Particle-in-Cell Magnetohydrodynamics

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Introduction

The power of magnetic fields to affect plasma dynamics on large scales is revealed dramatically by the magnificent Yohkoh x-ray photographs of the sun's corona. [Strong and Team, 1994] Field-aligned structures and bright striations reveal the presence of a magnetic field. Magnetic fields are as important in the dynamics of astrophysical structures, and in the interaction of the solar wind with the Earth's plasmasphere. The challenge is to capture the dynamics of magnetized plasmas in our simulations, and thus to understand them.

Clearly, there has been great progress in plasma simulation, so that some global scale phenomena have been modeled using both hybrid [Thomas and Winske, 1990] and full kinetic models [Pritchett, et al., 1996]. However, on length and time scales for which the plasma is at least approximately quasi-neutral, non-relativistic, and collisional, the reduced description given by magnetohydrodynamics (MHD) is a useful and economical alternative to kinetic simulations.

There has been rapid progress in numerical methods for MHD flow recently. Building on the upwind methods for the Euler equations developed by Godunov, Roe, Harten, and van Leer, new codes using directional splitting, adaptive mesh refinement, and expanded MHD equations have been developed [Gombosi, et al., 1996]. The new codes provide unequaled resolution of shocks and shock-shock interactions.

Nevertheless, there is still room for improvement. For example, explicit upwind methods are costly for problems with large variations in density and flow velocity. Further, unstable MHD flows often evolve without shocks, and modeling them requires methods with low dissipation and good conservation of vorticity. Thus we continue to study a general purpose particle-in-cell method, because it can model not only instability in low speed flows, but also compressible flow and even shocks if necessary.

FLIP MHD: A Particle-in-Cell Method for Magnetohydrodynamics

The FLIP, particle-in-cell (PIC) method is Galilean invariant[Brackbill and Ruppel, 1986]. Thus, the solutions are independent of the velocity of the fluid relative to the computation mesh . FLIP MHD extends this property to the MHD equations [Brackbill, 1991].

The FLIP algorithm solves the MHD equations in four steps which use both a particle and a grid description of the fluid. 1. Particle data is interpolated to the grid. 2. Finite difference equations are solved on the grid to advance the solution. 3. Changes in the grid data over a time step are interpolated to the particles to advance the particle data. 4. Particles are located on the grid for the next time step, thereby modeling convection.

The most important difference between FLIP and earlier PIC methods is in step 3. By interpolating changes in the solution from the grid to the particles, rather than by replacing the particle data with the new grid solution. Consequently, computational diffusion decreases with Δt . This change guarantees consistency, even with higher order interpolation, and reduces computational diffusion below that achievable with finite difference methods with a similar range of applicability.

Galilean invariance in FLIP MHD is achieved by making the magnetic field a particle variable. Each particle is assigned a magnetic moment, μ, from which a magnetization $\mathbf{M}$ is calculated on the grid by summation. From the magnetization $\mathbf{M}$, a solenoidal magnetic field $\mathbf{B}$ is calculated on the grid by projection,

$$\mathbf{B} = \mathbf{M} - \nabla\varphi, \quad \nabla^2\varphi = \nabla \bullet \mathbf{M}$$

The magnetic field, **B**, is advanced on the grid by solving Faraday's law. The magnetization, **M**, is calculated from,

$$\frac{d\mathbf{M}}{dt} = \frac{d\mathbf{B}}{dt} - (\nabla\mathbf{u}) \bullet \nabla\varphi$$

where **u** is the fluid velocity. Changes in the magnetization are interpolated to the particles to calculate the new particle magnetic moment, μ. This last step introduces some computational diffusion. However, the diffusion is small compared with that produced by, e.g., van Leer convection [Brackbill, 1991], and it can be reduced even further by a mass matrix formulation of the equations [Burgess, et al., 1992].

As with all PIC methods, there are two fundamental problems with FLIP that can limit its usefulness. The first problem is the finite grid or ringing instability, which occurs with both PIC kinetic and PIC fluid calculations and limits the minimum Mach number that can be modeled[Brackbill, 1988]. However, in contrast to PIC plasma simulations, PIC fluid calculations are not destroyed by the instability. In PIC fluid calculations momentum and energy conservation bound the growth of the instability to small amplitudes, and limit the effect of the instability to a migration of particles to cell centers. Thus, the ringing instability increases the approximation error to that which would have been obtained if there were one particle in each grid cell, regardless of the actual number of particles per cell. The ringing instability is effectively suppressed by implicitly differencing the dynamical equations . The second problem is that particles allow only limited variation in density within the problem domain unless the particle mass is allowed to vary from particle to particle, and from time step to time step. This problem is resolved by controlling the number of particles in each cell, and replacing particles in cells with too many or too few particles with the desired number. One successful approach requires that the new particles yield the same values of conserved variables on the grid, cell by cell [Lapenta and Brackbill, 1995]. Typically control is applied at intervals of ten or more time steps, so the impact of control on accuracy and cost is minimal.

FLIP has been validated by comparisons of analytically solvable problems, such as the Rayleigh-Taylor instability, confined eddy, and Kelvin-Helmholtz instability [Brackbill, 1991, Brackbill, 1993, Lapenta and Brackbill, 1994], and by comparisons with other numerical computations. In comparisons with second order, leapfrog calculations of the tearing instability in the Earth's magnetotail, FLIP MHD and leapfrog results were in good agreement [Birn, et al., 1995-accepted]. The cost of FLIP MHD was significantly higher, but the FLIP calculations could be continued long after the leapfrog algorithm began to exhibit numerical instability. In calculations of the global heliosphere in two dimensions, FLIP MHD calculations are in quantitative agreement with standard codes on the location and strength of the bow and heliospheric termination shocks without the magnetic field, and yield some insight into the effect of a magnetized interstellar medium on the size and shape of the heliosphere. Recently, multifluid calculations have been reported with plasma and neutral fluids interacting through charge exchange. The FLIP method has been validated by application to non-MHD problems. These are outside the scope of this paper, but the range of problems is illustrated by applications to glow discharges [Lapenta, et al., 1995], continuum mechanics [Sulsky, et al., 1994], and granular flow [Bardenhagen and Brackbill, 1997-submitted].

