

Jacobian-Free Newton-Krylov Method for GKM

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Outline

- Primer on Newton-Krylov Method
- Good preconditioning is the key
 - *Example: Wave-structure based preconditioner for MHD*
- JFNK for GKM

Related Work

- Chacon & co-workers (JCP 2002, 2003, 2006) developed JFNK methods with “physics-based” preconditioners
 - *Parabolization trick for the equations*
 - *Schur complement approach*
- M3d (Strauss, Park et al.) treats fast compressive wave implicitly
 - *Recently Fu & Breslau have extended to treating shear Alfvén wave implicitly*
- Glasser & co-workers use a static-condensation method in their fully implicit SEL code
- Rognlien et al. (J. Nuclear Matter 1992, JCP 2002) for edge plasmas
- Mousseau & Knoll (JCP 2000) - 2d Fokker-Planck for edge plasmas
- Reynolds, Samtaney & Woodward (JCP 2006) developed a fully implicit parallel JFNK method for 3D compressible MHD
 - *Recent work (2008) on development of a wave-structure based preconditioner*
- Excellent review paper by Knoll & Keyes (JCP 2004)

Nonlinearly Implicit : Introduction to Newton-Krylov

- Consider the equations of single-fluid resistive MHD written below in conservation form

$$\partial_t \rho + \nabla \cdot (\rho \mathbf{v}) = 0,$$

$$\partial_t (\rho \mathbf{v}) + \nabla \cdot \left(\rho \mathbf{v} \mathbf{v}^T - \mathbf{B} \mathbf{B}^T + \left(p + \frac{1}{2} \mathbf{B} \cdot \mathbf{B} \right) \bar{\mathbf{I}} \right) = \nabla \cdot \bar{\boldsymbol{\tau}},$$

$$\partial_t \mathbf{B} + \nabla \cdot \left(\mathbf{v} \mathbf{B}^T - \mathbf{B} \mathbf{v}^T \right) = \nabla \cdot \left(\eta \nabla \mathbf{B} - \eta (\nabla \mathbf{B})^T \right),$$

$$\begin{aligned} \partial_t e + \nabla \cdot \left((e + p + \frac{1}{2} \mathbf{B} \cdot \mathbf{B}) \mathbf{v} - \mathbf{B} (\mathbf{B} \cdot \mathbf{v}) \right) &= \nabla \cdot (\bar{\boldsymbol{\tau}} \mathbf{v} + \kappa \nabla T) \\ &+ \nabla \cdot \left(\eta \left(\frac{1}{2} \nabla (\mathbf{B} \cdot \mathbf{B}) - \mathbf{B} (\nabla \mathbf{B})^T \right) \right) \end{aligned}$$

- Condensing notation $\mathbf{U} = (\rho, \rho \mathbf{v}, \mathbf{B}, e)^T$

$$\partial_t \mathbf{U} = -\nabla \cdot \mathbf{F}_h(\mathbf{U}) + \nabla \cdot \mathbf{F}_v(\mathbf{U}) = \nabla \cdot \mathbf{F}(\mathbf{U}).$$

Nonlinearly Implicit : Introduction to Newton-Krylov

- The solution at the next time level to the entire system of equations is expressed as the solution to the following nonlinear equation

$$\mathcal{F}(U^{n+1}) = 0$$

$$\mathcal{F}(U^{n+1}) = U^{n+1} - U^n + (1 - \theta)R(U^{n+1}) + \theta R(U^n) = 0$$

$R(U)$ is the entire right hand side (contains divergence of hyperbolic and diffusive fluxes)

The number of unknowns is $8N^2$ for an $N \times N$ mesh

- This is solved using Newton's method

$$\delta U^k = - \left[\left(\frac{\partial \mathcal{F}}{\partial U} \right)^{n+1,k} \right]^{-1} \mathcal{F}$$

where $J(U^{n+1,k}) \equiv \left(\frac{\partial \mathcal{F}}{\partial U} \right)^{n+1,k}$ is the Jacobian; and $\delta U^k \equiv U^{n+1,k+1} - U^{n+1,k}$

