the model assumes an incompressible plasma).

The original magnetic reconnection simulation code was purely explicit as well as purely sequential. Although explicit, linear solves were present in order to

compute the potentials.

Starting from this original code we implemented a fully implicit parallel magnetic reconnection simulation code. This implicit code is built on top of PETSc. Our first attempt was a Krylov linear iteration (GMRES because of the lack of symmetry), within each nonlinear (Newton) iteration, with optimal multilevel preconditioning, using the geometric multigrid preconditioner from PETSc. However, for reasons that we have not yet fully understood, the multigrid preconditioner fails early in the simulation, breaking the outer Newton iteration.

Much better results were obtained after switching from optimal multilevel preconditioning to suboptimal one level preconditioning. Our current code, based on the additive Schwartz preconditioner from in PETSc, with ILU on subdomains, scales reasonably well, while matching the output of the original explicit code. The major difference is that the Newton-Krylov-Schwarz implicit code can take time-steps that are hundreds or thousands of times larger than the explicit code.

In the collaboration with CMRS we were also joined by TOPS members from University of Colorado at Boulder: Xiao-Chuan Cai and Serguei Ovtchinnikov. This investigation continues at present with our efforts focusing on optimal multilevel preconditioning as well as on suboptimal direct linear solves which, again, can be useful in particular regimes.

We started few other collaborations that are similar to the one with CMRS. In one of them, with Hank Strauss from New York University, member of CEMM, we consider another two dimensional model, this time for the tilt instability. Another two dimensional model that we consider in collaboration with Luis Chacon from Los Alamos National Laboratory corresponds to the Kelvin-Helmholtz instability.

In addition to the collaboration with people from the SciDAC application programs we have also contributed at the infrastructure level. We have continued to develop and improve Oblio, our sparse direct linear solver, at present a mature, robust tool that can solve sparse symmetric linear systems. Two other major projects on combinatorial algorithms are worth mentioning. Both projects investigate matchings in graphs, with immediate applications such as intelligent pivoting strategies for sparse linear solvers.

A list of talks given on this work are listed below.

1. “The Design of I/O-Efficient Sparse Direct Solvers”, Florin Dobrian and Alex Pothen; Supercomputing, Denver, Colorado, November 2001.
2. “Oblio: The Design of a Sparse Direct Solver Library”, Florin Dobrian and Alex Pothen; SIAM Annual Meeting, Montreal, Canada, June 2003.

3. "A Comparison between Three External Memory Algorithms for Factoring Sparse Matrices", Florin Dobrian and Alex Pothen; SIAM Conference on Linear Algebra, Williamsburg, Virginia, July 2003.
4. "The Design of a Memory-Efficient Sparse Direct Solver Library", Florin Dobrian and Alex Pothen, SIAM Conference on Parallel Processing, San Francisco, California, February 2004.
5. "Oblio: Design and Performance", Florin Dobrian and Alex Pothen; PARA 2004 Conference, Copenhagen, Denmark, June 2004.
6. "Evaluation of Parallel Implicit Methods for a Model MHD Problem", Florin Dobrian and David Keyes, SIAM Annual Meeting, Portland, Oregon, July 2004.
7. "Evaluation of Parallel Implicit Methods for a Set of Model MHD Problems", Florin Dobrian, Serguei Ovtchinnikov, Xiao-Chuan Cai and David Keyes; Domain Decomposition Conference, New York, New York, January 2005.
8. "Fast Approximation Algorithms for Preordering Sparse Matrices", Florin Dobrian, Mahantesh Halappanavar, Amit Kumar, Arijit Tarafdar and Alex Pothen, SIAM Conference on Computational Science and Engineering, Orlando, Florida, February 2005.

A list of papers published with support from this project are listed below.

1. "The Design of I/O Efficient Solvers", Florin Dobrian and Alex Pothen, Proceedings of Supercomputing 2001.
2. "Oblio: Design and Performance", Florin Dobrian and Alex Pothen, in State of the Art in Scientific Computing, J. Dongarra et al. (eds.), Lecture Notes in Computer Science, Vol. 3732, 10 pp., to appear.
3. "A comparison of three external memory algorithms for factoring sparse matrices", Florin Dobrian and Alex Pothen, Proceedings of SIAM Conference on Applied Linear Algebra, 11 pp., July 2003.
4. "Elimination structures in scientific computing", Alex Pothen and Sivan Toledo, in Handbook on Data Structures and Applications, Chapter 59, 29 pp., Dinesh Mehta and Sartaj Sahni (eds.), Chapman and Hall/CRC Press, 2004.

5. "Computational biomarker prediction: A case study for prostate cancer", M. Wagner, D. Naik and A. Pothen, *BMC Bioinformatics*, 5, 26 pp., 2004.
6. "What color is your Jacobian? Graph coloring for computing derivatives", A. Gebremedhin, F. Manne, and A. Pothen, *SIAM Review*, 76 pp., to appear.
7. "Parallel distance-k coloring algorithms for numerical optimization", Proceedings of Europar 2002, *Lecture Notes in Computer Science*, Vol. 2400, pp. 912-921, 2002.
8. "Domain Decomposed Fully Coupled Implicit Methods for a Magnetohydrodynamics Problem", Serguei Ovtchinnikov, Florin Dobrian, Xiao-Chuan Cai and David Keyes, to appear.
9. "Nonlinear Additive Schwartz Preconditioners and Applications in Computational Fluid Dynamics", Xiao-Chuan Cai, David Keyes and Leszek Marcinkowski, *International Journal of Numerical Methods in Fluids* 40:1463-1470, 2002.
10. "Using Automatic Differentiation for Second-order Matrix-free Methods in PDE-constrained Optimization", David Keyes, Paul Hovland, Lois McInnes and Widodo Samyono, *Automatic Differentiation of Algorithms: From Simulation to Optimization*, Springer, pp. 35-50, 2002.
11. "Nonlinearly Preconditioned Inexact Newton Algorithms", Xiao-Chuan Cai and David Keyes, *SIAM Journal on Scientific Computing*, 24:183-200, 2002.
12. "Using Krylov-Schwarz Methods in an Adaptive Mesh Refinement Environment", Kai Germaschewski, Amitava Bhattacharjee, Rainer Grauer, David Keyes and Barry Smith, *Lecture Notes in Computational Science and Engineering*, Springer, 41:115-124, 2003.
13. "Jacobian-free Newton-Krylov Methods: A Survey of Approaches and Applications", Dana Knoll and David Keyes, *Journal of Computational Physics*, 193:357-397, 2004.