A Fast, Scalable Parallel Solver for the HiFi Extended MHD Spectral Element Code

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Scalable Parallel Solver for Extended MHD

- **Jacobian-Free Newton-Krylov (JFNK)**
  PETSc SNES solver with Physics-Based Preconditioning. Time-centered solution of full nonlinear system of equations.

- **Physics Based Preconditioning (PBP)**
  Chacón. Reduces full hyperbolic linear system to smaller parabolic systems.
  - Partition 1: Mass matrix **M**
    mass density, plasma pressure, magnetic fields, currents
  - Partition 2: Approximate Schur complement matrix **S**
    fluid velocities

- **Static Condensation (SC)**
  Exploits C^0 continuity of spectral element representation. Uses small, local direct solves to eliminates cell interior degrees of freedom in terms of cell boundaries.

- **Solution of Reduced, Condensed Linear Systems**
  - Solver: CG for SPD matrices, GMRES for non-SPD.
  - Preconditioners
    - Schwarz overlap preconditioned by core-wise SuperLU_DIST.
      Fast and efficient but not scalable, increasing number of Krylov iterations
    - Algebraic multigrid, Hypre/BoomerAMG.
      Scalable for limited range of test cases; smoother requires nodal basis.

Using PETSc Runtime Options to Choose Solvers and Preconditioners

Fortran Source Code

```
c-----------------------------------------------------------------------
c     create linear solver for Schur solver.
c-----------------------------------------------------------------------
      CALL KSPCreate(comm,ctv%ksp,ierr)
      CALL KSPSetOptionsPrefix(ctv%ksp,TRIM(prefix),ierr)
      CALL KSPSetFromOptions(ctv%ksp,ierr)
```

PETSc Runtime Options File `petopt` for Schur Solver

```
-schur_ksp_type cg
-schur_ksp_rtol 1e-8
-schur_ksp_max_it 500
-schur_pc_type hypre
-schur_pc_hypre_type boomeramg
-schur_pc_hypre_boomeramg_max_iter 1
-schur_pc_hypre_boomeramg_tol 0
-schur_pc_hypre_boomeramg_coarsen_type HMIS
-schur_pc_hypre_boomeramg_interp_type ext+I
-schur_pc_hypre_boomeramg_strong_threshold .5
-schur_pc_hypre_boomeramg_relax_type_down SOR/Jacobi
-schur_pc_hypre_boomeramg_relax_type_up backward-SOR/Jacobi
-schur_pc_hypre_boomeramg_grid_sweeps_all 2
-schur_pc_hypre_boomeramg_truncfactor .5
-schur_pc_hypre_boomeramg_P_max 4
```

Weak Scaling Test Case: Sound Waves

Sound Waves

$$\frac{\partial p}{\partial t} + \nabla \cdot \mathrm{v} = 0, \quad \frac{\partial \mathrm{v}}{\partial t} + \nabla p = 0; \quad \frac{\partial^2 p}{\partial t^2} = \nabla^2 p$$