The size of the Jacobian matrix is $64N^4$

- The linear system at each Newton iteration is solved with a Krylov method in which an approximation to the linear system $J \delta U = -\mathcal{F}$ is obtained by iteratively building a Krylov subspace of dimension m

$$\mathcal{K}(r_0, J) = \text{span}\{r_0, Jr_0, J^2r_0, \dots, J^{m-1}r_0\}$$

Nonlinearly Implicit : Introduction to Newton-Krylov

- Commonly used Krylov methods which can handle asymmetric matrices
 - **GMRES (Generalized Minimum Residual)**
 - Long-recurrence Arnoldi orthogonalization method
 - Robust, guaranteed convergence, but heavy on memory requirement
 - **BICGSTab (Bi-conjugate Gradient Stabilized)**
 - Short-recurrence Lanczos biorthogonalization procedure
 - Residual not guaranteed to decrease monotonically, but less memory requirement
- Steps in a Newton-Krylov method
 1. Guess the solution $U^{n+1,0} (=U^n)$
 2. For each Newton iteration k
 1. Using a Krylov Method solve for δU^k
Solve $J \delta U^k = -F(U^{n+1,k})$ until $\|J \delta U^k + F(U^{n+1,k})\| < \text{ftol}$
 3. Update the Newton iterate: $U^{n+1,k+1} = U^{n+1,k} + \lambda \delta U^k$
 4. Check for convergence $\|F(U^{n+1,k+1})\| < \text{ftol}$

- Newton method converges quadratically if the approximate solution $U^{n+1,k+1}$ is close to the actual solution U^* (Constant C is not a fnc($U^{n+1,k+1}, U^*$))

$$\|U^{n+1,k+1} - U^*\| \leq C \|U^{n+1,k} - U^*\|^2$$
- **Jacobian-Free Newton-Krylov:** Krylov methods require only matrix-vector products to build up the Krylov subspace, i.e., only $J \delta U$ is required. This can be approximated as follows. Typically σ is chosen as square-root of machine zero. Thus, the entire method can be built from evaluations of the nonlinear function $F(U)$

$$J(U^k) \delta U^k \approx \frac{\mathcal{F}(U^{n+1,k} + \sigma \delta U^k) - \mathcal{F}(U^{n+1,k})}{\sigma}$$

Introduction to Newton-Krylov: Preconditioners

- Krylov methods can lead to slow convergence. This is especially true for MHD where the Jacobian is ill-conditioned. Preconditioners help alleviate the problem of slow convergence and are formulated as follows

$$\begin{aligned}(J(U^k)P^{-1})(P\delta U^k) &= -\mathcal{F}(U^{n+1,k}) \quad (\text{Right}), \\ (P^{-1}J(U^k))\delta U^k &= -P^{-1}\mathcal{F}(U^{n+1,k}) \quad (\text{Left}), \\ (P_L^{-1}J(U^k)P_R^{-1})(P_R\delta U^k) &= -P_L^{-1}\mathcal{F}(U^{n+1,k}) \quad (\text{Both}).\end{aligned}$$

- The basic idea of preconditioners is that the matrix JP^{-1} or $P^{-1}J$ is close to the identity matrix, i.e., P is a good approximation of J . Furthermore, to make preconditioning effective, P^{-1} should be computationally inexpensive to evaluate

- Two broad classes of preconditioners

1. **Algebraic:** These are of the “black-box” type. Obtained from relatively inexpensive techniques such as incomplete LU, multi-grid etc. These require storage for the preconditioner.
2. **Physics-based:** These may be derived from semi-implicit methods, and pay close attention to the underlying physics in the problem. Furthermore, these can still operate in the “Jacobian-Free” mode.
 1. Chacon, Knoll and co-workers (LANL) championed the “physics-based” preconditioners. Their work involves using “parabolizing” the wave terms and using multi-grid to solve approximate systems.

Wave-structure Based Preconditioner - Basic Idea

- The stiffness usually arises from the hyperbolic terms in the MHD equation
- Consider a system of hyperbolic conservation laws

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0,$$

$$\frac{\partial u}{\partial t} + J(u^0) \frac{\partial u}{\partial x} = 0,$$

$$\frac{\partial w}{\partial t} + \Lambda \frac{\partial w}{\partial x} = 0$$

- Linearizing about a background state $J(u^0)$ has real eigenvalues $\Lambda = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$ with linearly independent left (L) and right (R) eigenvectors
- Characteristic equations ($w = [L]u$)
- Solve implicitly
 - Using Crank-Nicholson and 4th order finite differences

$$\left(\frac{\partial u}{\partial x} \right)_i = a(u_{i+1} - u_{i-1}) + b(u_{i+2} - u_{i-2}),$$

$$a = (1.5\Delta x)^{-1}, \quad b = (-12\Delta x)^{-1}$$

- Leads to a linear system of the form $A U^{n+1} = R(U^n)$
 $K = a\Delta t J, \quad M = b\Delta t J$

