MULTISCALE MODELING OF HELIOSPHERIC PLASMAS

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Abstract

A new MHD code has been developed for massively parallel computers using adaptive mesh refinement (AMR) and a new 8-wave Riemann solver. The code was implemented on a Cray T3D massively parallel computer with 512 PEs. In the first application, which modeled the expansion of the solar wind from the solar surface, the code achieved 13 GFLOPS.

INTRODUCTION

Heliospheric phenomena have been a subject of interest virtually since the inception of the space program. Indeed, with Pioneer and Voyager in the outer heliosphere, Ulysses executing its polar passes, WIND in orbit upstream from Earth, SOHO observing the Sun and the inner heliosphere, the ISTP spacecraft studying the Earth's magnetosphere, and Galileo at Jupiter, this is an era of remarkable richness in revealing the full range of heliospheric phenomena. This wealth of data, however, will be of value only if we derive from these observations, and the subsequent interpretations, a clear understanding of the underlying and governing physical processes.

Even the best sets of observations are limited in space and time and they must be extended by sophisticated theoretical models into full 3D descriptions of heliospheric plasmas. It is here that a unifying multiscale, 3D model plays an essential role. The model must be sufficiently versatile to capture the complexity of the actual physical system from high gradient shocks and discontinuities, to spatially limited transition layers, to large volumes of slowly changing plasma flows.

Our long-term goal is to develop the first 3D, multiscale model of the heliosphere extending from the base of the solar corona to the free-streaming interstellar medium. In its fully developed form the model will self-consistently describe the complicated interplay between various physical processes controlling the structure and dynamics of the heliosphere, including the solar wind outflow, the generation, temporal and spatial evolution of transient interplanetary structures (such as coronal mass ejections or corotating interaction regions), as well as the heliosphere's interactions with the interstellar medium (including plasma and neutral gas), and with magnetized and non-magnetized solar system bodies.

Several years ago the federal goverment instituted the national High Performance Computing and Communications (HPCC) program to initiate advances in the state of the art of modern computer simulations and in new uses of high-speed computer networks. NASA actively participates in this federal program through several technical projects. One of these projects is the Earth and Space Sciences (ESS) project, which last year selected nine Grand Challenge Investigator Teams to develop applications at least 10 times faster than today. Our investigation, entitled "Multiscale Modeling of Heliospheric Plasmas" is one of the nine selected ESS Grand Challenge projects. This paper briefly outlines the method we use and it summarizes our first numerical results.

GOVERNING EQUATIONS

The governing equations of ideal magnetohydrodynamics describe the physics of a conducting fluid in which viscous and resistive effects are negligible. Under these assumptions, the governing equations for three-dimensional flow are conservation laws for mass, three momentum components, three magnetic field components, and energy. Conservation of mass is the same for the plasma as it is for a fluid, conservation of momentum and energy have electromagnetic terms that do not appear in the governing equation of classical fluid dynamics.

The dimensionless conservative form of the ideal MHD equations can be written in the following form:

$$\frac{\partial \tilde{\mathbf{W}}}{\partial \tilde{t}} + \left(\tilde{\nabla} \cdot \tilde{\mathbf{F}}\right)^T = \tilde{\mathbf{S}} \qquad (1)$$

where $\tilde{\mathbf{W}}$ and $\tilde{\mathbf{S}}$ are eight-dimensional state and source vectors, while $\tilde{\mathbf{F}}$ is an 8×3 dimensional flux diad. All quantities denoted by the symbol tilde are normalized with the help of physical quantities in the undisturbed upstream region

$$\begin{aligned}
\tilde{t} &= a_0 t / R_s && (2)\\
\tilde{\mathbf{r}} &= \mathbf{r}/R_s && (3)\\
\tilde{\rho} &= \rho/\rho_0 && (4)\\
\tilde{\mathbf{u}} &= \mathbf{u}/a_0 && (5)\\
\tilde{p} &= p/\rho_0 a_0^2 && (6)\\
\tilde{\mathbf{B}} &= \mathbf{B}/\sqrt{\mu_0 \rho_0 a_0^2} && (7)
\end{aligned}$$