Initial and Boundary Conditions

Periodic plane, traveling waves, initialized to longest wavelength,

$$k_x = k_y = \frac{2\pi}{L}$$

Unit Cell on Each Core

$$nx = ny = np = 8$$

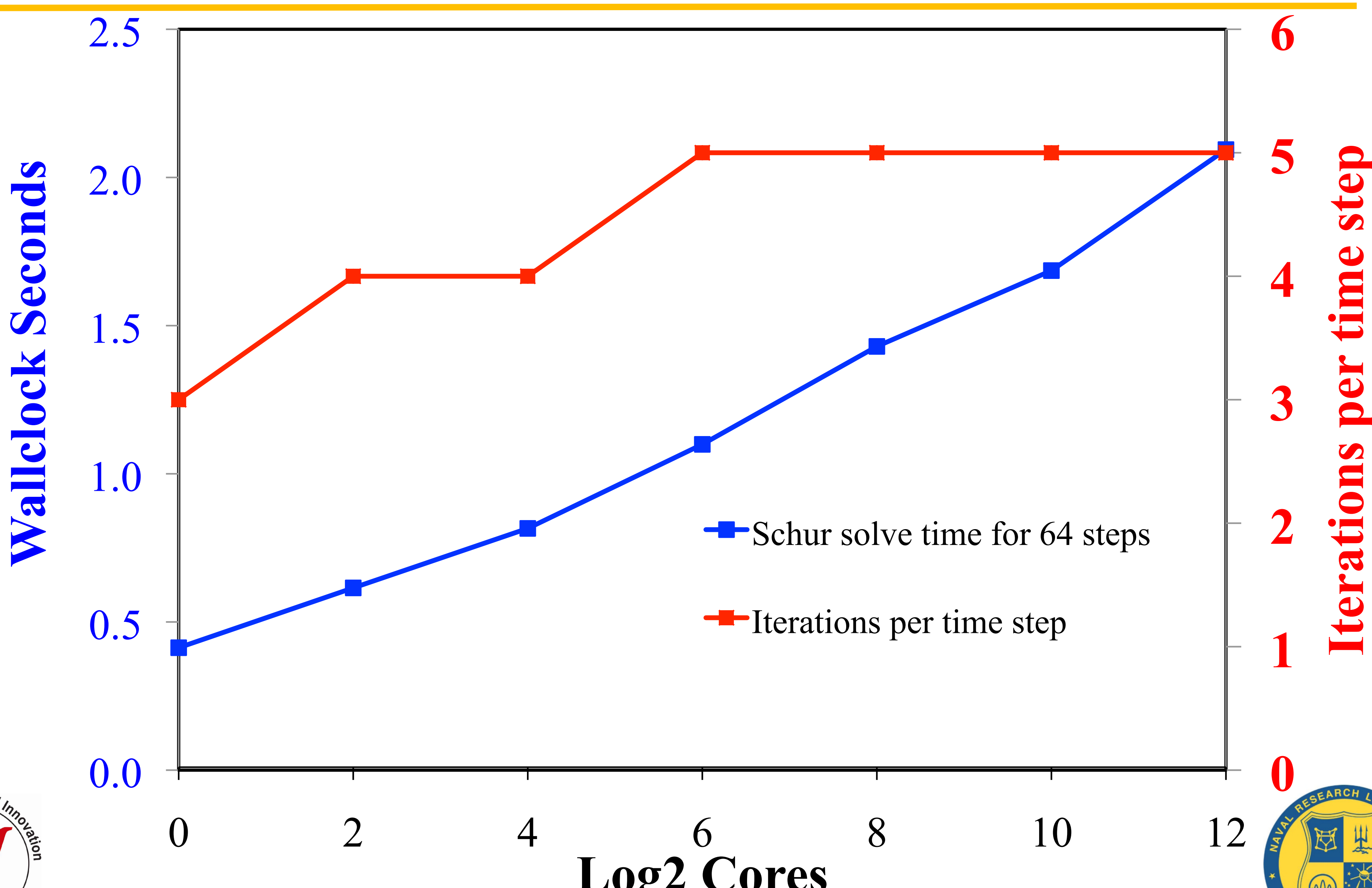
Weak Scaling Tests

L, nx, ny successively doubled, n_{core} successively quadrupled.

Condition Number

$$\kappa(\mathsf{S}) \sim \left(\frac{k_{\max}}{k_{\min}}\right)^2 \sim n_{\mathrm{core}}$$

Weak Scaling Test for Sound Waves



Weak Scaling Test Case: Ideal MHD Waves

Ideal MHD Waves

$$\rho \frac{\partial \mathbf{v}}{\partial t} = \mathbf{j} \times \mathbf{B} - \nabla p, \quad \mathbf{j} = \nabla \times \mathbf{b}$$

$$\frac{\partial \mathbf{b}}{\partial t} = \nabla \times (\mathbf{v} \times \mathbf{B}), \quad \nabla \cdot \mathbf{b} = 0$$

$$\frac{\partial p}{\partial t} + \gamma P \nabla \cdot \mathbf{v} = 0$$

Schur Complement, Ideal MHD Force Operator

$$\mathbf{B} \equiv B\mathbf{n}, \quad c_A^2 \equiv \frac{B^2}{\rho}, \quad c_S^2 \equiv \frac{\gamma P}{\rho}, \quad k_\parallel \equiv \mathbf{k} \cdot \mathbf{n} = k \cos\theta$$

$$\frac{\partial^2 \mathbf{v}}{\partial t^2} = c_A^2 \left\{ \nabla \times [\nabla \times (\mathbf{v} \times \mathbf{n})] \right\} \times \mathbf{n} + c_S^2 \nabla \nabla \cdot \mathbf{v}$$

Shear Alfvén Waves, Fast and Slow Magnetosonic Waves

$$\frac{\omega^2}{k^2} = c_A^2 \cos^2\theta, \quad \frac{1}{2} \left\{ \left(c_A^2 + c_S^2\right) \pm \left[\left(c_A^2 + c_S^2\right)^2 - 4 c_A^2 c_S^2 \cos^2\theta \right]^{1/2} \right\}$$

Initial conditions: longest-wavelength slow wave.