A =

$$A = \begin{bmatrix} I & K & M & 0 & 0 & 0 & \dots & -M & -K \\ -K & I & K & M & 0 & 0 & 0 & \dots & -M \\ -M & -K & I & K & M & 0 & 0 & \dots & 0 \\ 0 & -M & -K & I & K & M & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & 0 & -M & -K & I & K & M \\ M & 0 & \dots & 0 & 0 & -M & -K & I & K \\ K & M & 0 & \dots & 0 & 0 & -M & -K & I \end{bmatrix}$$

Wave-structure Based Preconditioner - Basic Idea

- Solve for all but the stiffness inducing waves
- Preconditioner Matrix is then

$$\tilde{K} = a\Delta t R \tilde{\Lambda} L$$

$$\tilde{M} = b\Delta t R \tilde{\Lambda} L$$

$$\tilde{\Lambda} = \text{diag}\{0, 0, \dots, \lambda_q, \lambda_{q+1}, \dots, \lambda_n\}$$

$$P = \begin{bmatrix} I & \tilde{K} & \tilde{M} & 0 & 0 & 0 & \dots & -\tilde{M} & -\tilde{K} \\ -\tilde{K} & I & \tilde{K} & \tilde{M} & 0 & 0 & 0 & \dots & -\tilde{M} \\ -\tilde{M} & -\tilde{K} & I & \tilde{K} & \tilde{M} & 0 & 0 & \dots & 0 \\ 0 & -\tilde{M} & -\tilde{K} & I & \tilde{K} & \tilde{M} & 0 & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots \\ 0 & \dots & 0 & 0 & -\tilde{M} & -\tilde{K} & I & \tilde{K} & \tilde{M} \\ \tilde{M} & 0 & \dots & 0 & 0 & -\tilde{M} & -\tilde{K} & I & \tilde{K} \\ \tilde{K} & \tilde{M} & 0 & \dots & 0 & 0 & -\tilde{M} & -\tilde{K} & I \end{bmatrix}$$

- Example: Ideal MHD, linearizing about a background state (low β tokamak parameters)
 $U^0 = \{\rho=1, u=0, B_x=0.1 \cos\alpha, B_y=0.1 \cos\alpha, B_z=1.0, p=0.01\}^T$
- Full matrix A has $\lambda_{max} \approx 342$
- Fast wave preconditioning $\lambda_{max} \approx 22$
 Fast + Alfvén wave $\lambda_{max} \approx 2$
 All waves: $\lambda_{max} = 1$
- Preconditioner is **exact** for a system of linear hyperbolic conservation laws in 1D

