NIMROD Fluid Development and Application

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Outline

• Nonlinear gyroviscous stress
• Temperature-dependent parallel viscosity
• Fluid electron stress
• Optimization efforts
• Pegasus injection computations
• HIT-II computations
• Plans for the coming year
Nonlinear gyroviscous stress: (with leverage from CEMM) NIMROD now has the Braginskii ion gyroviscous stress as one of the additive ion stress options.

- Only ion contributions to stress are significant for the center-of-mass flow velocity evolution.

\[
\rho \left( \frac{\partial \mathbf{V}}{\partial t} + \mathbf{V} \cdot \nabla \mathbf{V} \right) = \mathbf{J} \times \mathbf{B} - \nabla p - \nabla \cdot \Pi_i(\mathbf{V})
\]

\(\Pi_i\) is a combination of \(\Pi_{gv}\), \(\Pi_{\parallel}\), and \(\Pi_{\perp}\)

\[
\Pi_{gv} = \frac{m_i p_i}{4eB} \left[ \hat{b} \times \mathbf{W} \cdot \left( \mathbf{I} + 3\hat{b}\hat{b} \right) - \left( \mathbf{I} + 3\hat{b}\hat{b} \right) \cdot \mathbf{W} \times \hat{b} \right], \quad \left( \mathbf{W} = \nabla \mathbf{V} + \nabla (\mathbf{V}^T - \frac{2}{3} \mathbf{V} \cdot \mathbf{V}) \right)
\]

- Nonlinear effects in gyroviscosity arise from changes in \(\mathbf{B}\) (direction and magnitude) and \(p_i\).
- The NIMROD implementation includes new terms in the ‘dot-product’ routine for advancing velocity with matrix-free algebraic system solves.
- It was used for the OFES FY06 Performance Target ELM computation.
Aside: The ELM computation is an example of a large ($0 \leq n \leq 42$) parallel (384 processors) nonlinear two-fluid computation with gyroviscosity.

- The broad range of unstable modes shows nearest-neighbor (in n-space) coupling of modes resonant at about the same magnetic winding number, which is 3 in this case.
- The low-n distortion and high-n harmonics appear to lock the unstable ELMs together.

Number density in the $\phi=0$ plane at $t=7.92 \mu s$ shows three groups of ripples.

Temperature perturbations reach 100 eV at $t=7.72 \mu s$ ($T_{ped}=400$ eV). Perturbed plasma flow vectors are superposed.
Temperature-dependent parallel viscosity: A new option allows the coefficient for the parallel stress to include the collisional $T^{5/2}$ dependence.

- The Braginskii parallel stress is $\Pi_\parallel = \frac{p_i \tau_i}{2} (\hat{b} \cdot \mathbf{W} \cdot \hat{b})(\mathbf{I} - 3\hat{b}\hat{b})$
- The form of the coefficient is identical to that of parallel thermal conduction, so the same coding and data structures are used for both.
- The computed coefficient is 3D and available when run nonlinearily.
- Number density dependencies should cancel--a next step for nimuw.
- The implementation has been tested on compressive waves:
  
  for linear analysis with homogenous equilibria; solutions $\sim e^{i\mathbf{k} \cdot \mathbf{x}}$,
  
  $$\nabla \cdot \left[ 3\rho_0 \nu \left( \hat{b} \cdot \nabla \mathbf{V} \cdot \hat{b} - \frac{1}{3} \nabla \cdot \mathbf{V} \left( \hat{b}\hat{b} - \frac{1}{3} \mathbf{I} \right) \right) \right] \rightarrow -3\rho_0 \nu \left[ (\hat{b} \cdot \mathbf{k}) (\mathbf{V} \cdot \hat{b}) - \frac{1}{3} \mathbf{k} \cdot \mathbf{V} \left( \hat{b} \cdot \mathbf{k} \right) \hat{b} - \frac{1}{3} \mathbf{k} \right]
  $$

  For weakly damped ($k^2 \nu \ll \omega$) principal modes in the MHD regime,
  
  - Magnetoacoustic damping rate is $\frac{1}{6} \nu k^2$, \qquad $\nu \equiv \frac{k_B T_i \tau_i}{m_i}$
  - Ion acoustic damping rate is $\frac{2}{3} \nu k^2$
  - Alfvén waves are not damped.
Test computations excite standing waves in a periodic box.

