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**A Scalable Parallel Extended MHD Solver: Application of
Physics-Based Preconditioning to High-Order Spectral
Elements**

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We describe an application of physics-based preconditioning [L. Chacón, L., Phys. Plasmas **15**, 056103 (2008)] to a nonlinear initial-value extended MHD code using high-order spectral elements for spatial discretization.

HiFi is a 2D and 3D nonlinear fluid simulation code, written in Fortran 95, with principal emphasis on extended MHD and magnetic fusion energy. The code is separated into a large solver library and a much smaller application module which links to the library, using flux-source form for the physics equations. Realistic nonlinear and time-dependent boundary conditions have been developed.

Spatial discretization uses high-order C^0 spectral elements on a curvilinear grid. Grid cells are logically rectangular, with spectral elements a Cartesian product of 1D polynomial modal basis functions. Time discretization uses fully implicit Newton-Krylov method with adaptive time steps for efficient treatment of multiple time scales.

Computer time and storage are dominated by solution of large, sparse, ill-conditioned linear systems, arising from the implicit time step and multiple time scales. Static condensation is used to eliminate amplitudes of higher-order spectral elements in terms of linear elements. HiFi is built on the PETSc library [<http://www.mcs.anl.gov/petsc/petsc-as/index.html>] for efficient parallel operation and easy access to many advanced methods for linear and nonlinear system solution.

To achieve a weakly scalable parallel solution, we apply physics-based preconditioning, in which the physical dependent variables are partitioned into two sets as the basis of further reducing the order and increasing the diagonal dominance. In visco-resistive MHD, set 1 consists of density, pressure, magnetic flux function, and current, while set 2 consists of the momentum densities, The

linear system is expressed in block form as

$$\mathbf{L}\mathbf{u} = \mathbf{r}, \quad \mathbf{L} \equiv \begin{pmatrix} \mathbf{L}_{11} & \mathbf{L}_{12} \\ \mathbf{L}_{21} & \mathbf{L}_{22} \end{pmatrix}, \quad \mathbf{u} = \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix}, \quad \mathbf{r} = \begin{pmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \end{pmatrix}.$$

Any matrix of this block form can be formally factored to give

$$\mathbf{L} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{L}_{21}\mathbf{L}_{11}^{-1} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{L}_{11} & \mathbf{0} \\ \mathbf{0} & \mathbf{S} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{L}_{11}^{-1}\mathbf{L}_{12} \\ \mathbf{0} & \mathbf{I} \end{pmatrix},$$

with Schur complement matrix defined by

$$\mathbf{S} \equiv \mathbf{L}_{22} - \mathbf{L}_{21}\mathbf{L}_{11}^{-1}\mathbf{L}_{12}.$$

It is then straightforward to write the solution as

$$\mathbf{s}_1 = \mathbf{L}_{11}^{-1}\mathbf{r}_1, \quad \mathbf{s}_2 = \mathbf{r}_2 - \mathbf{L}_{21}\mathbf{s}_1, \quad \mathbf{u}_2 = \mathbf{S}^{-1}\mathbf{s}_2, \quad \mathbf{u}_1 = \mathbf{s}_1 - \mathbf{L}_{11}^{-1}\mathbf{L}_{12}\mathbf{u}_2.$$

solving only the reduced matrices \mathbf{L}_{11} and \mathbf{S} . We can introduce an approximation $\mathbf{P} \approx \mathbf{L}^{-1}$, use it as a preconditioner, and finish the solution with a preconditioned Krylov iteration, $(\mathbf{L}\mathbf{P})(\mathbf{P}^{-1}\mathbf{u}) = \mathbf{r}$. As long as the preconditioner \mathbf{P} constitutes a sufficiently accurate approximate inverse, the preconditioned Krylov iteration should converge rapidly, in just a few iterations, resulting in an effectively exact solution of the full problem.

The principal difficulty is that, while the block matrices \mathbf{L}_{ij} matrices are sparse, the presense of \mathbf{L}_{11}^{-1} makes \mathbf{S} matrix dense. To avoid this, we approximate \mathbf{S} by reversing the order of discretization and substitution, giving it the form of the well-known ideal MHD force operator. This leads to the approximate Schur complement

$$\mathbf{S} \approx \mathbf{L}_{22} - h^2\theta^2 \langle \nabla \cdot \mathbf{T} \rangle$$

where h is the time step, θ is the time-centering parameter, $\langle \dots \rangle$ represents spectral element discretization; and we express the force operator as

$$\begin{aligned} \mathbf{T} &= \left(\mathbf{B} \cdot \frac{\partial \mathbf{B}}{\partial t} + \frac{\partial p}{\partial t} \right) \mathbf{I} - \mathbf{B} \frac{\partial \mathbf{B}}{\partial t} - \frac{\partial \mathbf{B}}{\partial t} \mathbf{B} \\ &= [\mathbf{B} \cdot \nabla \times (\mathbf{v} \times \mathbf{B}) - \gamma p \nabla \cdot \mathbf{v} - \mathbf{v} \cdot \nabla p] \mathbf{I} \\ &\quad - \mathbf{B} \nabla \times (\mathbf{v} \times \mathbf{B}) - \nabla \times (\mathbf{v} \times \mathbf{B}) \mathbf{B}. \end{aligned}$$

in flux-source form, as required by our spectral element discretization.

The matrices \mathbf{L}_{11} and \mathbf{S} which must be solved have reduced order and are more diagonally dominant than the full Jacobian. They are further reduced by static condensation and then solved by GMRES, preconditioned by additive-Schwarz blockwise LU. This physics-based preconditioning is then followed by Newton-Krylov iteration on the full nonlinear system, using matrix-free GMRES. The convergence rate is measured by the number of KSP iterations required for the

block solves, reflecting the condition number of the preconditioning matrices, and by the number of iterations in the final Newton-Krylov solve, reflecting the accuracy of the approximate Schur complement. Inaccuracy in the Schur complement influences the rate of convergence but not the final solution.

Future efforts will be devoted to weak scaling tests on large parallel computers; exploration of other methods of solution for the reduced preconditioning equations; and extending the approximate Schur complement to include two-fluid effects.