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High Performance Parallel Methods for Space Weather Simulations

Grant number: NAG5-9406
Principal Investigator: Tamas I. Gombosi
Performance Period: 5/1/2000 - 4/30/2003
Final Technical Report

June 4, 2003

Dr. Joseph H. Bredekamp
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Dear Joe:

This is the final report of our NASA AISRP grant entitled "High Performance Parallel Methods for Space Weather Simulations" (award number: NAG5-9406). The main thrust of the proposal was to achieve significant progress towards new high-performance methods which would greatly accelerate global MHD simulations and eventually make it possible to develop first-principles based space weather simualtions which run much faster than real time. I am pleased to report that with the help of this award we made major progress in this direction and developed the first parallel implicit global MHD code with adaptive mesh refinement.

The main limitation of all earlier global space physics MHD codes was the explicit time stepping algorithm. Explicit time steps are limited by the Courant-Friedrichs-Lewy (CFL) condition, which essentially ensures that no information travels more than a cell size during a time step. This condition represents a non-linear penalty for highly resolved calculations, since finer grid resolution (and consequently smaller computational cells) not only results in more computational cells, but also in smaller time steps.

In global MHD simulations of space plasmas the CFL condition is controlled by two factors: (1) the smallest cell size in the simulation, and (2) the fast magnetosonic speed in high magnetic field, low plasma density regions. In a typical magnetosphere simulation with a smallest cell size of about 0.25 R_{E} the CFL condition limits the time step to about 10^{-2} s. This small step is primarily controlled by the high fast magnetosonic speed (due to the high Alfvén speed) in the near-Earth region.

There are several ways to increase the time step in an MHD simulation and thus decrease the time to solution: a "slow speed-of-light" version of the so-called "*Boris* correction," and implicit time stepping. The "Boris correction" corrects the fact that in non-relativistic MHD the Alfvén speed (and the fast magnetosonic speed) can exceed the speed of light in low density, high magnetic field regions.

The "slow speed-of-light Boris correction" is used to increase the time step in global MHD simulations of the magnetosphere by artificially reducing the value of the speed of light. Since the CFL condition is controlled by the fastest wave speed in the simulation domain (which usually happens in regions where the computational cells are the smallest), one can increase the time step by a factor of 10 to 100 by limiting the speed of light to $c/100 - c/500$. This is a fairly efficient way of code speedup which is also easy to implement. However, this speed-up comes at a cost of accuracy in the temporal evolution, and the more the Alfvén speed is limited the more the fast physics is compromised. In practice, the benefit seems to outweigh the penalty up to a point. However, the penalty also gives us a reason to go looking for an alternative.

An alternative method is to use implicit methods in the code. This is the method we use to speed up our adaptive MHD code BATS-R-US. As it will be described below, we implemented a parallel implicit time stepping algorithm and we achieved a factor of $100 - 1,000$ increase in the MHD timestep. The implicit time stepping was achieved with considerable computational overhead, but we still gained a factor of $10 - 100$ code speedup from this improvement.

We combined explicit and implicit time stepping in our magnetosphere simulations. Magnetosphere simulations usually include large volumes where the Alfvén speed is quite low (tens of km/s), where the local CFL number would allow large explicit time steps (tens of seconds to several minutes). In these regions implicit time stepping is a waste of computational resources. Since our parallel implicit technique is fundamentally block based, we only treat those blocks implicitly where the CFL condition would limit the explicit time step to less than ~ 10 s. Needless to say, this combined explicit-implicit time stepping represents more computational challenges (such as separate balancing of explicit and implicit blocks), but the gain is so high that it is worth the price.

With our objective in mind, a parallel implicit Newton-Krylov-Schwarz (NKS) method has been developed and implemented for improving the performance and efficiency of the upwind finite-volume scheme for solving the equations of MHD. We are using a high-resolution upwind treatment of the convective fluxes, and a central treatment of the viscous fluxes. All of this is carried out using the block-adaptive data structure used in our MHD code. Newton-Krylov methods are iterative techniques that have proven to be very effective in the solution of sparsely discretized nonlinear

PDEs. They are based on inexact Newton iteration and a Krylov method, such as GMRES, and can be applied in a Jacobian-free manner. In the last ten years, these approaches have gained wide acceptance and have been applied to the solution of many problems in science and engineering.

Newton-Krylov methods require preconditioning for scalability in the algorithmic, or convergence rate, sense. One successful approach to the high-performance parallelization of these methods that is data-placement consistent with the best domain decomposition parallelization of the Newton-Krylov method is additive Schwarz preconditioning. The action of the Schwarz preconditioner is carried out independently on subdomain problems. This approach appears to be well suited to fully exploiting the potential of distributed-memory multi-processor machines. Keyes and co-researchers have achieved some very encouraging first results in parallel implementations of NKS algorithms. In general, good parallel efficiency was achieved up to 6144 processors (ASCI Red). Specifically, the parallel efficiency between 128 and 3072 processors was 70%.

