Status and Plans for the NIMROD Code Development Project

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OUTLINE

I. NIMROD introduction
   A. Participants
   B. Objectives
   C. Product

II. Physics Kernel
   A. Revised formulation
   B. Development status
   C. Linear solver

III. Benchmarking
   A. Plan
   B. Linear results for comparison

IV. Graphical User Interface

V. Preprocessing

VI. Postprocessing
   A. XDRAW
   B. IBM Data Explorer
OBJECTIVES


2. Provide a flexible computational tool for alternates.

3. Explore the use of concurrent engineering and quality function deployment in large-scale code development.

PRODUCT

**Non-Ideal MHD with Rotation: Open Discussion**

- Time-dependent, time-split, implicit fluid simulation code.
- Realistic, flexible geometry via finite element discretization of the poloidal plane.
- Pseudospectral representation of the periodic direction.
- Block decomposition of the computational domain for parallel computing on message passing architectures.
- Graphical User Interface for easy use.
- Multi-level graphics for routine and publication quality output.
PHYSICS KERNEL

Original numerical formulation:

\( \mathbf{J}_S \text{ equations} \rightarrow \text{Ampere’s law} \rightarrow \text{implicit } \mathbf{E} \text{ equation.} \)

Unacceptable coupling of shear and compressional Alfven waves.

Revised formulation:

Generalized Ohm’s law \( \rightarrow \) Faraday’s law \( \rightarrow \) implicit \( \mathbf{B} \) equation.

Better numerical properties (see Glasser, et al.)
Time-discrete Equations (Cold Plasma)

\[ Z = -q_i/q_e \]
\[ \nu = Z e m_e/m_i \]
\[ m = m_i/Z_e + m_e \]
\[ n = n_e, \text{ electron number density} \]
\[ \rho = mn = m_i n(1 + \nu)/Z_e, \text{ mass density} \]
\[ M = m_i J_i/q_i + m_e J_e/q_e, \text{ momentum density} \]
\[ f_\Omega = \text{numerical time-centering parameter} \]

\[ \frac{\Delta J_s}{\Delta t} + \frac{f_\Omega q_s}{m_s} B^* \times J_s^{n+1} = \frac{n_s q_s^2}{m_s} \mathbf{E} + \frac{(f_\Omega - 1) q_s}{m_s} B^* \times J_s^n \]

\[ \mathbf{E} = 1 \frac{\Delta \mathbf{J}}{\varepsilon_0 \omega_p^2 \Delta t} + f_\Omega B^* \times \left( \frac{1}{\rho} M^{n+1} - \frac{1 - \nu}{1 + \nu} \frac{1}{en} J^{n+1} \right) \]
\[ + (1 - f_\Omega) B^* \times \left( \frac{1}{\rho} M^n - \frac{1 - \nu}{1 + \nu} \frac{1}{en} J^n \right) \]

\[ M^{n+1} = M^n + \Delta t \left( f_\Omega \Delta \mathbf{J} + J^n \right) \times B^* \]

\[ \mathbf{E}_{imp} = \frac{1}{\varepsilon_0 \omega_p^2} \frac{\Delta \mathbf{J}}{\Delta t} + \frac{f_\Omega^2 \Delta t}{\rho} \left( B^{*2} - B^* B^* \right) \cdot \Delta \mathbf{J} - \frac{1 - \nu}{1 + \nu} \frac{f_\Omega}{en} B^* \times \Delta \mathbf{J} \]

\[ \mathbf{E}_{exp} = \frac{1}{\rho} \left[ B^* \times M^n + f_\Omega \Delta t \left( B^{*2} - B^* B^* \right) \cdot J^n \right] - \frac{1 - \nu}{1 + \nu} \frac{1}{en} B^* \times J^n \]

\[ \Delta \mathbf{B} + \nabla \times \mathbf{Z} \cdot \nabla \times \Delta \mathbf{B} = -\Delta t \nabla \times \mathbf{E}_{exp} \]

\[ \mathbf{Z} = \frac{c^2}{\omega_p^2} \mathbf{I} + \frac{f_\Omega^2 \Delta t^2}{\mu_0 \rho} \left( B^{*2} - B^* B^* \right) - \frac{(1 - \nu)}{1 + \nu} \frac{f_\Omega \Delta t}{\mu_0 en} B^* \times \mathbf{I} \]
Present Status

• Revised formulation including conforming/nonconforming approximation options.
• Two types of grid blocks: 1) rectangular blocks of structured quadrilateral cells, 2) blocks of unstructured triangles.
• Cold plasma equations (except semi-implicit term for Hall dynamics).
• Nonzero electrical resistivity (implicit).
• F90 conjugate gradient solver with diagonal preconditioning for blocks of triangles and either diagonal or direct, domain-decomposition preconditioning on rectangular blocks.
• Message passing for parallel computing (see Plimpton, et al.).

