

Newton-Krylov Solves in NIMROD

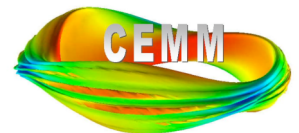
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Outline

- Algebraically nonlinear terms in implicit leapfrog
- Newton iteration
- Convergence criteria
- Other possible improvements
- Summary

In the present implicit leapfrog, advection and Hall-**E** are centered only approximately.

Velocity advance:

$$m_i n^{j+1/2} \left(\frac{\Delta \mathbf{V}}{\Delta t} + \frac{1}{2} \mathbf{V}^j \cdot \nabla \Delta \mathbf{V} + \frac{1}{2} \Delta \mathbf{V} \cdot \nabla \mathbf{V}^j \right) - \Delta t L^{j+1/2} (\Delta \mathbf{V}) + \nabla \cdot \Pi_i (\Delta \mathbf{V})$$

← Newton-like step
 ← staggering-centered

$$= \mathbf{J}^{j+1/2} \times \mathbf{B}^{j+1/2} - m_i n^{j+1/2} \mathbf{V}^j \cdot \nabla \mathbf{V}^j - \nabla \left[n^{j+1/2} \left(T_e^{j+1/2} + Z^{-1} T_i^{j+1/2} \right) \right] - \nabla \cdot \Pi_i (\mathbf{V}^j)$$

Number density advance:

$$\frac{\Delta n}{\Delta t} + \frac{1}{2} \nabla \cdot \left(\mathbf{V}^{j+1} \cdot \Delta n - D \nabla \Delta n \right) = -\nabla \cdot \left(\mathbf{V}^{j+1} \cdot n^{j+1/2} - D \nabla n^{j+1/2} \right)$$

← staggering-centered
 ← predict/correct if nl coefficient

For the magnetic advance, the time-averaged n is known.

Temperature advances:

$$\frac{3\bar{n}}{2} \left(\frac{\Delta T_\alpha}{\Delta t} + \frac{1}{2} \mathbf{V}_\alpha^{j+1} \cdot \nabla \Delta T_\alpha \right) + \frac{\bar{n}}{2} \Delta T_\alpha \nabla \cdot \mathbf{V}_\alpha^{j+1} + \frac{1}{2} \nabla \cdot \mathbf{q}_\alpha (\Delta T_\alpha)$$

averaged
stagger (&p/c)
p/c if \mathbf{B} -dependent

$$= -\frac{3\bar{n}}{2} \mathbf{V}_\alpha^{j+1} \cdot \nabla T_\alpha^{j+1/2} - \bar{n} T_\alpha^{j+1/2} \nabla \cdot \mathbf{V}_\alpha^{j+1} - \nabla \cdot \mathbf{q}_\alpha (T_\alpha^{j+1/2}) + Q_\alpha^{j+1/2}$$

Magnetic advance:

$$\frac{\Delta \mathbf{B}}{\Delta t} - \frac{1}{2} \nabla \times (\mathbf{V}^{j+1} \times \Delta \mathbf{B}) + \frac{1}{2} \nabla \times \frac{1}{\bar{n}e} (\mathbf{J}^{j+1/2} \times \Delta \mathbf{B} + \Delta \mathbf{J} \times \mathbf{B}^{j+1/2}) + \frac{1}{2} \nabla \times \eta \Delta \mathbf{J}$$

stagger
Newton-like
averages

$$= -\nabla \times \left[\frac{1}{\bar{n}e} (\mathbf{J}^{j+1/2} \times \mathbf{B}^{j+1/2} - \bar{T}_e \nabla \bar{n}) - \mathbf{V}^{j+1} \times \mathbf{B}^{j+1/2} + \eta \mathbf{J}^{j+1/2} \right]$$

Correct after \mathbf{B} advance.

The discrepancies from nonlinear centering are small, but they may affect nonlinear stability.

- The momentum-density advection and Hall terms are among the hyperbolic parts of the system.
- Analysis for linear waves shows that these terms must be time-centered for numerical stability.

V-advance: solution field is $\Delta\mathbf{V}$, and nonlinearly centered advection is

$$m_i n^{j+1/2} \left(\mathbf{V}^j + \frac{1}{2} \Delta\mathbf{V} \right) \cdot \nabla \left(\mathbf{V}^j + \frac{1}{2} \Delta\mathbf{V} \right)$$

B-advance: solution field is $\Delta\mathbf{B}$, and nonlinearly centered Hall is

$$\nabla \times \left\{ \frac{1}{\mu_0 \bar{n} e} \left[\nabla \times \left(\mathbf{B}^{j+1/2} + \frac{1}{2} \Delta\mathbf{B} \right) \right] \times \left(\mathbf{B}^{j+1/2} + \frac{1}{2} \Delta\mathbf{B} \right) \right\}$$

Both terms are bilinear, and minor changes allow iteration.