where t=time, $\mathbf{r}$=radius vector, ρ=mass density, $\mathbf{u}$=bulk flow velocity, p=pressure, and $\mathbf{B}$=magnetic field vector. The subscript 0 refers to values at the solar surface, R_s is the radius of the Sun and a_0 is the hydrodynamic sound speed at the solar surface. It follows from this normalization procedure that the normalized state and flux vectors are:

$$\tilde{\mathbf{W}} = \begin{pmatrix} \tilde{\rho} \\ \tilde{\rho}\,\tilde{\mathbf{u}} \\ \tilde{\mathbf{B}} \\ \tilde{\varepsilon} \end{pmatrix} \qquad (8)$$

$$\tilde{\mathbf{F}} = \begin{pmatrix} \tilde{\rho}\,\tilde{\mathbf{u}} \\ \tilde{\rho}\,\tilde{\mathbf{u}}\,\tilde{\mathbf{u}} + \left(\tilde{p} + \frac{1}{2}\tilde{B}^2\right)\mathbf{I} - \tilde{\mathbf{B}}\tilde{\mathbf{B}} \\ \tilde{\mathbf{u}}\tilde{\mathbf{B}} - \tilde{\mathbf{B}}\tilde{\mathbf{u}} \\ \tilde{\mathbf{u}}\left(\tilde{\varepsilon} + \tilde{p} + \frac{1}{2}\tilde{B}^2\right) - \left(\tilde{\mathbf{B}} \cdot \tilde{\mathbf{u}}\right)\tilde{\mathbf{B}} \end{pmatrix}^T \qquad (9)$$

where $\tilde{\varepsilon}$ is the normalized internal energy density:

$$\tilde{\varepsilon} = \frac{1}{2}\left[\tilde{\rho}\,\tilde{u}^2 + \frac{2\tilde{p}}{\gamma - 1} + \tilde{B}^2\right] \qquad (10)$$

Equation (1) is a coupled system of eight partial differential equations — conservation laws for the mass, momentum, magnetic flux, and internal energy.

SOLUTION ALGORITHM

Equation (1) was solved on a solution-adaptive Cartesian mesh using an upwind-differencing approach. The method is called *Multiscale Adaptive Upwind Scheme for Magnetohydrodynamics* (MAUS-MHD).

MAUS-MHD is based on two key ingradients that are extremely well suited to heliosphere modeling. The first is a data structure that allows for adaptive refinement of the mesh in regions of interest (*De Zeeuw and Powell,* 1992), and the second is an upwind scheme (*van Leer*, 1979) based on a new approximate Riemann solver for ideal MHD. The details of the new numerical method have already been published in several papers (*Gombosi et al.,* 1994; *Powell,* 1994; *Powell,* 1996; *Gombosi et al.,* 1996) and a comprehensive description of the entire method is presently in preparation (*Powell et al.*, 1997). The approach has been applied to the interaction of the solar wind with comets and non-magnetized planets, as well as strongly magnetized planets.

Adaptive refinement and coarsening of a mesh is a very attractive way to make optimal use of computational resources. It becomes particularly attractive for problems in which there are disparate spatial scales. For problems like the heliosphere, in which typical spatial scales can differ by orders of magnitude, an adaptive mesh is a virtual necessity. The primary difficulty in implementing an adaptive scheme is related to the way in which the solution data are stored; the data structure must be much more flexible than the simple array-type storage used in the majority of scientific computations.

