

A fully implicit 3D extended magnetohydrodynamics algorithm

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Introduction

The extended magnetohydrodynamics model (XMHD) includes effects such as nonlinear transport and two-fluid (Hall) effects. XMHD supports multiple, disparate time scales that make explicit time-differencing approaches extremely inefficient. While a fully implicit implementation promises efficiency without sacrificing numerical accuracy [1], the nonlinear nature of the XMHD system and the numerical stiffness of its fast waves make this endeavor very difficult.

Newton-Krylov methods are, however, ideally suited for such a task. They combine Newton's method for nonlinear convergence and Krylov techniques to solve the associated Jacobian (linear) systems. Krylov methods can be implemented in a Jacobian-free fashion (avoiding forming and storing the Jacobian matrix), and can be preconditioned for efficiency [2, 3]. The preconditioning step considers an inexpensive approximation to the Jacobian inverse to enhance the Krylov iteration convergence rate, and can be easily incorporated into the Krylov algorithm. Here, we advocate “physics-based” preconditioning strategies [2, 3], in which knowledge of the physics is exploited to derive well-conditioned (diagonally dominant) approximations to the original system that are amenable to optimal multilevel solver technologies.

The focus of this document is to discuss progress in the preconditioning strategy for the 3D primitive-variable extended MHD formalism (including two-fluid physics). It complements previously presented work at this meeting [4], which focused on resistive MHD and demonstrated the feasibility of the concept. We will demonstrate here the potential of the concept to deliver large CPU speedups (~ 30) vs. explicit approaches.

Implicit Time Integration and Newton-Krylov methods

Traditionally, computational methods for MHD have been mostly based on explicit and semi-implicit methods. While conceptually simple, explicit techniques are inappropriate for multiple-time-scale problems, since they must resolve the fastest time scale supported by the model. Semi-implicit methods can effectively step over explicit time-step constraints, but concern exists about their accuracy for large time steps. Implicit methods, however, can step over fast time scales to accurately resolve the dynamical time scale, but a large-scale system of nonlinear equations must be solved every time step. Nevertheless, large CPU speedups over explicit methods are possible [2, 3, 4], as will be shown here.

To invert the large-scale system of nonlinear equations, we employ Newton-Krylov (NK) methods [5]. These are Newton-based methods which employ Krylov subspace techniques (GMRES in this work) to iteratively solve the associated linear systems. Krylov methods feature two main advantages: they can be implemented Jacobian-free, and they can be preconditioned. Preconditioning consists in operating on the system matrix \mathbf{J} with an operator \mathbf{P}^{-1} (preconditioner) such that \mathbf{JP}^{-1} (right preconditioning) or $\mathbf{P}^{-1}\mathbf{J}$ (left preconditioning) is well-conditioned (i.e., $\mathbf{P}^{-1} \approx \mathbf{J}^{-1}$). Here, we focus on right preconditioning, where the equivalent system $(\mathbf{JP}^{-1})(\mathbf{P}\delta\mathbf{v}) = -\mathbf{G}(\mathbf{v})$ is considered. Notice that the preconditioned system is equivalent to the original system for any nonsingular operator \mathbf{P}^{-1} . Thus, the choice of \mathbf{P}^{-1} does not affect the accuracy of the final solution, but crucially determines the efficiency of the algorithm.

The linear Jacobian systems that result from coupled multi-physics, multiple-time-scale systems are very ill-conditioned due to the presence of fast-time-scale phenomena (e.g., waves). An important new class of preconditioners for NK methods that addresses stiff hyperbolic systems (such as XMHD) is referred to as physics-based or PDE-based (e.g., see [2, 3, 4]). Hyperbolic systems are generally unsuitable for multilevel approaches (e.g., multigrid), which are desirable because they result in a number of Krylov iterations per time step virtually independent of the problem size [2, 3, 4]. Physics-based methods attempt to reformulate such hyperbolic systems into parabolic ones, which are better suited for multilevel methods. We term this procedure “parabolization”. In Ref. [4], we discussed the procedure for resistive MHD. Its generalization for XMHD is described in the next section.

