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TITLE: **IMPLICIT ADAPTIVE GRID PLASMA SIMULATION**

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Implicit Adaptive Grid Plasma Simulation

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1. Introduction

In a plasma simulation, the nonlinear interactions among the charged particles and the fields they generate are calculated by solving particle equations of motion self-consistently with Maxwell's equations. Standard methods simulate plasmas by solving explicit approximations to the equations of motion with a representative sample of charged particles. Explicit methods must resolve all time scales, including the fastest, the electron plasma oscillations, for numerical stability. Because plasmas exhibit a wide range of natural frequencies, ranging from electromagnetic waves and electron plasma oscillations at high frequencies, to sound waves and mass motion at low frequency, it is clearly impossible to cover this range of length and time scales with a small time step.

Reduced equations, such as the gyrokinetic model [*Lee*, 1983], the hybrid model [*Byers et al.*, 1978, *Winske*, 1985], or the δf method [*Kotschenreuther et al.*, 1990] remove the most restrictive constraints on the time step by removing some of the physics. Implicit methods [*Brackbill and Forslund*, 1985, *Langdon and Barnes*, 1985], remove this constraint by giving unconditional stability. With the implicit formulation, one can choose the time step to resolve the time scale of interest, rather than restrict the time step to a small value to maintain numerical stability.

The principal approximation in the hybrid model is the replacement of kinetic electrons by a fluid model. The ions remain kinetic. The hybrid approximation removes the electron time scale from the problem, and permits one to model the ion time scale. However, one must introduce an electron energy equation to complete the model, e.g. an adiabatic law, and thus, for example, the electron entropy increase through a shock cannot be learned from the simulations. The energy partition between ions and electrons, and the electron dissipation are modeled rather than derived from first principles [*Winske*, 1985].

The two basic implicit formulations, the direct and implicit moment methods, also reduce the cost by reducing the number of equations that must be solved, but differently from the hybrid method. The direct method extrapolates particle motion forward in time along unperturbed particle orbits [*Langdon and Barnes*, 1985], and the implicit moment method calculates the fields in which the particles move by solving coupled field and moment equations self-consistently [*Brackbill and Forslund*, 1985]. Closure is given by data from the simulation particles. Both the direct and implicit moment methods give accurate estimates of the evolution of the charge and current density when the (electron) particle displacement per time step is smaller than the grid spacing, $\frac{v_{the}\Delta t}{\Delta x} = \frac{\lambda_D}{\Delta x}\omega_{pe}\Delta t < 1$, where λ_D is the Debye length. This inequality can be satisfied with very large time steps when the grid spacing is large compared with the shielding length. (Of course, when the shielding length is small the finite grid instability may be a problem [*Lapenta and Brackbill*, 1994].)

2. Implementation of Implicit Methods

Obviously, an implicit algorithm is computationally more complex than an explicit code, especially in the solution of the implicit equations, because the solution of the implicit

equations requires that one advance the moment and field equations self-consistently to achieve stability. One actually solves a second order PDE for **E**,

$$(c\theta\Delta t)^2 \nabla \times \nabla \times \mathbf{E}^\theta + \mu \cdot \mathbf{E}^\theta = \mathbf{E}^0 = (c\theta\Delta t)\frac{4\pi}{c}\hat{\mathbf{J}}$$

in which the implicit susceptibility is given by,

$$\mu \cdot \mathbf{E} = \mathbf{E} + \Sigma_s \omega_{ps}^2 \Delta t^2 \frac{\mathbf{E} + \alpha_s \mathbf{E} \times \mathbf{B} + \alpha_s^2 \mathbf{E} \cdot \mathbf{BB}}{1 + \alpha_s^2 B^2} \ .$$

and $\mathbf{E}^\theta$ is the unknown electric field at mid-time step [*Vu and Brackbill*, 1992]. The terms on the right hand side are from the previous time step, or calculated explicitly from the particle data.

When the spatial derivatives appearing in the equation for the electric field are approximated by finite differences, there results a system of equations that can be written in matrix form. The matrix is non-symmetric with variable coefficients. The $\mathbf{E} \times \mathbf{B}$ term in the equation is, like the convective derivative in fluid flow, anti-symmetric. Direct methods could, in principle, be applied [*Vu and Brackbill*, 1992]. However, in two and three dimensions the size of the matrix and the cost of Gaussian elimination is prohibitive. Instead, one must use iterative methods for nonsymmetric, sparse matrices. In CELEST3D, an implicit moment code in three dimensions, the GMRES method gives satisfactory results [*Saad and Schultz*, 1986].