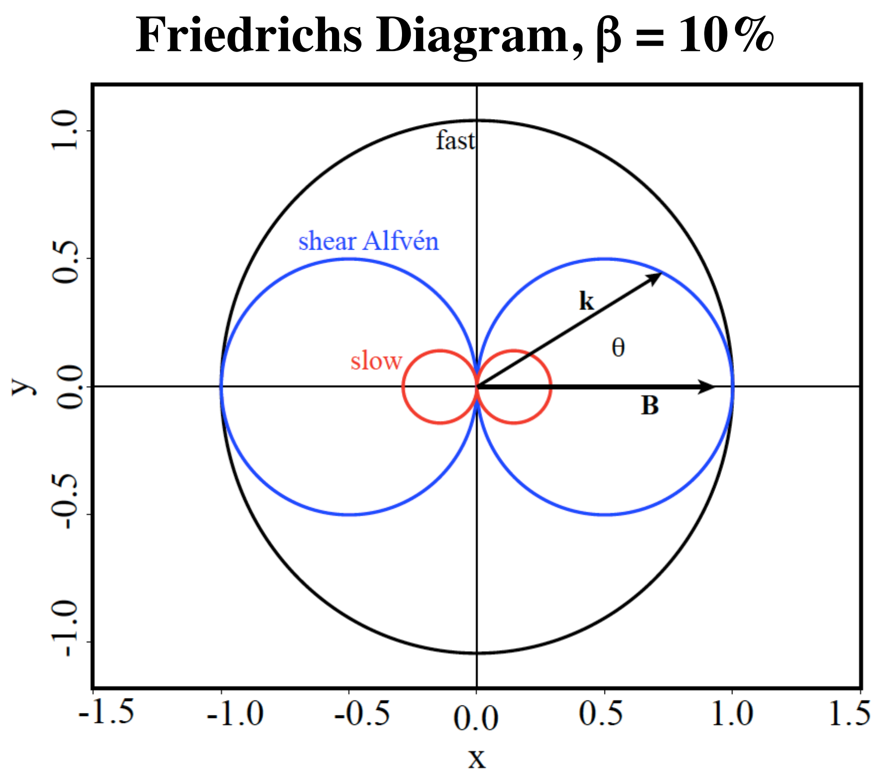
Condition Number

$$\kappa(\mathbf{S}) \sim \left(\frac{k_{\max}}{k_{\min}} \right)^2 \left(\frac{\omega_{\text{fast}}}{\omega_{\text{slow}}} \right)^2$$

