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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 [1] to spectral element discretization. HiFi is a 2D and 3D nonlinear fluid simulation code, written in Fortran 95 for efficient operation on distributed-memory parallel computers, with 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. A large range of realistic nonlinear and time-dependent boundary conditions has been developed.

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

The greatest on computer time and storage is due to the need to solve large, sparse, ill-conditioned linear systems, resulting from multiple time scales. Static condensation is used to eliminate amplitudes of higher-order spectral elements in terms of linear elements by small, local direct solves, leaving reduced-order and better-conditioned matrices, to be solved by distributed parallel iterative methods. HiFi is built on the PETSc library [2] for efficient parallel operation and access to advanced methods of linear and nonlinear system solution. Our goal is weakly scalable parallel solution as problem size and number of parallel processors are scaled up.

Our approach is physics-based preconditioning [1], in which the physical dependent variables are partitioned into two sets as the basis of further reducing the order and increasing the diagonal dominance. For example, 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

$$\mathbf{L}\mathbf{u} = \mathbf{r}, \quad \mathbf{L} \equiv \begin{pmatrix} \mathbf{L}_{11} & \mathbf{L}_{12} \\ \mathbf{L}_{21} & \mathbf{L}_{22} \end{pmatrix}, \quad \mathbf{u} = \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \end{pmatrix}, \quad \mathbf{r} = \begin{pmatrix} \mathbf{r}_1 \\ \mathbf{r}_2 \end{pmatrix}. \tag{1}$$

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

$$\mathbf{L} = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{L}_{21}\mathbf{L}_{11}^{-1} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{L}_{11} & \mathbf{0} \\ \mathbf{0} & \mathbf{S} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{L}_{11}^{-1}\mathbf{L}_{12} \\ \mathbf{0} & \mathbf{I} \end{pmatrix}, \tag{2}$$

with Schur complement matrix defined by

$$\mathbf{S} \equiv \mathbf{L}_{22} - \mathbf{L}_{21}\mathbf{L}_{11}^{-1}\mathbf{L}_{12}. \tag{3}$$

After factorization, a formal inverse can be expressed as

$$\mathbf{L}^{-1} = \begin{pmatrix} \mathbf{I} & -\mathbf{L}_{11}^{-1}\mathbf{L}_{12} \\ \mathbf{0} & \mathbf{I} \end{pmatrix} \begin{pmatrix} \mathbf{L}_{11}^{-1} & \mathbf{0} \\ \mathbf{0} & \mathbf{S}^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ -\mathbf{L}_{21}\mathbf{L}_{11}^{-1} & \mathbf{I} \end{pmatrix}, \tag{4}$$

in which only the solutions of the smaller block matrices $\mathbf{L}_{11}$ and $\mathbf{S}$ are required, thereby already simplifying solution. It is then straightforward to solve the system:

$$\mathbf{s}_1 = \mathbf{L}_{11}^{-1}\mathbf{r}_1, \quad \mathbf{s}_2 = \mathbf{r}_2 - \mathbf{L}_{21}\mathbf{s}_1, \quad \mathbf{u}_2 = \mathbf{S}^{-1}\mathbf{s}_2, \quad \mathbf{u}_1 = \mathbf{s}_1 - \mathbf{L}_{11}^{-1}\mathbf{L}_{12}\mathbf{u}_2. \tag{5}$$

Exact solution of $\mathbf{S}$ is impractical because, while the $\mathbf{L}_{ij}$ are sparse, the presense of $\mathbf{L}_{11}^{-1}$ in Eq. (3) makes $\mathbf{S}$ dense.. We introduce an approximation $\mathbf{P} \approx \mathbf{L}^{-1}$, use it as a preconditioner, and finish the solution with a preconditioned Krylov iteration, $(\mathbf{L}\mathbf{P})\left(\mathbf{P}^{-1}\mathbf{u}\right) = \mathbf{r}$. As long as $\mathbf{P}$ constitutes a sufficiently accurate approximate inverse, the preconditioned Krylov iteration should converge rapidly, resulting in an effectively exact solution of the full problem.

We approximate $\mathbf{S}$ by reversing the order of discretization and substition, giving it the form of the well-known ideal MHD force operator, expressed in terms of the divergence of a stress tensor. This leads to the approximate Schur complement

$$\mathbf{S} \approx \mathbf{L}_{22} - h^2\theta^2 \langle \nabla \cdot \mathbf{T} \rangle \tag{6}$$

with h the time step, θ the time-centering parameter, and brackets representing spectral element discretization. The stress tensor is given by

$$\begin{aligned} \mathbf{T} &= \left(\mathbf{B} \cdot \frac{\partial \mathbf{B}}{\partial t} + \frac{\partial p}{\partial t} \right) \mathbf{I} - \mathbf{B}\frac{\partial \mathbf{B}}{\partial t} - \frac{\partial \mathbf{B}}{\partial t}\mathbf{B} \\ &= \left[\mathbf{B} \cdot \nabla \times (\mathbf{v} \times \mathbf{B}) - \gamma p \nabla \cdot \mathbf{v} - \mathbf{v} \cdot \nabla p \right] \mathbf{I} \\ &\quad -\mathbf{B}\nabla \times (\mathbf{v} \times \mathbf{B}) - \nabla \times (\mathbf{v} \times \mathbf{B})\,\mathbf{B}. \end{aligned} \tag{7}$$

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

The matrices $\mathbf{L}_{11}$ and $\mathbf{S}$ 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 is 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 Newton iterations, reflecting the accuracy of the approximate Schur complement. Inaccuracy influences the rate of convergence but not the final solution.

Future efforts will be devoted to weak scaling tests to determine the limits of this approach on large parallel computers; exploration of other methods of solution for the reduced preconditioning equations, available through PETSc; and extending the physics content of the approximate Schur complement to include two-fluid effects.

Bibliography

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