We have decided to take the most flexible possible AMR approach, in order to give us parameters which can be chosen to optimize parallel performance of the code. To this end, we have chosen a block-based tree structure, which is a generalization of the cell-based tree used in our earlier work (*De Zeeuw and Powell,* 1992). The root of the block-based tree is a structured coarse grid that covers the entire flow domain. The root block can have an arbitrary number of children blocks, where each child block is one level more refined than the parent block (i.e. $\Delta x_{child} = \Delta x_{parent}/2$, $\Delta y_{child} = \Delta y_{parent}/2$, $\Delta z_{child} = \Delta z_{parent}/2$). This data structure devolves to the cell-based tree in the limit of child blocks that are $1 \times 1 \times 1$. This data structure is more general, however, allowing arbitrary block sizes. The advantages of allowing arbitrary block sizes for the refinement are:

- Larger blocks have better surface-area to volume ratios, yielding lower communication overheads than smaller blocks.
- Block sizes can be chosen to make load-balancing easier, allowing the decomposition of the domain to be done at a higher level (i.e. portions of the grid are farmed out to the processors on a block-by-block basis, rather than on a micro-managed cell-by-cell basis).
- Because the data for the cells inside each block can be stored in an array data structure, indi-

rect addressing is avoided for flow-solver loops, and greater locality of data is obtained, leading to more possibilities for efficient use of the cache on each processor.

The mesh is generated in such a way that important geometric and flow features are resolved. The geometry is resolved by recursively dividing blocks in the vicinity of the sun until a specified cell-size is obtained. A larger block-size is specified for the remainder of the mesh. Flow features are resolved by obtaining a solution on this original mesh, and then automatically refining cells in which the flow gradients are appreciable, and coarsening cells in which the flow gradients are negligible.

The MAUS-MHD upwind scheme is a finite-volume method, in which the governing equations are integrated over each cell of the mesh. This way the governing equations given by equation (1) become a set of coupled ordinary differential equations in time, which can be solved by a suitable numerical integration procedure. In MAUS-MHD, an optimally smoothing multistage scheme (*van Leer et al.*, 1989) is used. To carry out the multistage time-stepping procedure for (1), an evaluation of the flux tensor at the interfaces between cells of the mesh (a so called "Riemann solver") is required.

Previous upwind-type schemes for MHD (*Brio and Wu*, 1988; *Zachary and Colella*, 1992) have been based on the one-dimensional Riemann problem obtained by noting that, for one-dimensional problems, the $\nabla \cdot \mathbf{B} = 0$ condition reduces to the constraint that $B_x = \text{const}$. Methods based on this approach require a separate procedure for updating the component of the the magnetic field normal to a cell face in multi-dimensional problems. Typically, this requires the use of a projection scheme which solves a global elliptic equation every few time-steps to project out the numerical divergence that accumulates (*Zachary and Colella*, 1992; *Tanaka* 1993]).

In MAUS-MHD a new approach is taken (*Powell* 1994; *Powell*, 1996). The governing equations for 3D MHD are derived without explicitly enforcing $\nabla \cdot \mathbf{B} = 0$ *a priori*, and a numerical procedure that is stable for this system is derived. Since the finite-volume scheme is a collocated one, truncation-error levels of $\nabla \cdot \mathbf{B}$ can be generated by the scheme, and the algorithm must "clean" itself from these errors in a stable manner. The resulting equations are those given in 1, with the source term $\mathbf{S}$ (not truly a source term, since it is proportional to derivatives of the magnetic field) defined by

$$\tilde{\mathbf{S}} = -\tilde{\nabla} \cdot \tilde{\mathbf{B}} \begin{pmatrix} 0 \\ \tilde{\mathbf{B}} \\ \tilde{\mathbf{u}} \\ \tilde{\mathbf{B}} \cdot \tilde{\mathbf{u}} \end{pmatrix} \tag{11}$$

This form of the equations resolves the degeneracy of the characteristic equation system and one can derive eight non-degenerate eigenvectors and eigenvalues. A more complete derivation of the equations and the Riemann solver are given in (*Powell*, 1996).