- Equilibrium temperature is varied while keeping pressure the same.
- The tests shown here have 20 quadratic elements along the wave. (overkill)
- $\omega \Delta t \sim 0.2-0.3$.
- A single sine wave is not excited due to temporal staggering, but the secondary mode gets smaller as $\Delta t$ is reduced.
- The equilibrium internal energy is left out of the energy diagnostic.
- Viscous heating is not used, allowing us to measure decay from the energy.

Probe histories for the sound wave.

Energy histories for the sound wave.

Damping rate results:
- MA wave at $T_i=1$: 0.066/0.064, $T_i=0.5$: 0.012/0.011 predicted/observed
- Sound wave $T_i=1$: 0.263/0.257, $T_i=0.5$: 0.047/0.046
Parallel electron stress [with CEMM leverage]: Like other forces on the electron fluid, the force from parallel stress appears as an electric-field contribution in Ohm’s law.

- The combined Faraday’s/Ohm’s law is

\[
\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \left[ \eta J - \mathbf{V} \times \mathbf{B} + \frac{1}{ne} \left( \mathbf{J} \times \mathbf{B} - T_e \mathbf{n} \cdot \nabla - \nabla \cdot \Pi_e \right) \right]
\]

and the collisional form of the parallel stress is:

\[
\Pi_e = -3\eta_0 \left( \mathbf{\hat{b}} \cdot \nabla \mathbf{V}_e \cdot \mathbf{\hat{b}} - \frac{1}{3} \nabla \cdot \mathbf{V}_e \right) \left( \mathbf{\hat{b}} \mathbf{\hat{b}} - \frac{1}{3} \mathbf{I} \right)
\]

with \( \mathbf{V}_e = \mathbf{V} - \left( \frac{1}{1 + Z_m e / m_i} \right) \frac{1}{ne} \mathbf{J} \equiv \mathbf{V} - \frac{1}{ne} \mathbf{J} \)

- An implicit computation of this stress can be used in NIMROD’s magnetic advance.
  - The fluid stress will allow direct modeling of the Pfirsch-Schlüter regime.
  - The implicit operator will be used to stabilize nonlocal kinetic stress computations. [Held, PoP 11, 2419 (2004)]
Implementation of parallel electron stress with basis functions having $C^0$ continuity requires an auxiliary field.

• NIMROD’s polynomial spaces are sufficiently general to represent functions with square-integrable first derivatives.

• Since electron velocity depends on the curl of $\mathbf{B}$, adding electron stress to Ohm’s law implies that $d\mathbf{B}/dt$ depends on fourth-order derivatives of $\mathbf{B}$.

• Just like ODE systems, introducing auxiliary fields is a way to have fewer derivatives appearing explicitly.

• With $\theta$-centering in the time advance, we define $\nu = \sqrt{3\Delta t\eta_0\theta}/e\sqrt{\mu_0}$ and

$$f - \nu \left[ \mathbf{b} \cdot \nabla \left( \frac{\nabla \times \Delta \mathbf{B}}{n} \right) \right] = -\frac{3\eta_0\mu_0\Delta t}{\theta} \left\{ \mathbf{b} \cdot \nabla \left( \mathbf{v} - \frac{1}{ne} \mathbf{J}^n \right) \right\}$$

The auxiliary field $f$ is essentially the parallel component of the electron stress, and the $\nu$-coefficient is defined to make implicit terms symmetric.

$$\Delta \mathbf{B} = \nabla \times \left\{ \frac{1}{n} \nabla \cdot \left[ \nu f \left( \mathbf{b} \mathbf{b} - \frac{1}{3} \mathbf{I} \right) \right] \right\} = -\Delta t \nabla \times \mathbf{E}_{other}$$

• The note on the “sovinec_research” page of [www.cptc.wisc.edu](http://www.cptc.wisc.edu) provides more details.
The linear parts of the electron stress for spatially uniform $\eta_0$ have been implemented.

