NIMROD Project Overview

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Project Overview

- NIMROD models the macroscopic dynamics of magnetized plasmas by evolving the visco-resistive Magnetohydrodynamic (MHD) equations and extended models for two fluid and kinetic effects.
- NIMROD has been in development for 11 years and continues to evolve today.
- The project is a collaboration across many institutions
  - University of Wisconsin
  - University of Washington
  - Utah State University
  - University of Colorado
  - University of Tulsa
  - Tech-X Corp - Boulder, Colorado
  - General Atomics - San Diego, CA
- Primarily funded by the DOE
  - Center for Extended MHD Modeling (CEMM) SciDAC
  - Plasma Science and Innovation Center (PSI Center)

The Science

- NIMROD evolves fluid based models of magnetized plasmas.
- A finite element representation is employed in the poloidal plane.
- A finite Fourier series representation is used in the toroidal direction.
- NIMROD is currently being used to model both laboratory and astrophysical plasmas.

$$\frac{\partial \vec{B}}{\partial t} = -\nabla \times \vec{E} + \boxed{\kappa_b \nabla\, \nabla \cdot \vec{B}} \qquad \vec{E} = -\vec{v} \times \vec{B} + \eta \vec{J}$$

$$\frac{\partial n}{\partial t} + \nabla \cdot (n\, \vec{v}) = \boxed{\nabla \cdot (D\, \nabla n)} \qquad \mu_o \vec{J} = \nabla \times \vec{B}$$

$$\rho\, \frac{\partial \vec{v}}{\partial t} + \rho\, (\vec{v} \cdot \nabla)\, \vec{v} = -\nabla p + \vec{J} \times \vec{B} + \nabla \cdot \nu\, \rho \nabla \vec{v}$$

$$\frac{n}{\gamma - 1}\left(\frac{\partial T}{\partial t} + (\vec{v} \cdot \nabla) T\right) = -\frac{p}{2} \nabla \cdot \vec{v} - \nabla \cdot \vec{q} + Q$$

Parallel Programming Model

- Code is implemented in F90 with couplings to external C packages.
- Parallel communications use MPI (distributed memory).
    - Blocks of finite elements are distributed across processors.
    - Fourier components are distributed across processors.
- Most large computations are performed at NERSC
    - Bassi
    - Seaborg
- Smaller computations are performed on local beowulf clusters.

Computational Methods

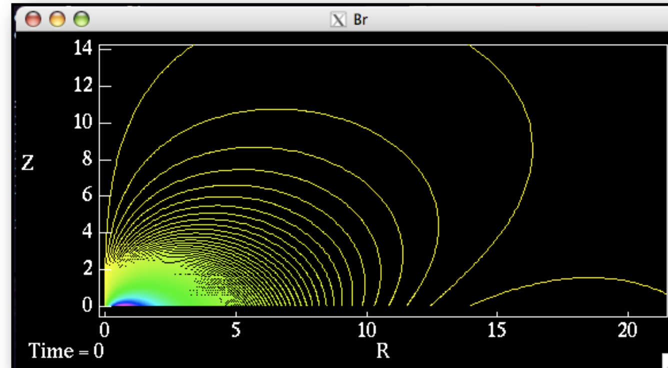
- NIMROD solves time dependent PDE's as initial value problems using implicit methods.
- 2-D and 3-D operations produce algebraic systems which must be solved during each time step (~10,000's over a nonlinear simulation).
    - Conjugate gradient method
    - GMRES
- 3-D couplings in the toroidal direction are computed with FFT's in matrix-free solves.
- 2-D systems represent coupling over the finite element mesh only.
    - Calculated using high-order Lagrange type finite elements.
    - Matrix elements are computed.
    - The 2-D coupling matrices are also generated for preconditioning the 3-D matrix-free solves
    - Direct factorization for preconditioning - SuperLU