Preconditioning strategy for XMHD

We consider the compressible, two-fluid (single temperature), extended MHD model, given by (normalized using Alfvénic units):

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (1)$$

$$\frac{\partial \mathbf{B}}{\partial t} + \nabla \times \mathbf{E} = 0, \quad (2)$$

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot [\rho \mathbf{u} \mathbf{u} - \mathbf{B} \mathbf{B}] + \overleftrightarrow{T} (p + B^2/2) - \rho \nu \nabla \mathbf{u} = 0, \quad (3)$$

$$\frac{\partial T_e}{\partial t} + \mathbf{u} \cdot \nabla T_e + (\gamma - 1) T_e \nabla \cdot \mathbf{u} = 0, \quad (4)$$

where the plasma is assumed polytropic $p \propto \rho^\gamma$, with γ the polytropic constant, $p = \rho(T_i + T_e)$ the pressure, $T_{i,e}$ the ion/electron temperatures, and ρ the particle density. The electric field \mathbf{E} is given by the extended Ohm’s law:

$$\mathbf{E} = -\mathbf{u} \times \mathbf{B} + \eta \nabla \times \mathbf{B} - \frac{d_i}{\rho} (\mathbf{j} \times \mathbf{B} - \nabla p_e), \quad (5)$$

where $d_i = c/\omega_{pi}$ is the ion skin depth, and is a measure of the importance of two-fluid physics for a given simulation. In these equations, \mathbf{u} is the plasma velocity, \mathbf{B} is the magnetic field, η is the resistivity, ν is the kinematic viscosity.

The XMHD model in Eqs. 1-5 supports dispersive waves with dispersion relation $\omega \sim k^2$, such as the whistler and kinetic Alfvén waves. In explicit methods, the presence of dispersive waves results in explicit CFL time step limits $\Delta t_{CFL} \sim \Delta x^2$, substantially slowing down their numerical integration. In implicit methods, dispersive waves result in very poorly conditioned matrices, of difficult treatment via iterative methods. In the context of Krylov methods, adequate treatment of dispersive waves puts a premium on preconditioning. We proceed here to demonstrate a proof of principle for a preconditioner strategy for XMHD. For this, we focus on the cold ion limit, $T_e \gg T_i$. In this limit, $p \approx p_e$, and therefore the Ohm's law (Eq. 5) reads:

$$\mathbf{E} \approx -\mathbf{u} \times \mathbf{B} + \eta \nabla \times \mathbf{B} - \frac{d_i}{\rho} (\mathbf{j} \times \mathbf{B} - \nabla p) = -\mathbf{u} \times \mathbf{B} + \eta \nabla \times \mathbf{B} - d_i (\partial_t \mathbf{u} + \mathbf{u} \cdot \nabla \mathbf{u} - \nu \nabla^2 \mathbf{u}). \quad (6)$$

With this simplification in mind, the linearized XMHD model in Eqs. 1-4 has the following coupling structure:

$$\mathbf{J} \delta \mathbf{x} \approx \begin{bmatrix} D_\rho & 0 & 0 & U_{\rho\mathbf{u}} \\ 0 & D_T & 0 & U_{T\mathbf{u}} \\ 0 & 0 & D_{\mathbf{B}} & U_{\mathbf{u}\mathbf{B}} + U_{\mathbf{u}\mathbf{B}}^H \\ L_{\rho\mathbf{u}} & L_{T\mathbf{u}} & L_{\mathbf{B}\mathbf{u}} & D_{\mathbf{u}} \end{bmatrix} \begin{pmatrix} \delta \rho \\ \delta T \\ \delta \mathbf{B} \\ \delta \mathbf{u} \end{pmatrix} = - \begin{pmatrix} \mathbf{G}_\rho \\ \mathbf{G}_T \\ \mathbf{G}_{\mathbf{B}} \\ \mathbf{G}_{\mathbf{u}} \end{pmatrix},$$