With N being either operator, and the superscript j indicating the time level at the start of an advance,

$$N\left(X^j + \frac{1}{2}\Delta X, X^j + \frac{1}{2}\Delta X\right) = \underbrace{N(X^j, X^j)}_{\text{explicit}} + \frac{1}{2}\underbrace{\left[N(X^j, \Delta X) + N(\Delta X, X^j)\right]}_{\text{linearly implicit}} + \frac{1}{4}\underbrace{N(\Delta X, \Delta X)}_{\text{new}}$$

To iterate with minimal changes, let ΔX_k be the k -th iteration for $X^{j+1} - X^j$.

$$\begin{aligned} L(\Delta X_k) + \frac{1}{2}N\left(X^j + \frac{1}{2}\Delta X_{k-1}, \Delta X_k\right) + \frac{1}{2}N\left(\Delta X_k, X^j + \frac{1}{2}\Delta X_{k-1}\right) \\ = -N(X^j, X^j) + R^j + \frac{1}{4}N(\Delta X_{k-1}, \Delta X_{k-1}) \quad , \end{aligned}$$

where L is linear and remaining RHS is R , is equivalent to Newton:

$$F(\Delta X_{k-1}) + \left. \frac{\delta F}{\delta \Delta X} \right|_{\Delta X_{k-1}} (\Delta X_k - \Delta X_{k-1}) = 0 \quad \text{for} \quad F = L + N - R$$

Coding changes are minimal.

- Loop around linear solve.
- Reuse original RHS, $-N(X^j, X^j) + R^j$ and add $\frac{1}{4}N(\Delta X_{k-1}, \Delta X_{k-1})$.
 - There are new RHS integrands.
- When performing each matrix-free linear solve, use the last iterate, $X^j + \frac{1}{2}\Delta X_{k-1}$, in the linearized terms.
- Save ΔX_k as the guess for the next linear solve.
- Find $\frac{1}{4}N(\Delta X_k, \Delta X_k)$ and test for convergence.

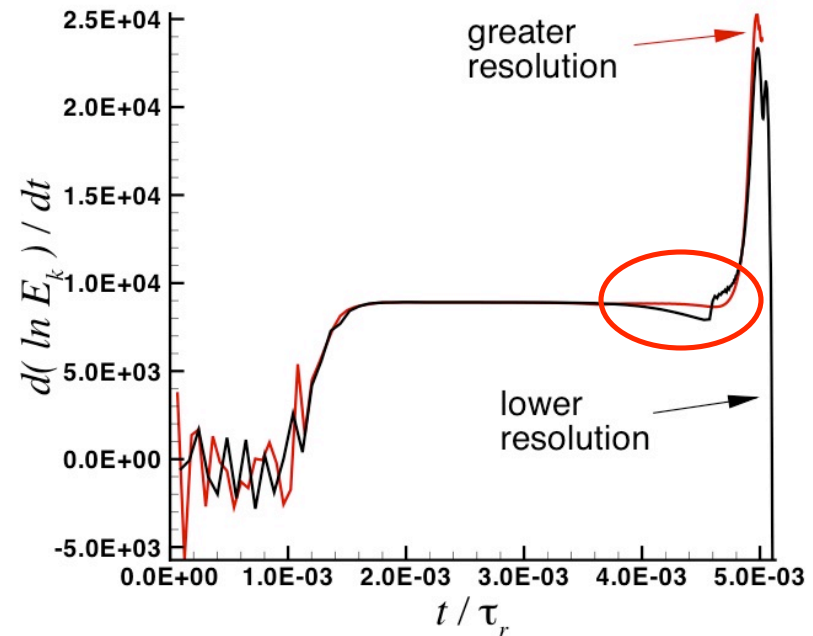
$$\frac{\frac{1}{4}\|N(\Delta X_k, \Delta X_k) - N(\Delta X_{k-1}, \Delta X_{k-1})\|}{\|R^j - N(X^j, X^j)\|} \leq \textit{tolerance}$$

For bilinear N,
numerator = norm
of nonlinear resid.
(using last Newt. it.)

- First test cases do not show significant changes.
- Computational cost is about 15%.

Other possible developments: two-fluid internal kink may benefit from 3D linear force operator.

- Time step in nonlinear two-fluid internal kink computations has been limited for accuracy.
- Before the crash, the evolution is quasi-static, so the largest truncation error is likely in the force-balance.



- First case has a 20×20 mesh, degree of polynomials is 8, and $0 \leq n \leq 42$.
- Second case has a 24×32 mesh, degree of polynomials is 8, and $0 \leq n \leq 85$.
- The computations limit Δt by nearly 2 orders of magnitude from linearly accurate Δt before the crash. Minimum CFL is ~ 600 .

A 3D linear force operator can be used in the matrix-free velocity operation.

- It will be similar to other 3D operators, except test-function terms are more complicated.
- After integration by parts, MHD wave terms include

$$\int \nabla \times (\mathbf{A}_v^* \times \mathbf{B}) \cdot \nabla \times (\Delta \mathbf{V} \times \mathbf{B}) dVol$$

where \mathbf{B} is 3D.

- Dot product in integrand should be done in real space.
- Transform of $\nabla \times (\mathbf{A}_v^* \times \mathbf{B})$ is needed for the three *vector* test functions \mathbf{A}_r , \mathbf{A}_z , and \mathbf{A}_ϕ .

Bug-fix topics

- Pressure noise caused problems in computations with toroidal equilibria when $\text{grad}(p)$ is computed directly from n , and T .
 - Returning to p -expansion patches problem.
- Code for recovering from failed linear solves had bugs.
 - Temporary computation pointers were not deallocated after a failed solve-> memory leak.
 - Multi-layer computations with '2D' matrices did not communicate 'converged' status. This can cause a parallel computation to hang.

Conclusions

- Newton-Krylov iteration for the implicit leapfrog is practical and has been implemented.
- More testing is needed to evaluate its importance.
- A 3D linear ideal MHD force operator is being considered.