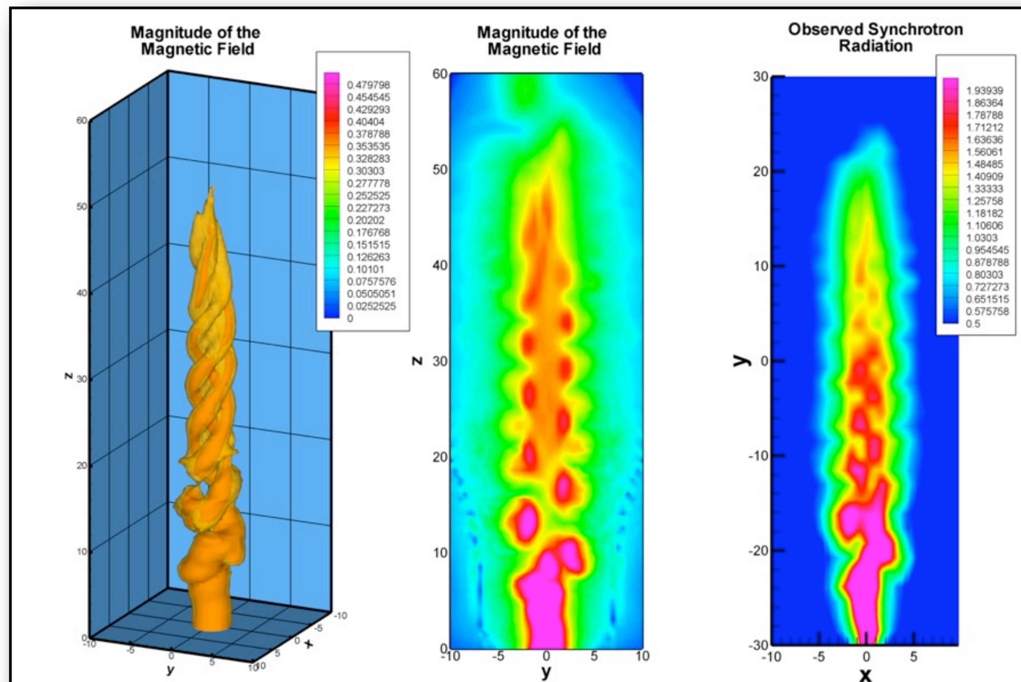
I/O Patterns and Strategy

- A dump file containing the field data is created periodically during the computation.
  - Can be up to 100's of megabytes in size
- The calculation can be restarted from the dump files.
- A single process writes the dump file after collecting field data from all of the other processes

Visualization and Analysis

- Nimplot is a custom post processing application which is used to convert NIMROD dump files for plotting.
- Xdraw is used for quick visualization.
- Tecplot is generally used for more advanced data analysis.
- Exploring using VisIt (Lawrence Livermore) for our advanced data analysis.





Performance

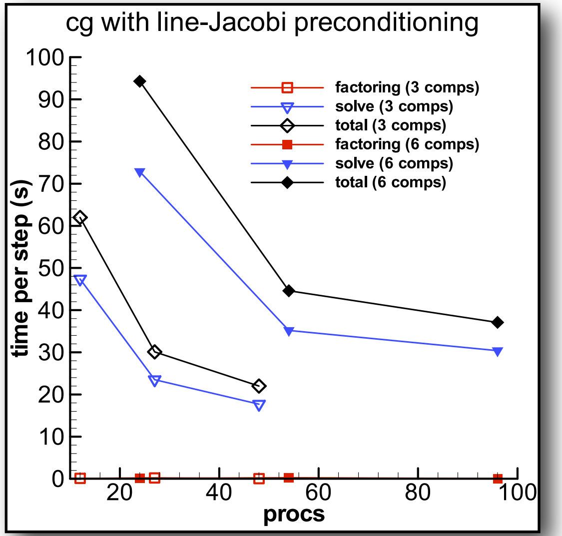
- Solving algebraic systems is the dominant performance issue.
- Iterative methods scale well but tend to perform poorly on ill-conditioned systems.
- Collaborations with TOPS Center researcher Sherry Li led us to parallel direct methods with reordering using SuperLU
    - Improved NIMROD performance by a factor of 5 in nonlinear simulations
- Algebraic solves remain our limit in scaleability
    - SuperLU developers are working on strategies for improving scaleability
    - Using an incomplete factorization may help the scaling for our application
    - Exploring coupling NIMROD to PETSc to access HYPER for multi-grid