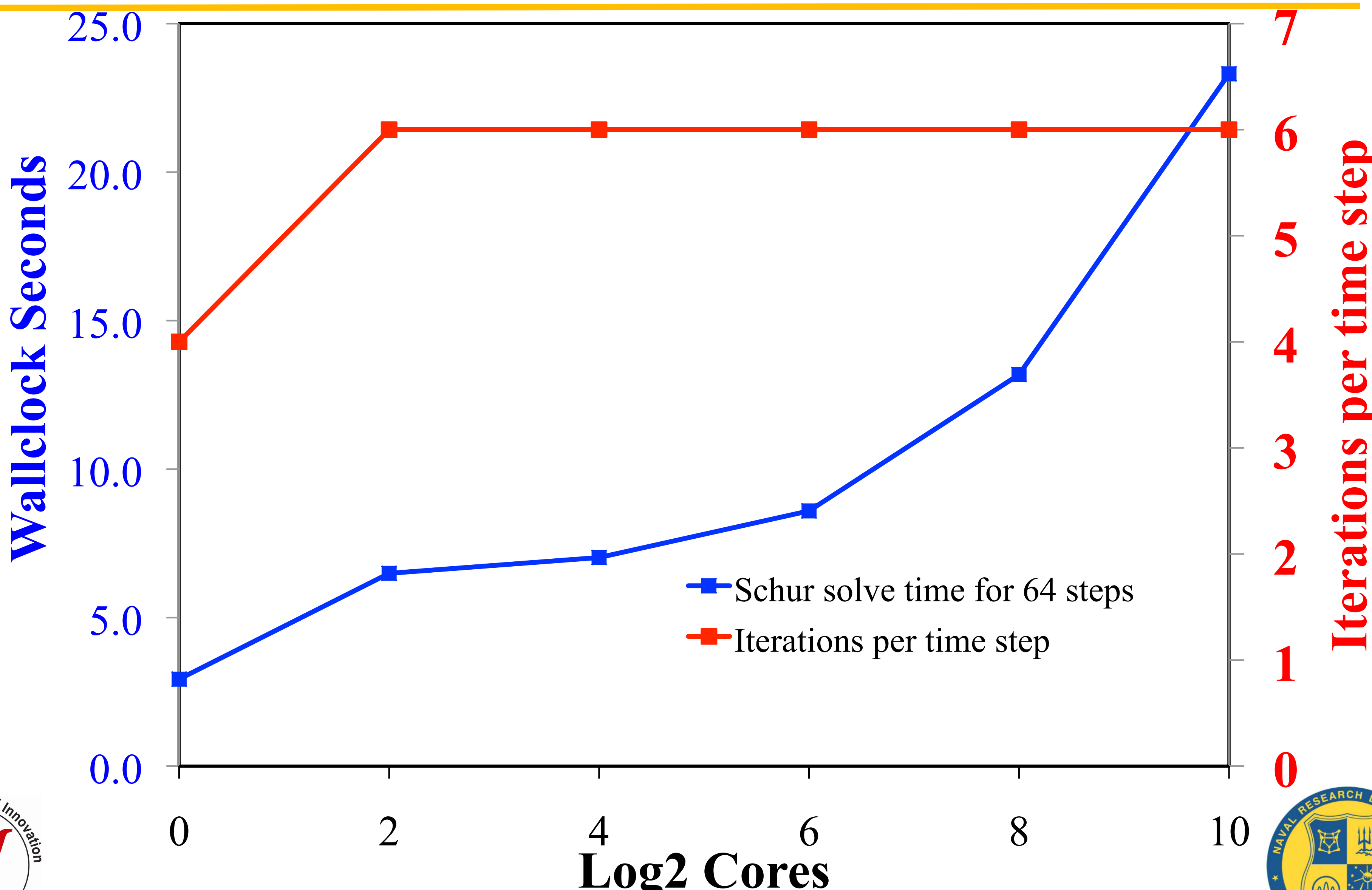
Friedrichs Diagram

Shear Alfvén Waves, Fast and Slow Magnetosonic Waves

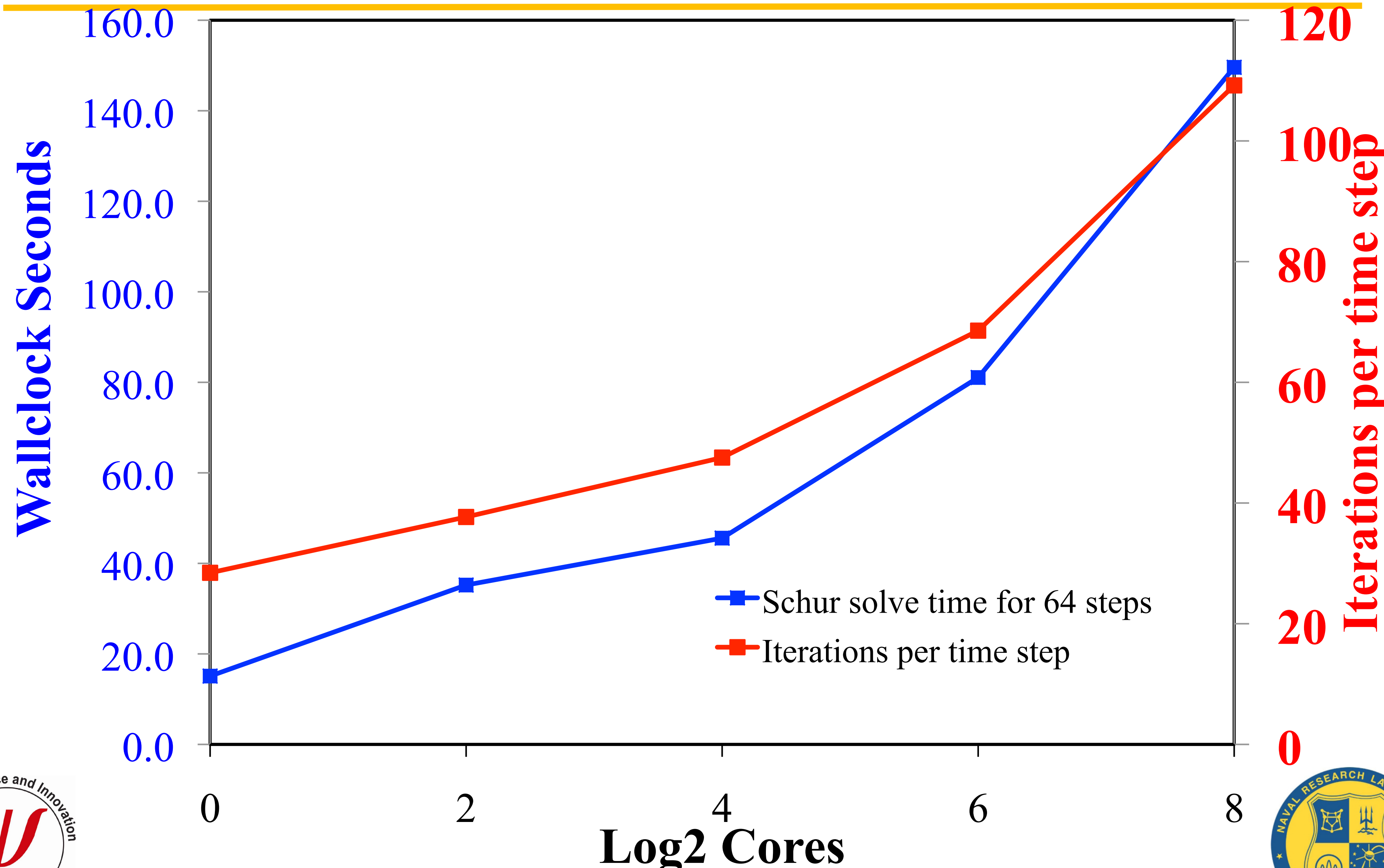
$$\frac{\omega^2}{k^2} = c_A^2 \cos^2\theta, \quad \frac{1}{2}\left\{\left(c_A^2 + c_S^2\right) \pm \left[\left(c_A^2 + c_S^2\right)^2 - 4c_A^2 c_S^2 \cos^2\theta\right]^{1/2}\right\}$$