- The NIMROD implementation presently has all of the linear terms for $\Pi_e$ when $\eta_0$ is spatially uniform.
- Whistler tests for NIMROD have $\mathbf{k}$ and $\mathbf{B}_0$ in various orientations in the finite element plane and in the periodic (Fourier) coordinate.
- Electron stress alone in a uniform background and $\mathbf{B} \sim e^{i k \cdot x - i \omega t}$ has
  \[
  -i \omega \mathbf{B} \sim -i \mathbf{k} \times \left\{ \begin{array}{c}
- \mathbf{h} \cdot i \mathbf{k} \left( -i \mathbf{k} \times \mathbf{B} \right) \cdot \mathbf{b} \end{array} \right\} \sim -(\mathbf{k} \cdot \mathbf{h})^2 \left( \mathbf{k} \times \mathbf{h} \right) \left( \mathbf{k} \times \mathbf{h} \right) \cdot \mathbf{B}
  \]
- The whistler dispersion relation is
  \[
  \omega^2 + \left( \omega_0^2 \frac{k^2}{k^2} \right) \left( i \frac{3\eta_0 \mu_0 k^2}{B_0^2 k^2} \omega - 1 \right) = 0 , \quad \omega_0^2 \equiv \Omega_i^2 d^4 k^4
  \]
  and for weak damping, $\omega_r^2 \equiv \omega_0^2 \frac{k^2}{k^2}$, $\omega_i \equiv -\omega_0^2 \left( \frac{3\eta_0 \mu_0 k^2 k^2}{2 B_0^2 k^4} \right)$
- Implementing nonlinear terms is the next step for this project.
Optimization efforts: improving serial and parallel performance is also important for meeting application needs.

- Numerical quadrature computations in rblocks now have ‘nqty’-specific coding for scalars and 3-vectors.
  - This allows explicit unrolling of inner-most loops.
  - Can be added for other nqty values.
- Intensive integrand computations have been modified to use explicit looping instead of array syntax.
  - The extent of optimization with array syntax is up to the compiler.
  - Temporary array-syntax computations need arrays instead of scalars, and this clogs memory access.
- In biquartic computations, the above changes reduce matrix computation times by 30-40%.
- Reordering data before FFT calls transforms data from all quadrature points simultaneously, reducing the number of mpi calls.
- The next step is to extend this idea throughout NIMROD’s FE integration to allow longer loops and further reduce the number of FFT calls.
Pegasus injection computations: simulated evolution from an axisymmetric thermal channel shows relaxation.

- Temperature (left) and \( \lambda \) (right) before and after relaxation.
- Final flux and RB.

- \( T \)-dependent thermal and electrical conduction are used with \( B_\phi \) boundary conds.
- Computations starting from non-axisymmetric channels have also progressed but are computationally costly.
**HIT-II specific development and application:** with new boundary conditions, simulations with experimentally relevant specifications are possible.

- Applying $B_\phi$ at the injector ‘gap’ and $E_{radial}$ at the absorber ‘gap’ allows control of the final electrostatic potential without precluding or fixing inductive changes.
- Flow at the absorber is $\mathbf{E} \times \mathbf{B}$ drift, and flow at the injector conserves mass.
- Recent meshing work has NIMROD modeling a realistic domain.

Mesh for realistic HIT-II domain.

Sequence of $\psi$ and $RB_\phi$ contours from 2D MHD.
Initial studies used a rectangular cross section for simplicity and reproduced global characteristics from HIT-II.

- A series of zero-beta nonlinear computations scans $I_{TF}$ with fixed $I_{inj}$.
- Moderate $\psi_{inj}$ spread is “NSTX-like” or less and peaks at 6 mWb.

2D simulation results of toroidal current with varied vacuum toroidal field--compare with Fig. 17 of Redd, et al. Windup at lowest $I_{TF}$ (=75 kA) is 5.8.

3D simulation results show increasing relaxation as vacuum toroidal field is reduced.
Saturation of the MHD instability increases plasma current and windup, in addition to amplification of poloidal flux.

- Windup increases at saturation in the simulation, possibly related to building-current observation in HIT-II.

Comparison of 2D and 3D simulation results on plasma current. $I_p$ builds past the 2D-only level when relaxation occurs, similar to HIT-II result reported in IEEJ by Redd, et al.

Fluctuation amplitude at $S \sim 10,000$ before loss of mode is $\sim 1\%$ for steady drive without thermal effects.

- Temperature evolution with $T$-dependent transport is a next step.
Plans for the Coming Year

• Improve fluid algorithm efficiency.
  • Modify quadrature-point storage to have the quad-point index inside the Fourier index, and hide this within the existing array indices for integrand operations.
  • Modify numerical integration routines to avoid outer loops.
  • Test for scalar and parallel efficiency.
• Modify fluid transport coefficients to have correct number-density dependencies.
  • Presently, all scale with $n^1$, except in problem-specific modifications for GEM, CDX-U, etc.
  • Should have parallel~$n^0$, gyro~$n^1$, perpendicular~$n^2$.
• Perform EC simulation studies.
  • Use efficiency improvements on Pegasus helical current channel.
  • Include temperature evolution, $T$-dependent resistivity and thermal conduction, and realistic current waveform for HIT-II.
• Begin two-fluid HIT-II studies with improved preconditioning from SciDAC work.
Numerical Algorithm: NIMROD uses an implicit leapfrog method to advance the two-fluid equations.