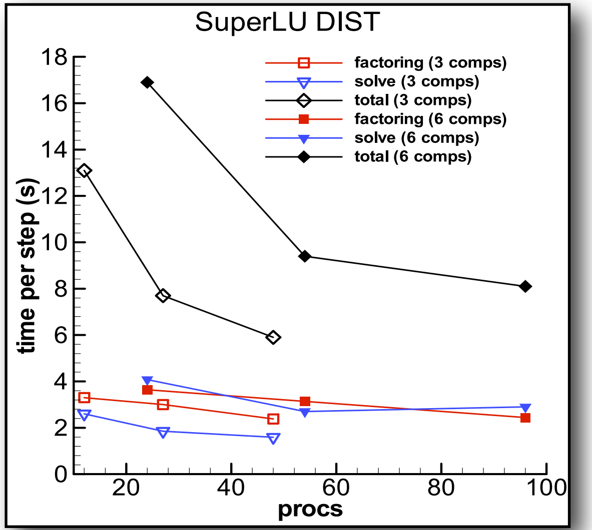
Tools

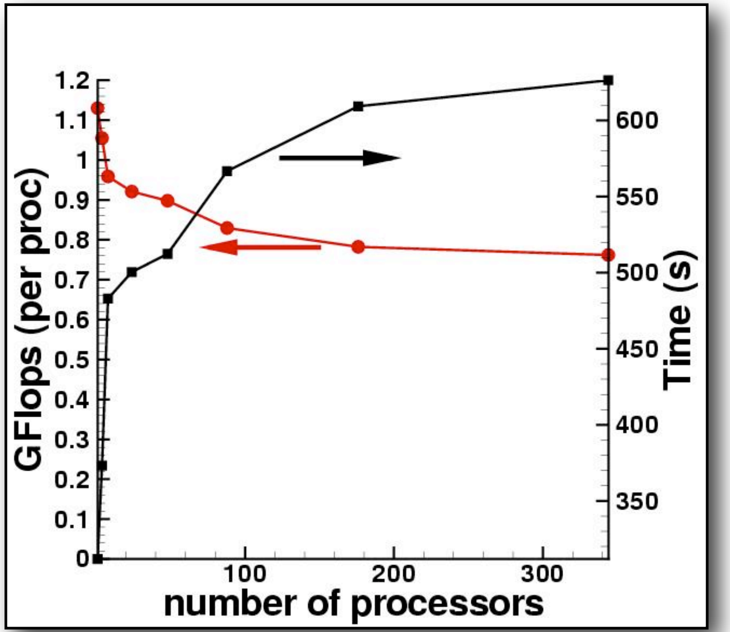
- Code debugging is performed using Totalview and command line based debuggers (gdb).
- Gprof has been used for optimization.
- HELP!!!!!

Scalability

- The fluid component of NIMROD scales to hundreds of processors.
  - Achieved using the distributed version of SuperLU.
- Nonlocal closures to the MHD equations more easily scale to thousands of processors.







Roadmap

- A relatively new algorithm for two fluid physics has been implemented
  - This makes the algebraic systems non-symmetric
  - Preconditioning of toroidal coupling in 3D systems is needed
- Computations with much greater resolution are needed to simulate realistic parameters for laboratory plasmas.
- Simulations with kinetic modeling will be more computationally intensive but scale more readily than fluid-only computations.
- NIMROD will be a component of integrated plasma modeling.