The Schwarz preconditioning with the block-based data structure and Cartesian mesh domain decomposition procedure is very appropriate for high performance MHD codes. Use of additive overlapping Schwarz preconditioning in conjunction with a Newton-Krylov method for the parallel implicit solution of the ideal and resistive MHD equations on block-based adaptive Cartesian mesh are implemented in several stages. Initially, an inexact matrix-free Newton's method is adopted, GMRES is used as the Krylov subspace method, and the effects of granularity of the subdomains, domain overlap, and subdomain solvers and preconditioners on the performance of the method have been investigated. This way we developed an effective parallel implicit NKS solver for the MHD equations while still achieving both high parallel performance and good scalability. Attention was be given to both parallel performance issues, such as load balancing and message passing, and serial performance issues, such as memory and cache usage and inner loop optimizations. Portability of the implicit NKS solvers across different hardware platforms has also been ensured.

Very truly yours,

Tamas I. Gombosi

Refereed Publications

1. T.I. Gombosi, K.G. Powell, D.L. De Zeeuw, C.R. Clauer, K.C. Hansen, W.B. Manchester, A.J. Ridley, I.I. Roussev, I.V. Sokolov, Q.F. Stout, and G. Tóth, Solution Adaptive MHD for Space Plasmas: Sun-to-Earth Simulations, *Computing in Science and Engineering*, submitted, 2003.
2. T.I. Gombosi, D.L. De Zeeuw, K.G. Powell, A.J. Ridley, I.V. Sokolov, Q.F. Stout, and G. Tóth, Adaptive Mesh Refinement MHD for Global Space Weather Simulations, in "*Space Plasma Simulation*", edited by J. Büchner, C. T. Dum, M. Scholer, *Lecture Notes in Physics*, *615*, 251-279, Springer, Berlin-Heidelberg-New York, 2003.
3. T.I. Gombosi, G. Tóth, D.L. De Zeeuw, K.C. Hansen, K. Kabin, and K. G. Powell, Semi-relativistic magnetohydrodynamics and physics-based convergence acceleration, *J. Computational Phys.*, *177*, 176-205, 2002.
4. A.J. Ridley, D.L. De Zeeuw, T.I. Gombosi, and K.G. Powell, Using steady-state MHD results to predict the global state of the magnetosphere-ionosphere system, *J. Geophys. Res.*, *106*, 30,067-30,076, 2001.
5. C.R. Clauer, T.I. Gombosi, D.L. De Zeeuw, A.J. Ridley, K.G. Powell, B. van Leer, Q.F. Stout, C.P.T. Groth, and T.E. Holzer, High-performance computer methods applied to predictive space weather simulations, *IEEE Trans. Plasma Sci.*, *28*, 1931-1937, 2000.
6. D.L. De Zeeuw, T.I. Gombosi, C.P.T. Groth, K.G. Powell, and Q.F. Stout, An Adaptive MHD Method for Global Space Weather Simulations, *IEEE Trans. Plasma Sci.*, *28*, 1956-1965, 2000.

Presentations

1. G. Toth, D.L. De Zeeuw, A.J. Ridley, O. Volberg, T.I. Gombosi, Evaluation of Implicit Timestepping Schemes for Global Magnetosphere Simulations *2003 Spring AGU/EGS Meeting*, Nice, France, April 7-11, 2003.
2. T.I. Gombosi, and the CSEM Team, Sun-to-Earth simulations with a first-principles based coupled space weather model, invited talk, *34th COSPAR General Assembly*, Houston, TX, October 10-19, 2002.
3. T.I. Gombosi, D.L. De Zeeuw, K.G. Powell, I.V. Sokolov, Q.F. Stout, G. Tóth, Adaptive Mesh Refinement MHD for Space Plasma Simulations, *22nd Annual International Conference of the Center for Non-Linear Studies: Frontiers of Simulation*, invited talk, Los Alamos, NM, August 19-23, 2002.

4. T.I. Gombosi, C.R. Clauer, D.L. De Zeeuw, K.C. Hansen, W.B. Manchester, K.G. Powell, A.J. Ridley, I. Roussev, I.V. Sokolov, G. Tóth, R.A. Wolf, S. Sazykin, T.E. Holzer, B.C. Low, A.D. Richmond, R.G. Roble, Towards an Operational Sun-to-Earth Model for Space Weather Forecasting, invited talk, *2002 Spring AGU Meeting*, Washington, D.C., May 28-31, 2002.
5. T. Gombosi, D. De Zeeuw, A. Ridley, Global Simulations of Ionospheric Control of the Magnetosphere, invited talk, *10th International Ionospheric Effects Symposium*, Alexandria, Virginia, May 7-9, 2002.
6. T.I. Gombosi, D.L. De Zeeuw, K.G. Powell, I.V. Sokolov, Q.F. Stout, G. Tóth, Adaptive Mesh Refinement MHD for Space Plasma Simulations, *2002 International Sherwood Fusion Theory Conference*, Rochester, NY, April 22-24, 2002.
7. T.I. Gombosi, Comprehensive Solar-Terrestrial Environment Model for Space Weather Predictions: Progress of the Space Weather MURI Project, *Space Weather Week*, Boulder, CO, April 16-19, 2002.