The Riemann solver based on the eight equations given by (1) and (11), as shown in (*Gombosi et al.*, 1994; 1996; *Powell* 1994; *Powell*, 1996), has substantially better numerical properties than one based on the form in which the source term is not accounted for. Such a Riemann solver gives a consistent update for the component of the magnetic field normal to a cell face, such that the resulting numerical scheme treats $(\nabla \cdot \mathbf{B})/\rho$ as a passive scalar. Any $(\nabla \cdot \mathbf{B})/\rho$ that is created numerically is passively convected, and, in the steady state, $(\nabla \cdot \mathbf{B})/\rho$ is constant along streamlines. with this treatment $\nabla \cdot \mathbf{B} = 0$ is satisfied to within truncation error, once it is imposed as an initial condition to the problem. The resulting scheme is stable to these truncation-level errors in the divergence of $\mathbf{B}$, and does not require a projection scheme.

Given the eigenvalues and right eigenvectors of equations (1) and (11) (*Powell* 1994; *Powell*, 1996), the flux through an interface is given by

$$\Phi\left(\tilde{\mathbf{W}}_L, \tilde{\mathbf{W}}_R\right) = \frac{1}{2}\left(\Phi_L + \Phi_R\right) - \frac{1}{2}\sum_{k=1}^{8} |\lambda_k|\, \alpha_k \mathbf{R}_k \tag{12}$$

where the subscripts L and R refer to quantities at the left and right sides of the interface, while λ_k and $\mathbf{R}_k$ are the k^{th} eigenvalue and right eigenvector (these can be found in (*Gombosi et al.*, 1994; *Powell*, 1996)), α_k is the inner product of the k^{th} left eigenvector with the state difference, $\tilde{\mathbf{W}}_R - \tilde{\mathbf{W}}_L$, while the quantities, Φ_L and Φ_R, are simply $\tilde{\mathbf{F}}(\tilde{\mathbf{W}}_L)\cdot\mathbf{n}$ and $\tilde{\mathbf{F}}(\tilde{\mathbf{W}}_R)\cdot\mathbf{n}$, respectively (where $\mathbf{n}$ is the normal vector of the interface).

The advantages of the flux-based approach described above are:

1. The flux function is based on the eigenvalues and eigenvectors of the Jacobians of $\tilde{\mathbf{F}}$ with respect to $\tilde{\mathbf{W}}$, leading to an upwind-differencing scheme which respects the physics of the problem being solved,

