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:

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

Newton-like step

staggering-centered

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

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 **B**-dependent

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

Magnetic advance:

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

stagger

Newton-like

averages

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

Correct after **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

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

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

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

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,

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

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

$$L(\Delta X_k)+\frac{1}{2}\mathrm{N}\left(X^j+\frac{1}{2}\Delta X_{k-1},\Delta X_k\right)+\frac{1}{2}\mathrm{N}\left(\Delta X_k,X^j+\frac{1}{2}\Delta X_{k-1}\right)$$

$$=-\mathrm{N}\left(X^j,X^j\right)+R^j+\frac{1}{4}\mathrm{N}(\Delta X_{k-1},\Delta X_{k-1}) \qquad ,$$

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

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

Coding changes are minimal.

- Loop around linear solve.
- Reuse original RHS, $-\mathrm{N}\left(X^j, X^j\right) + R^j$ and add $\frac{1}{4}\mathrm{N}(\Delta X_{k-1}, \Delta X_{k-1})$.
    - 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 $\frac{1}{4}\mathrm{N}(\Delta X_k, \Delta X_k)$ and test for convergence.

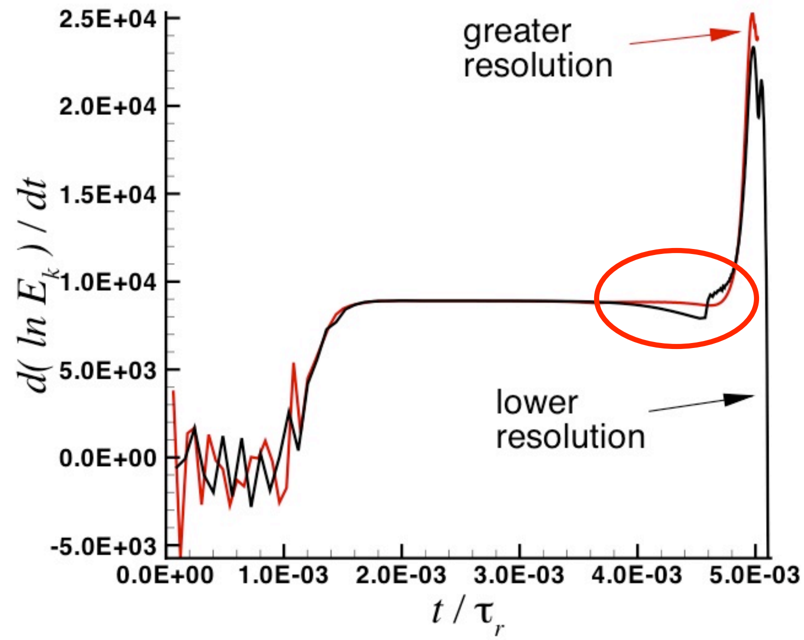
$$\frac{\frac{1}{4}\left\|\mathrm{N}(\Delta X_k, \Delta X_k) - \mathrm{N}(\Delta X_{k-1}, \Delta X_{k-1})\right\|}{\left\|R^j - \mathrm{N}\left(X^j, X^j\right)\right\|} \le tolerance$$

For bilinear N, numerator = norm of nonlinear residual (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 $0 \le n \le 42$.
- Second case has a 24×32 mesh, degree of polynomials is 8, and $0 \le n \le 85$.
- 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

$$\int \nabla \times \left(\mathbf{A}_{\nu}^{*} \times \mathbf{B}\right) \cdot \nabla \times (\Delta\mathbf{V} \times \mathbf{B})\, dVol$$

where **B** is 3D.

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

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.