FLIP3D MHD

FLIP3D MHD is a straightforward extension of FLIP MHD to three dimensions. The computational mesh is logically rectangular and composed of hexahedral cells of arbitrary size and shape. Interpolation between the grid and particles is by a tensor product of b-splines. The interpolation is performed on a uniform grid in natural coordinates. Natural coordinates are defined by mapping each hexahedral cell in physical space on to a unit cube. Kinematic variables, position and velocity, are interpolated using trilinear interpolation. Thermodynamic variables and the magnetization are interpolated using triquadratic interpolation. The support of the b-splines is a fixed number of cells in natural coordinates, so that the size of a particle will vary from cell to cell on a nonuniform grid. The basic techniques are the same in most details to those reported earlier for two dimensions [Brackbill and Ruppel, 1986]. The grid is a moving-mesh adaptive grid [Brackbill, 1993]. The grid can be uniform and fixed, as in the examples that will be presented here. A uniform grid costs less per computation cycle, since particles are much more easily located on a uniform grid. Adaptive mesh refinement is a natural extension of this technology that has not been explored.

The dynamical equations are solved on a Lagrangian grid, i.e. one which moves with the fluid velocity at every point. A staggered mesh formulation is used. Spatial differencing assures that differencing at grid vertices and cell centers are conjugate operations [Sulsky, 1990]. Thus momentum is conserved, and energy is conserved with implicit differencing in time. Details of the time differencing are described in [Brackbill, 1991]. Details of the spatial differencing are discussed in [Pracht and Brackbill, 1976].

The implicit MHD equations are solved using a conjugate residual solver [O'Rourke and Amsden,], with a block-diagonal Jacobi preconditioner. The elements of the Jacobian are calculated by numerical differentiation, and the iteration is matrix-free. Thus, modifications to include additional physics require modifications to the residual calculation only. The multigrid preconditioner described here by Knoll et al. would reduce this time by reducing the number of iterations required for convergence. The projection to calculate **B** uses a gmres solver. The cost of the projection is small.

Unstable MHD Flow

FLIP3D MHD is applied to study differential rotation of a magnetized plasma., which may enhance reconnection in the interaction of the solar with the Earth's magnetosphere. When it encounters the Earth's magnetosphere, the solar wind is deflected around the equator and over the poles. At the subsolar point, the flow stagnates. As one traces the flow away from the subsolar point, it accelerates as it follows the magnetopause, the boundary between stationary terrestrial plasma and the solar wind plasma. At a distance that increases with the angle between the flow and the equatorial plane, there is sufficient shear across the magnetopause to cause the Kelvin-Helmholtz instability to grow to significant amplitude. The variation with angle is due to the stabilizing influence of the magnetic field. Flow parallel to the field. e.g. over the pole, is stable. (Whether the instability actually occurs in the magnetosphere is still a matter of controversy, with theorists on one side arguing that it must occur and observationalists on the other arguing that the evidence that it does occur is ambiguous.)

Computational MHD studies of the Kelvin-Helmholtz instability in two dimensions [Miura, 1995, Miura, 1995, Wu, 1986] predict current amplification and enhanced reconnection [Brackbill, 1993, Wu, 1986], but these results are for low beta flow parallel to the magnetic field One asks whether reconnection is enhanced in three dimensions, even when the vorticity is parallel to the magnetic field.

In the flow geometry described above, it is clear the Kelvin-Helmholtz instability will be strongest in the low-latitude boundary layer . This will cause differential rotation of magnetic flux tubes, with significant rotation at the equator, and a diminishing rotation as one moves toward the poles. Differential rotation is considered by Moffatt in a kinematic model [Moffatt, 1978pp65-70]. For differential rotation of an initially uniform magnetic field with a perpendicular plane of symmetry, $\mathbf{A} \bullet \mathbf{B}$ is nonzero even though the helicity is zero. Further, differential rotation produces a parallel current. Where $\omega = \nabla \times \mathbf{u}$ is the vorticity, $\mathbf{J} = \nabla \times \mathbf{B}$ is the current density, and $\mathbf{E}$ the electric field, the variation in the parallel vorticity along a magnetic field line is a source of parallel current,

$$\mathbf{B} \bullet \frac{\partial \mathbf{J}}{\partial t} = \mathbf{B} \bullet \nabla(\mathbf{B} \bullet \omega) + \mathbf{B} \bullet \nabla^2 \mathbf{E} - (\mathbf{B} \bullet \nabla)(\mathbf{u} \bullet \mathbf{J})$$

When there is resistance to electric current, the parallel current will cause the helicity to change

$$\frac{\partial \mathbf{A} \bullet \mathbf{B}}{\partial t} + \nabla \bullet (\varphi \mathbf{B} + \mathbf{E} \times \mathbf{A}) = -2(\eta \mathbf{J} \bullet \mathbf{B})$$

where η is the resistivity.[Hornig and Rastatter, 1997]

Does the change in $\mathbf{A} \bullet \mathbf{B}$ correspond to reconnection? Results with FLIP3D MHD suggest that it will when the magnetic field reverses direction across a shear layer through localized breakdown of ideal MHD" [Birn, et al., 1997].

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