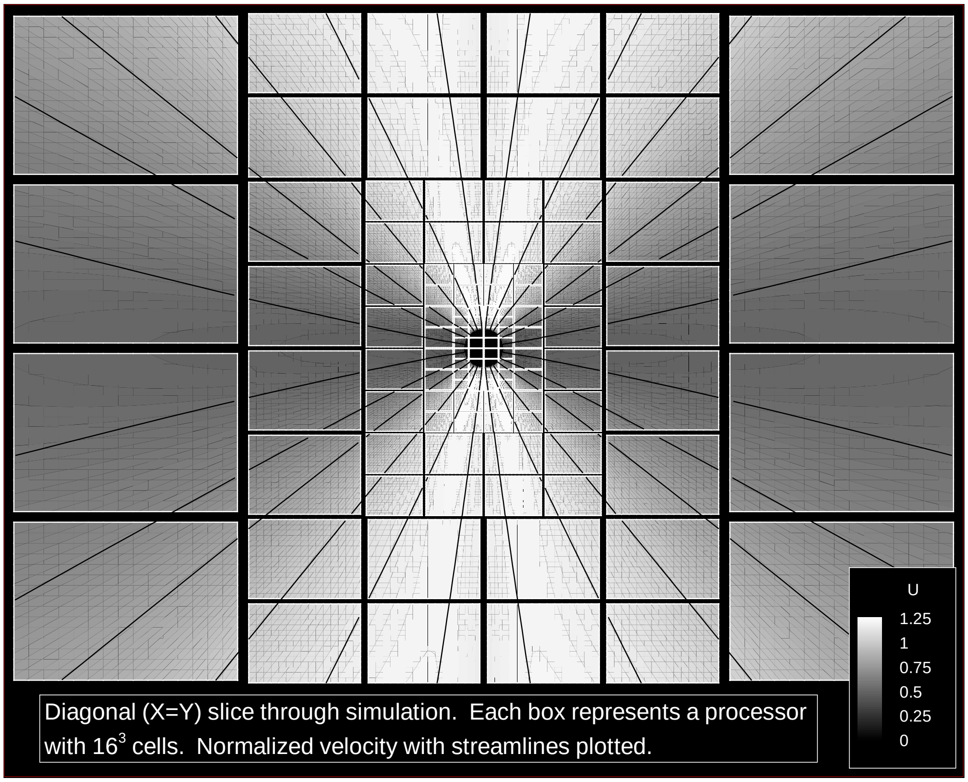

Figure 1: Velocity magnitude (grayscale) and streamlines.

2. The scheme provides capturing of shocks and other high-gradient regions without oscillations in the flow variables,

3. The scheme has just enough dissipation to provide a nonoscillatory solution, and no more,

4. The scheme provides a physically consistent way to implement boundary conditions that are stable and accurate: a physically consistent flux can be calculated at all boundaries by use of the approximate Riemann solver.

PARALLEL IMPLEMENTATION

The MAUS-MHD code was implemented in FORTRAN90, using a domain-decomposition approach. Blocks of cells, stored as 3D arrays, were locally stored on each processor in such a way as to achieve a balanced load — each processor held blocks containing the same number of cells (16^3 in this run). At each iteration, messages containing cell-center states (density, momentum, magnetic field and energy) were passed between neighboring processors. The message-passing was implemented using the Edinburgh 32-bit MPI package. Special care had to be taken at refinement interfaces, where a block of cells at one level of refinement abuts a block that is one level finer or coarser than itself. The approach taken to assure stability and conservation at these interfaces is described in (*DeZeeuw and Powell,* 1992; *Powell*, 1996). The difference in refinement level also requires that interpolation and restriction operators be applied before passing data between processors.

The first case run with the code was a simulation of the emanation of the solar wind from the sun. It models the 3D expansion of the solar wind from 1 R_s to 16 R_s. The inner boundary condition describes a stationary sphere of hot plasma with an embedded dipole field. Due to the low interplanetary pressure, plasma expands into the interplanetary medium. The converged solution shows that the solar wind originating from the polar regions is much faster than the solar wind originating from the equatorial region, due to the presence of the solar magnetic field. This fact was observed with the Ulysses spacecraft, but until now no numerical model was able to reproduce this observation. Figure 1 shows the $x = y$

meridional plane of the solution. The block structure of the parallel implementation is shown together with the magnitude of the plasma velocity (gray scale) and the solar wind flow lines (solid lines).

PARALLEL PERFORMANCE

The code used a total of 5 levels of refinement and 512 blocks of 16x16x16=4096 cells for over 2 million total cells. A Cray T-90 Hardware Performance Monitor (HPM) count gave 1.94×10^7 floats per processor per timestep. A total of 4.02×10^{13} floats were computed in the simulation, which ran for 3088 seconds. The resulting performance of the code was 13.0 GFLOPS.

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BIOGRAPHIES

Tamas I. Gombosi is Professor of Space Science and Professor of Aerospace Engineering. He has extensive experience in solar system astrophysics. His research areas include generalized transport theory, modeling of planetary environments, heliospheric physics, and more recently, multiscale MHD modeling of solar system plasmas. He is Interdisciplinary Scientist of the Cassini/Huygens mission to Saturn and its moon, Titan. Professor Gombosi is Senior Editor of the Journal of Geophysical Research – Space Physics. He is Program Director and Co-Principal Investigator of the NASA HPCC ESS Computational Grand Challlenge Investigator Team at the University of Michigan.

Kenneth G. Powell is Associate Professor of Aerospace Engineering. His research areas include: solution-adaptive schemes, genuinely multidimensional schemes for compressible flows, and, most recently, numerical methods for magnetohydrodynamics. He was a National Science Foundation Presidential Young Investigator from 1988-1994. He is Co-Principal Investigator of the NASA HPCC ESS Computational Grand Challlenge Investigator Team at the University of Michigan.