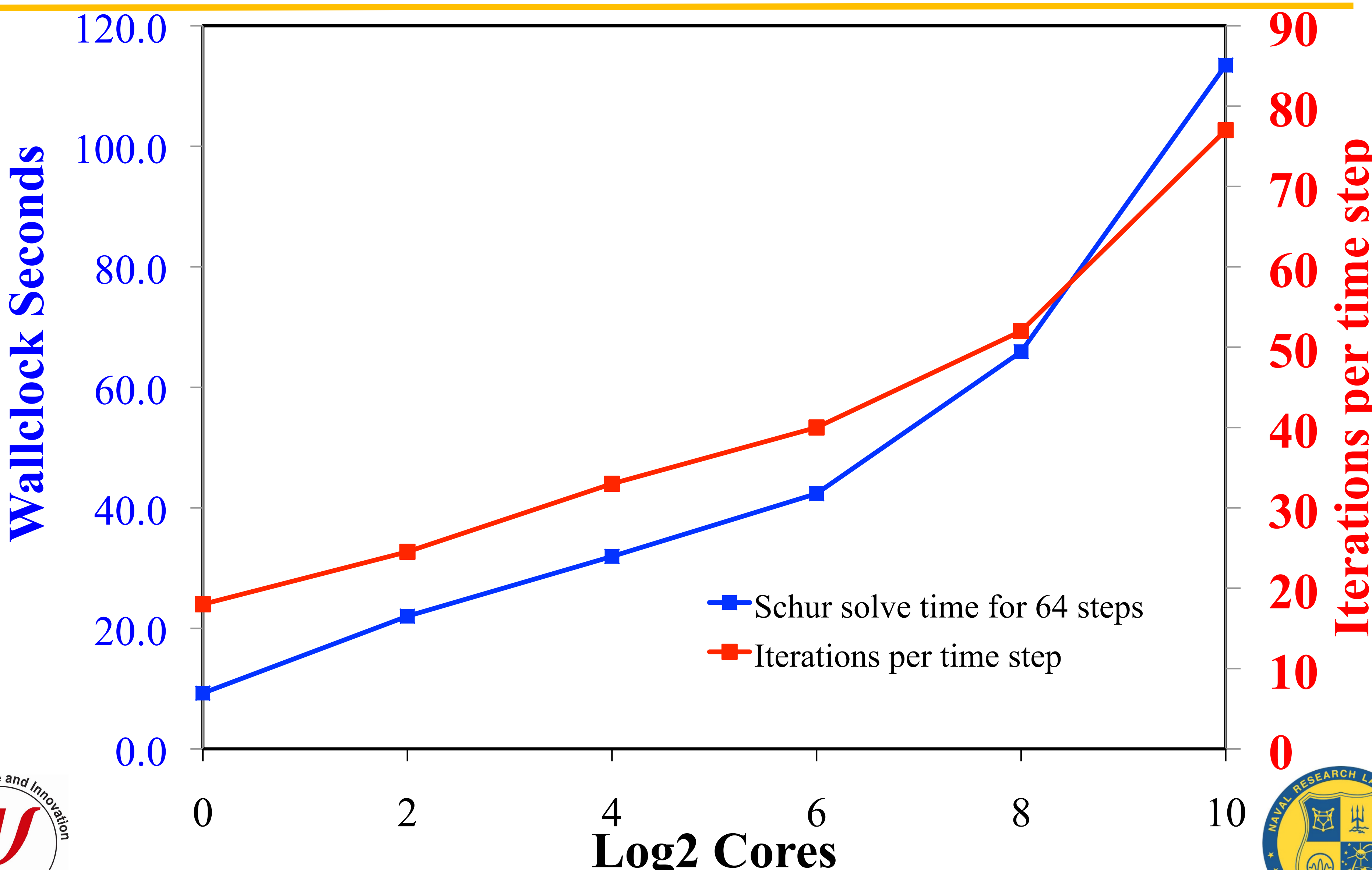
Weak Scaling Test for MHD Waves, θ = 45



Weak Scaling Test for MHD Waves, θ = 75



Weak Scaling Test for MHD Waves, θ = 5



Conclusions About Scaling Tests

- Results are excellent for sound waves and for MHD waves with $\theta = 45°$.
- Hypre/BoomerAMG appears not to handle MHD-type anisotropy well. Results for $\theta = 75°$ and $5°$ scale badly.
- The Hypre Team, (Rob Falgout, Ulrike Yang, Tzanio Kolev) have provided assistance in optimizing runtime parameters of BoomerAMG Algebraic Multigrid and will study this problem further, using data files we've sent.
- Additive Schwarz preconditioner with core-wise Superlu provides an alternative which is reliable and reasonably fast, but not scalable. Increasing number of iterations.

Status of 3D Implementation

- Extension to a 3rd dimension of the HiFi code is straightforward because of the uniformity of spectral element representation in all directions.
- Enhanced source code for static condensation and new source code for physics-based preconditioning have been ported to 3D HiFi code.
- 3D sound wave test problem has been set up and run successfully.
- Preliminary testing of solvers has been successfully demonstrated.
- PETSc profiling has been used to determine timing of multiple code stages. Bottleneck in Gaussian quadratures for matrix elements and rhs. Solution: flatten 3D indices to a single index, reduce memory access time and number of nested do-loops.
- Collaboration with HYPRE Team, Rob Falgout, to understand and improve scaling of BoomerAMG on MHD waves.
- Future 3D Tests:
  - Sound waves
  - Ideal MHD waves
  - Merging spheromaks

The Limits of Scalable Computing?


THE TOPS IN FLOPS

SUPERCOMPUTERS ARE NOW RUNNING OUR SEARCH ENGINES AND SOCIAL NETWORKS. BUT THE HEADY DAYS OF STUNNING PERFORMANCE INCREASES ARE OVER BY PETER KOGGE

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