In-progress and Planned Development

• Multiple toroidal modes and FFTs for pseudospectral operations.
• Pressure evolution equation including anisotropic thermal conduction.
• Explicit advection terms.
• Neoclassical closure terms.
• Arbitrary unit vectors.
• \( \nabla \cdot \mathbf{B} \) cleaning.
• Multi-grid preconditioning for cg solver.
NIMROD Physics Kernel Development

1996 1997

Project Organization

Algorithm Decisions

Cold Plasma Development

Pressure and Density Equations

Multiple Toroidal Modes and FFTs

Blocks of Unstructured Triangles

Neoclassical Closures

Projected

Actual
Force-free, Ideal Linear Results for Comparison
(Computed by S. A. Galkin, Keldysh Institute of Applied Mathematics with the TWIST-R and RESTOR codes.)
BENCHMARKING

NIMROD VALIDATION PLAN (DRAFT 9/20/96 Rev. 1)

I. Stable linear oscillations (MHD limit only)
   A. Uniform Bphi, no current
      1. Zero beta, 2-D
         a. Compressional Alfvén waves, plasma
            oscillations, whistler waves, all cases
            have perfectly conducting plasma
            i) Rectangular region - frequency known
               analytically * Uniform grid
                  - Explicit
                  - Implicit
               * Non uniform grid
                  - Explicit
                  - Implicit
            ii) Cylindrical region
               * Multiple blocks with seams
      2. Zero beta, 3-D
         a. Compressional Alfvén waves, plasma
            oscillations, whistler waves - n=0 -
            Repeat the above test to assure there are
            no surprises.
         b. Torsional Alfvén waves, n > 0 - Compare
            frequency with analytic (?) solutions and
            with GATO. (Initialize with GATO)
eigenfunction?) Both explicit and implicit cases. i) Single block grid
   ii) Multiple block grid with seams
3. Finite beta, 2-D
   a. Electron sound waves (turn off ions)
   b. Ion sound waves (both species on)
   c. Drift waves
4. Finite beta, 3-D redo 2-D cases

B. Force-free toroidal equilibria - Comparision with GATO frequencies and eigenfunctions. (Are there any analytic equilibria of this sort?)

II. Linear unstable modes, 3D (Ideal MHD limit)

A. Internal modes (perfectly conducting boundary at separatrix).
   1. Force-free toroidal equilibria (are there any that we understand?)
   2. Finite beta

   a. Solov'ev equilibrium - Internal kink modes
      i) Berger, et al, paper (growth rates and eigenfunctions)
      ii) comparison of marginal points with Berger, et al., and DCO

   b. Numerical equilibria - Compare growth rates and eigenfunctions with GATO, Keldish codes, marginal points with DCON

      i) DIIIID
      ii) TFTR
      iii) ITER
      iv) etc, etc, etc........

B. External modes - vacuum region - Comparisons with GATO.

III. Linear unstable modes (Resistive MHD)
A. Compare with Carreras, et al (n = 2 tearing mode in a circular cross section torus) - Growth rate and eigenfunction

B. Any other known toroidal solutions (Keldish codes?)

C. Marginal points (DCON?)

IV. Linear unstable modes with 2-Fluid effects

A. Cylindrical case (Pic3d comparison) 1. Ideal
   (1,1) mode
   2. Resistive (2,1) mode
B. Toroidal case (QIP3D comparison)
   1. Resistive (1,1) mode
   2. Resistive (2,1) mode

V. Nonlinear evolution (Ideal and resistive MHD) - We need to identify a nonlinear codes.
   A. Internal modes???
   B. External modes (requires moving separatrix)???

VI. Thermal Conductivity - Test pollution of perpendicular transport in highly anisotropic cases. Impose islands and see how well temperature conforms to the flux surfaces.

VII. Nonlinear evolution with 2-Fluid effects
   A. Cylindrical case (Pic3d comparison)
      1. Ideal (1,1) mode
      2. Resistive (2,1) mode
   B. Toroidal case (QIP3D comparison)
      1. Resistive (1,1) mode
      2. Resistive (2,1) mode

VIII. Neo-Classical effects - We need to define a suite of test problems here, too.
IX. Comparison with experiment - We need help here, too.
Shear Alfven Wave Tests

• Uniform rectangular grid, doubly periodic, 1m on a side.
• Neither $k$ nor $B$ are aligned with the grid ($k_x=k_y=2\pi$, $k_z=2^{3/2}\pi$).

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GRAPHICAL USER INTERFACE
(NIMEXEC and supporting scripts)

Tcl scripts presently provide:
• job status information and control
• convenient input file editing
• links to preprocessing and postprocessing codes

Future developments will allow remote job control.

See demonstration.

PREPROCESSING
(NIMSET & FLUXGRID)

• Read equilibrium code output.
• Generate grid based on flux surfaces.
• Generate block connections and vertex connections within blocks of unstructured triangles.
• Initialize physical fields such as $B_0$ and momentum density perturbations.
• Write an initial dump file.
POSTPROCESSING

Routine graphics (XDRAW):
- Grid plots
- Spatial slicing
- Slices showing temporal dependence
- Time-history traces
- Contour plotting of multi-block problems is being developed by N. Popova

IBM Data Explorer
- Multi-dimensional movies
- Sophisticated, 3D data rendering available

See demonstration.