Quentin F. Stout is Professor of Computer Science. His research interests are in parallel computing, especially in the areas of scalable parallel algorithms and in overcoming inefficiencies caused by interactions among communication, synchronization, and load imbalance. This work has been applied to a variety of industrial and scientific parallel computing problems, as well as to fundamental problems in areas such as sorting, graph theory, and geometry. He is Co-Principal Investigator of the NASA HPCC ESS Computational Grand Challlenge Investigator Team at the University of Michigan.

Edward S. Davidson is Professor of Computer Science. He developed a variety of systematic methods for computer performance evaluation, including a hierarchical simulation-based approach to cost-effective computer design, a lattice based evaluation methodology for evaluating the individual and joint impact of a set of possible architectural features, Markov and analytic models for realistic evaluation of memory hierarchies, and a methodology for evaluating branch and data dependence in instruction pipelines that achieves a separation between application-dependent and architecture-dependent analysis.

Daren L. DeZeeuw is Assistant Research Scientist at the Space Physics Research Laboratory. His interests involve the development and implementation of algorithms to solve the multidimensional Euler and MHD equations using octree-based unstructured Cartesian grids with adaptive refinement and multigrid convergence acceleration. He is one of the primary developers of the code described in this paper.

Lennard A. Fisk is Professor and Chair, Department of Atmospheric, Oceanic and Space Sciences. His area of expertize is heliospheric physics and the propagation of energetic particles in the solar system. Between 1987 and 1993 he served as NASA's Associate Administrator for Space Science and Applications. In this position he was responsible for the planning and direction of all NASA programs concerned with space science and for the institutional management of the Goddard Space Flight Center in Greenbelt, Maryland and the Jet Propulsion Laboratory in Pasadena, California.

Clinton P.T. Groth is Assistant Research Scientist at the Space Physics Research Laboratory. His research interests involve generalized transport theory and the development of higher-order moment closures for the solution of the Boltzmann equation via advanced numerical methods with applications to both rarefied gaseous and anisotropic plasma flows. This research has led to a new hierarchy of moment closures with many desirable mathematical features that appears to offer improved modeling of transitional rarefied flows.

Timur J. Linde is graduate student in the Department of Aerospace Engineering. He is developing a new three-dimensional model of the interaction of the solar wind wind with the local interstellar medium using an octree-based MHD code with adaptive mesh refinement.

Hal G. Marshall is Associate Research Scientist at the Center for Parallel Computing. His interests focus on scientific computing using massively parallel computers. He is one of the primary developers of the code described in this paper.

Philip L. Roe is Professor of Aerospace Engineering. In 1976, he was asked to undertake research into numerical methods for solving the compressible flow (Euler) equations, with instructions to "find something new." The outcome of this work became known as the "Roe solver", a formula for the interface flux in a finite-volume code, that is now a standard feature in numerous commercial and industrial codes. Later, he initiated an effort to link the algorithms for multidimensional partial differential equations even more closely with the appropriate physics, a project that has attracted an international team of collaborators. This effort is now essentially complete for two-dimensional gasdynamics. Not only are the results superior to those of the earlier approach, but the algorithm, as a byproduct, minimizes message passing. Most of the tools are in place to make the extensions to three dimensions and more complex equations.

Bram van Leer is Professor of Aerospace Engineering. In the 1970s he became dissatisfied with the available finite-difference methods for shocked flows, which were either too diffusive or oscillatory, and designed a grand plan to bring CFD to a uniformly higher level. This he did singlehandedly at Leiden Observatory during the years 1972-77, as reported in the 5-part article series "Towards the ultimate conservative differences scheme." Starting from Godunov's method (1959) he formulated higher-order, yet non-oscillatory, upwind-differencing methods for the Euler equations; such methods became the industry's standard in the 1980's and are called MUSCL-type, after the first code of its kind. His current research interest lies in convergence acceleration of steady-flow computations, in particular, the development of truly effective multigrid methods for high-Reynolds-number flows, using local preconditioning to remove the stiffness of the governing equations.