- The number density appearing in the advances of $T$ and $B$ is time-averaged, as is the temperature appearing in the magnetic advance.
- A Newton-like computation is used for momentum advection and the Hall term.

\[
\begin{align*}
m_i n_i^{j+1/2} & \left( \frac{\Delta V}{\Delta t} + \frac{1}{2} V^j \cdot \nabla \Delta V + \frac{1}{2} \Delta V \cdot \nabla V^j \right) - \Delta t L^{j+1/2} (\Delta V) + \nabla \cdot \Pi_i (\Delta V) = J^{j+1/2} \times B^{j+1/2} \\
- m_i n_i^{j+1/2} V^j \cdot \nabla V^j - \nabla \left[ n_i^{j+1/2} \left( T_e^{j+1/2} + Z^{-1} T_i^{j+1/2} \right) \right] - \nabla \cdot \Pi_i (V^j) \\
\Delta n + \frac{1}{2} \nabla \cdot \left( V^{j+1} \cdot \Delta n - D \nabla \Delta n \right) & = - \nabla \cdot \left( \frac{3n}{2} \left( \Delta T_\alpha + \frac{1}{2} V^\alpha \cdot \Delta T_\alpha \right) \right) + \frac{n}{2} \Delta T_\alpha \nabla \cdot V^\alpha_j + \frac{1}{2} \nabla \cdot \mathbf{q}_\alpha (\Delta T_\alpha) \\
& = - \frac{3n}{2} V^\alpha_j \cdot \nabla T_\alpha^{j+1/2} - n T_\alpha^{j+1/2} \nabla \cdot V^\alpha_j - \nabla \cdot \mathbf{q}_\alpha (T_\alpha^{j+1/2}) + Q_\alpha^{j+1/2} \\
\frac{\Delta B}{\Delta t} - \frac{1}{2} \nabla \times \left( V^{j+1} \times \Delta B \right) + \frac{1}{2} \nabla \times \frac{1}{n_e} \left( J^{j+1/2} \times \Delta B + \Delta J \times B^{j+1/2} \right) + \frac{1}{2} \nabla \times \eta \Delta J \\
& = - \nabla \times \left[ \frac{1}{n_e} \left( J^{j+1/2} \times B^{j+1/2} - T_e \nabla n \right) - V^{j+1} \times B^{j+1/2} + \eta J^{j+1/2} \right]
\end{align*}
\]

- A corrector step for temperature is used for $B$- or $T$-dependent thermal conduction.
Grad-Shafranov reasoning for bubble burst & $I_p \sim \psi_{inj}$

- Lowest-order force-balance holds throughout--not model-specific.
- Assume: $d << a$, $\Delta F << F$ (F=RB$\phi$ so 2nd is equivalent to $I_{inj} \ll I_{TF}$)
- GS eqn for $p=0$ is $\mu_0 R J_\phi = \Delta^* \psi = -FF'$

1. Estimate for vacuum (homogeneous) solution: $\Delta^* \psi \sim \frac{\partial^2 \psi}{\partial R^2} \sim \frac{\partial^2 \psi}{\partial Z^2} \sim \frac{\Delta \psi}{d^2}$

2. For CHI in STs, $F = \mu_0 I_{TF} / 2\pi$, $\Delta F = \mu_0 I_{inj} / 2\pi$, $\Delta \psi = \psi_{inj}$

3. To change the vacuum distribution significantly (leading to bubble-burst in the case of $d << a$), we must have $FF' \equiv F \frac{\Delta F}{\Delta \psi} \sim \frac{\Delta \psi}{d^2}$

4. Therefore, burst occurs for $I_{inj} \sim \frac{4\pi^2 \psi_{inj}^2}{\mu_0 d^2 I_{TF}}$

5. The final state maintains $\Delta^* \psi \sim \psi_{inj} / d^2$ relation. A flux balloon without relaxation, for example, will have a thickness $(d)$, stretched around the chamber perimeter.

6. Estimate $I_p$: $I_p = \int dA J_\phi = \frac{1}{\mu_0} \int dA \frac{\Delta^* \psi}{R} \equiv \left( \frac{2\pi a d}{\mu_0 R_0} \right) \left( \frac{\psi_{inj}}{d^2} \right) \sim \psi_{inj}$ and geometry
Simulations using the realistic mesh for HIT-II have also produced flux amplification.

Poloidal flux contours after relaxation show the amplified-flux. Contours of constant $R B_\phi$ from the same time.