By comparison, the numerical approximation of the particle equations of motion is straightforward. However, the errors due to large time steps must be controlled. The properties of the leapfrog and Euler methods with large time steps are described in several references [*Vu and Brackbill*, 1995].

3.   When should implicit methods be used

One must be convinced that an implicit plasma simulation is worth the extra cost if one is to choose it over the less expensive and simpler hybrid simulation. We will discuss three examples where a kinetic description of the electrons appears to be essential to a correct solution.

The earliest is the discovery of a propagating, self-generated magnetic field in a laser heated plasma [*Forslund and Brackbill*, 1982]. There electron drifts in the magnetic and electric fields resulted in energy deposition patterns that were visible to the eye [*Yates et al.*, 1982].

More recently, numerical simulations of the slow-mode switch-off shock with kinetic electrons give significantly different results from hybrid simulations with fluid electrons [*Brackbill and Vu*, 1993]. With appropriate downstream boundary conditions there results a more coherent trailing magnetic wave with fewer back-streaming ions than with the hybrid model under the same conditions. In addition, the trailing magnetic wave is more strongly damped. One underlying cause of these differences is that with kinetic effects, there is a more equal sharing of shock-induced entropy increases between ions and electrons than there is in comparable hybrid calculations. The increased sharing results in lower ion temperatures downstream and greater electron energy transport from downstream to upstream. (In the slow shock calculations, $\omega_{pe}\delta t = 50$ and $\lambda_D/\delta x = 9 \cdot 10^{-4}$, where λ_D is the electron Debye length. That is, the time step is 50 times larger and the grid spacing 1000 times larger than allowed in an explicit calculation.)

In hybrid simulations of a contact discontinuity, an electron pressure gradient causes a barrier potential to form that suppresses the interpenetration of hot and cold particles

across the discontinuity [*Wu et al.*, 1994]. The barrier potential is observed to increase with the electron temperature. In implicit simulations with kinetic electrons, where the electrons are free to move relative to the ions, the barrier potential does not form and the contact discontinuity rapidly diffuses [*Brackbill and Lapenta*, 1996]. The latter result is the correct one. In the hybrid model, the fluid electron energy equation contains insufficient physics to model the energy transport that occurs due to relative motion of electrons and ions.

In these examples, the time step is much larger than the electron plasma period. Since the maximum frequency that can be represented by a numerical calculation with time step Δt is the Nyquist frequency, $2\pi/\Delta t$, the essential contribution of the electrons cannot be on the fast time scale. In fact, unresolved waves , those for which $\omega \Delta t > 2\pi$, are strongly damped numerically. The essential contribution appears to be that the solution of the electron kinetic equations captures certain essential features of the correct electron energy equation, such as electron energy transport and the correct electron pressure, which are not correctly modeled by the fluid electron equations.

4. Multiple length scale problems and adaptive grids

All parts of the physical domain for a plasma physics modeling problem may not have equal importance, for example collisionless shocks and magnetic reconnection. Multiple length scale problems are effectively modeled using solution adaptive grids [*Brackbill*, 1993] . Such grids, which move grid points from one place to another to concentrate zones in certain regions, focus the computational effort in the regions of short length scales. Furthermore, by decreasing the concentration of zones in regions of long length scales, one can avoid wasting computational resources where they are not needed. An adaptive grid is especially useful if the location of regions with strong gradients is not know a priori.

On an adaptive mesh, variation in the grid spacing to resolve gradients may result in large cells having too many particles, and small cells having too few. The variation in the number of particles per cell can be an obstacle to parallelization, it certainly can limit the accuracy of the method if some cells have too few particles, and it imposes a limit on the adaptability of the mesh by imposing a lower bound on the grid spacing to prevent cells with too few particles.

The dynamic control algorithm should be selective so that it can change the number of particles in selected cells; and dynamic, so that it can act as necessary to keep the number of particles in a cell within a prescribed range [*Lapenta and Brackbill*, 1994] .

The algorithm replaces N particles located in a cell by $N+1$ particles, if a particle is split, or $N-1$ particles, if two particles are coalesced. In splitting and coalescing, no knowledge of the distribution in velocity is assumed. This knowledge is difficult to derive from the data in a cell, and approximations, such as the first few moments of the distribution, are insufficient. Thus, the algorithm splits one particle into two with the same velocity, or coalesces two particles with nearly the same velocity into one.

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