where subscripts label the relevant dependent variables. The diagonal blocks D contain advection/diffusion contributions, and are “easy” to invert using multilevel techniques. Off-diagonal blocks L and U contain all hyperbolic couplings, and are the source of hyperbolic stiffness in the MHD model. Note the Jacobian matrix has an “arrow” structure. This coupling structure is identical to that of the resistive MHD model [4], but with a new contribution $U_{\mathbf{u}\mathbf{B}}^H$, coming from the modified Ohm's law in Eq. 6. To derive an approximate inverse of this Jacobian matrix, we proceed as in the resistive MHD case [4] by factorizing the following 2×2 block matrix:

$$\mathbf{J} \delta \mathbf{x} = \begin{bmatrix} M & U \\ L & D_{\mathbf{u}} \end{bmatrix} \begin{pmatrix} \delta \mathbf{y} \\ \delta \mathbf{u} \end{pmatrix} = - \begin{pmatrix} \mathbf{G}_{\mathbf{y}} \\ \mathbf{G}_{\mathbf{u}} \end{pmatrix}, \quad (7)$$

with M containing the diagonal blocks for ρ , \mathbf{B} , and T , and approximating $M^{-1} \approx \Delta t I$ in selected places (which amounts to neglecting ion advection and transport time scales) to obtain:

$$\begin{aligned} \delta \mathbf{y}^* &= -M^{-1} \mathbf{G}_{\mathbf{y}} \\ \delta \mathbf{u} &\approx P_{SI}^{-1} [-\mathbf{G}_{\mathbf{u}} - L \delta \mathbf{y}^*]; \quad P_{SI} = D_{\mathbf{u}} - \Delta t L U \\ \delta \mathbf{y} &\approx \delta \mathbf{y}^* - \Delta t U \delta \mathbf{u} \end{aligned}$$

We employ multigrid methods (MG) to approximately invert P_{SI} and M , since both are block-diagonally dominant by construction. The nature of P_{SI} is changed vs. the resistive MHD model by the additional block U_{vB}^H , which results, after the Schur complement treatment, in PDE systems of the form $\partial_t \delta \mathbf{u} - d_i \mathbf{B}_0 \times (\nabla \times \nabla \times \delta \mathbf{u}) = \dots$. We have analytical proof that such systems can in fact be dealt with effectively with multigrid methods.

We demonstrate the performance of such a preconditioner with the tearing mode problem in 2D Cartesian geometry described in Ref. [6], with $d_i = 0.05$. We employ classical MG V(3,3) cycles (with under-damped Jacobi as a smoother and linear tolerance of 10^{-2}) to approximately invert M and P_{SI} . We have fixed the time step to $\Delta t = 1$, which spans anywhere from 100 explicit CFL time steps for the coarsest grid to 3000 for the finest. Grid scaling results are presented in Table 1. Notice from the table that the CPU speedup increases sharply as the grid is refined, reaching a factor of 30 for the finest grid considered. Notice also that the solver does better as the grid is refined. This is due to the fact that differences in spatial truncation errors between the preconditioner and the nonlinear function matter less as the grid is refined.

Grid	Nonlinear its. per Δt	GMRES its. per Δt	CPU (s)	CPU_{exp}/CPU	$\Delta t/\Delta t_{exp}$
32x32	5	22	25	0.44	110
64x64	5	12	66	1.4	238
128x128	5	8	164	6.2	640
256x256	4	7	674	30	3012

Table 1: Grid convergence study for $d_i = 0.05$. Computations span 1 time step.

References

- [1] D. A. Knoll, L. Chacón, L. Margolin, and V. A. Mousseau, *J. Comput. Phys.* **185**, 583 (2003).
- [2] L. Chacón, D. A. Knoll, and J. M. Finn, *J. Comput. Phys.* **178**, 15 (2002).
- [3] L. Chacón and D. A. Knoll, *J. Comput. Phys.* **188**, 573 (2003).
- [4] L. Chacón, in *Proceedings of the 32nd European Physical Society Conference on Plasma Physics* (Tarragona, Spain, 2005).
- [5] C. T. Kelley, *Iterative methods for linear and nonlinear equations* (SIAM, Philadelphia, 1995).
- [6] L. Chacón, *Comput. Phys. Comm.* **163**, 143 (2004).