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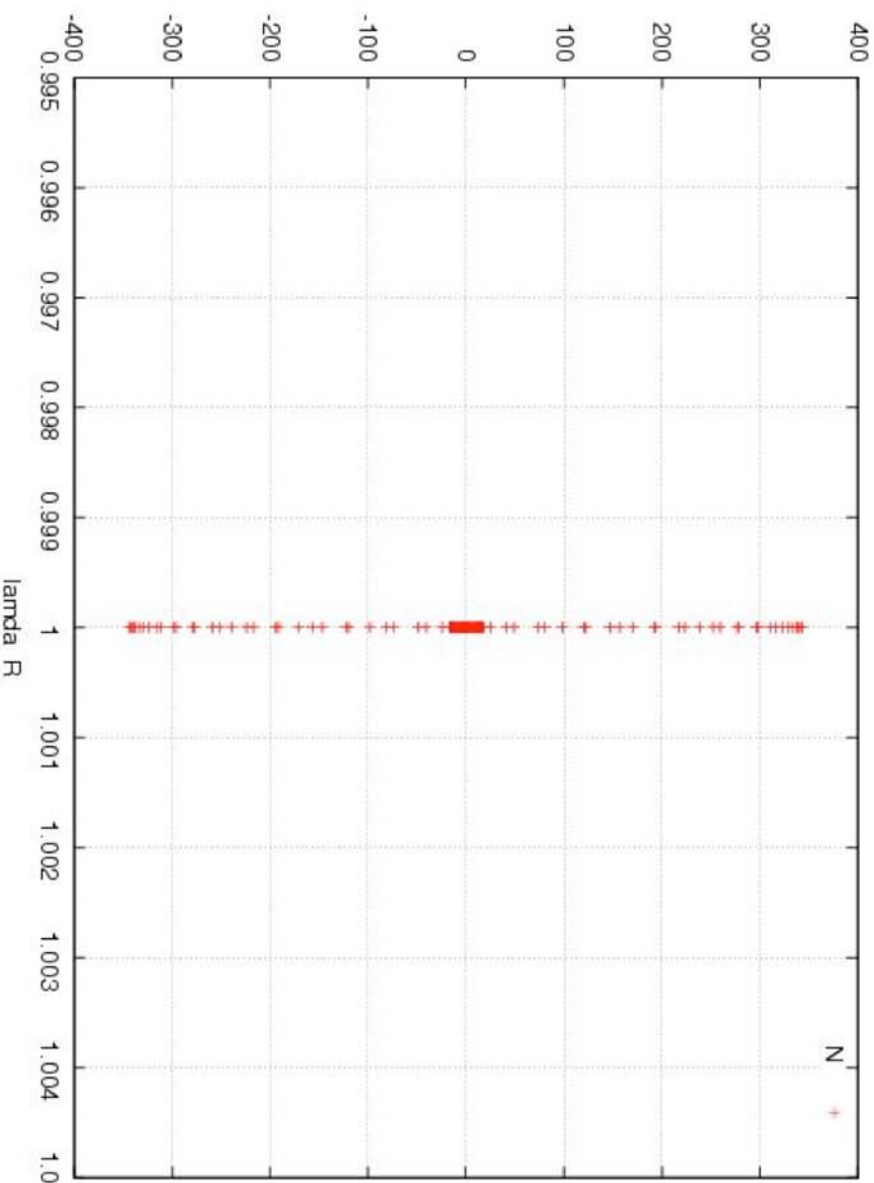
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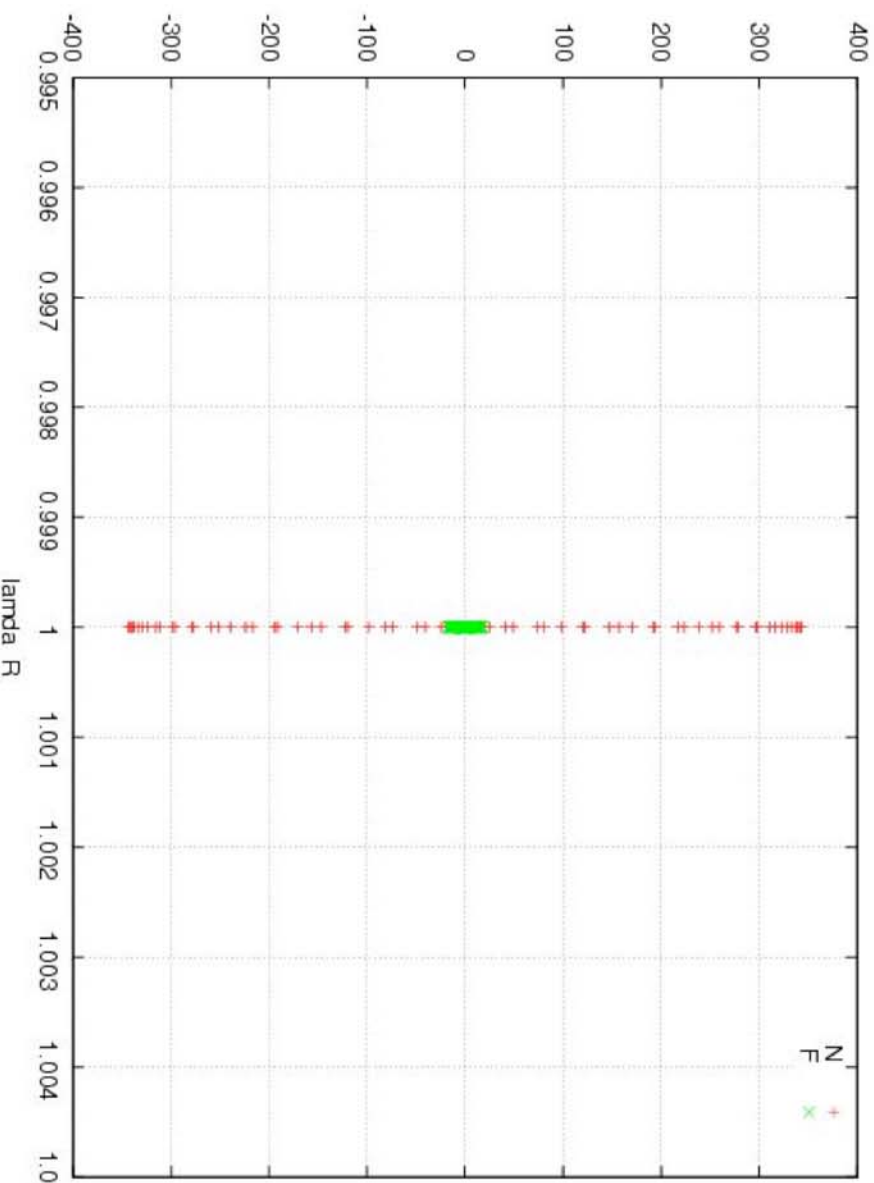
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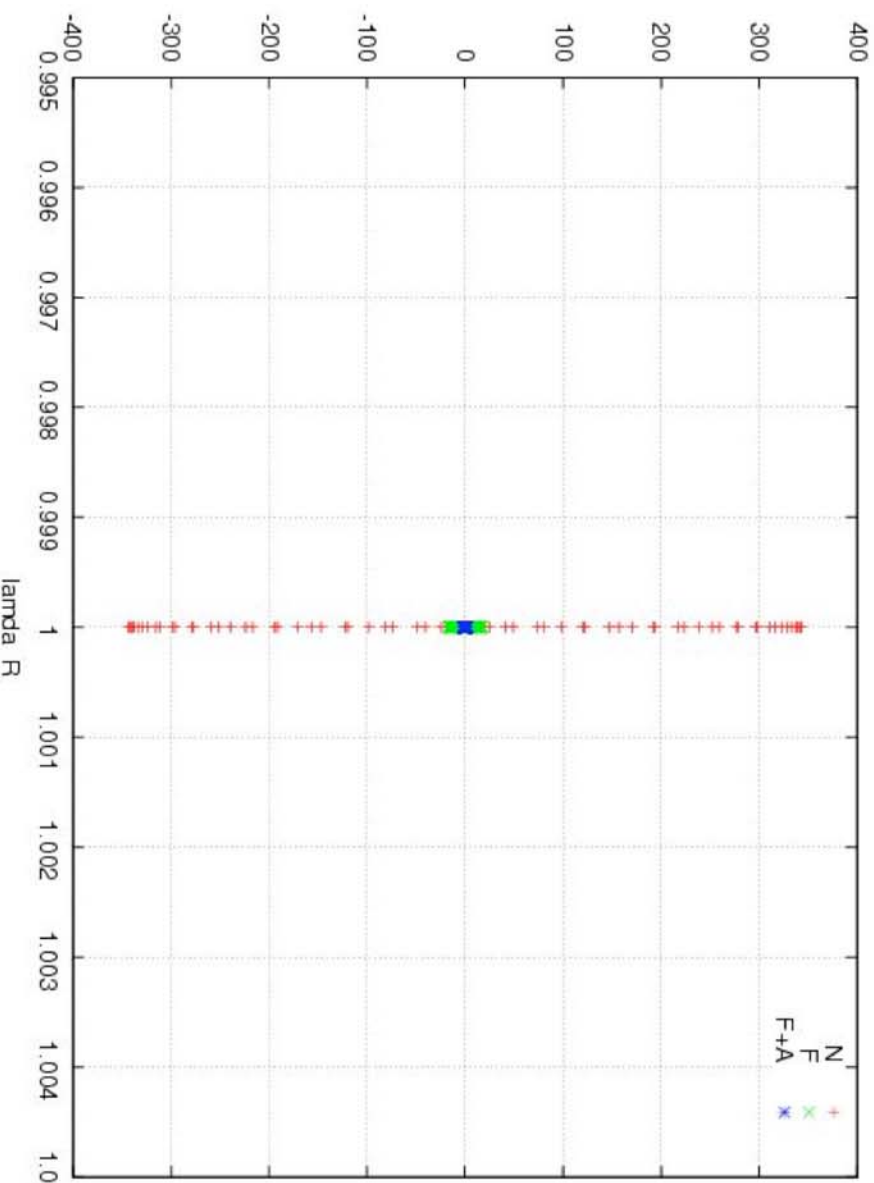
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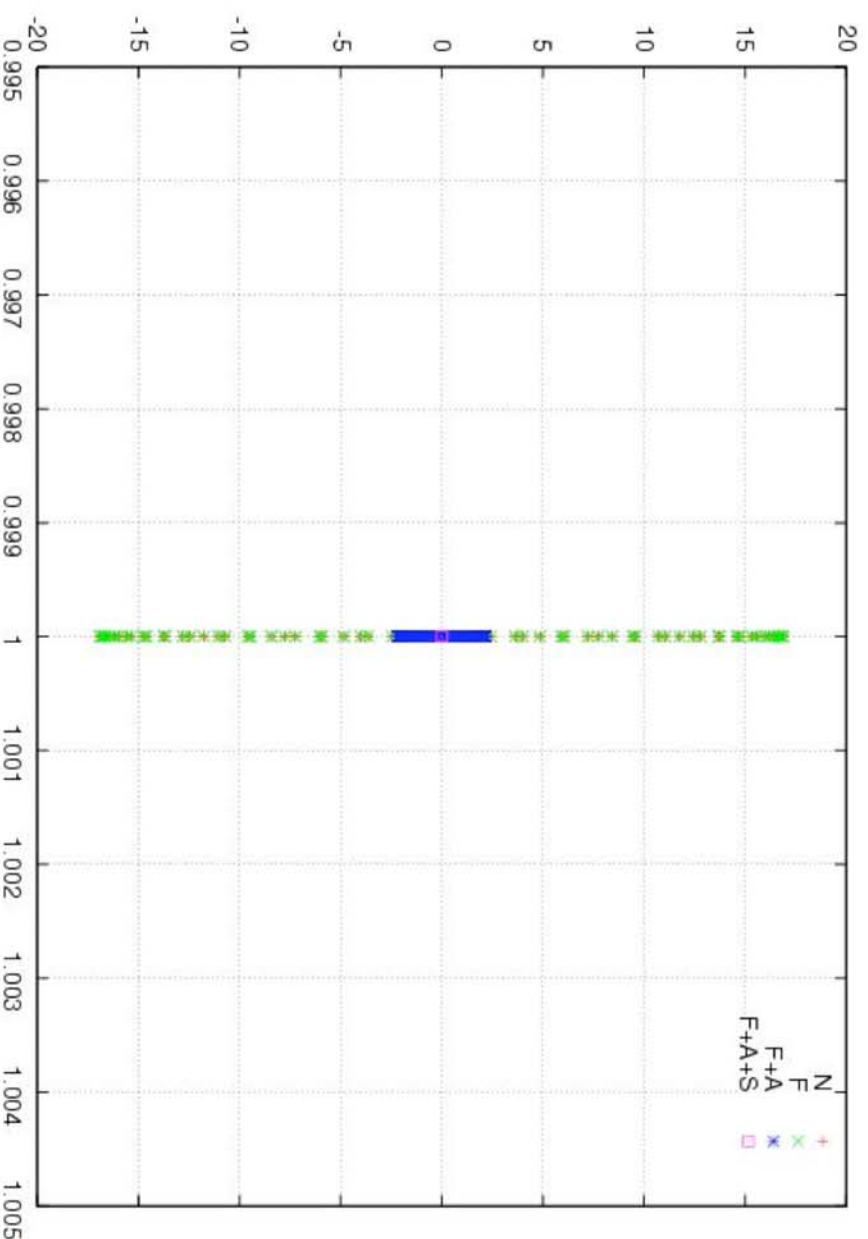
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JFNK: Resistive MHD - Preconditioner

- Instead of solving $J \delta U = -g$ solve $(J P^{-1}) (P \delta U) = -g$, i.e., right preconditioning is employed
- The preconditioner is split into a hyperbolic and a diffusive component

$$P^{-1} = P_h^{-1} P_d^{-1} = J(\mathbf{U})^{-1} + \mathcal{O}(\Delta t^2)$$

- Denoting by (\cdot) the location of the linear operator action, the ideal MHD Jacobian is

$$\begin{aligned} J_h(\mathbf{U}) &= I + \bar{\gamma} [J_x \partial_x(\cdot) + J_y \partial_y(\cdot) + J_z \partial_z(\cdot)] \\ &= I + \bar{\gamma} [J_x L_x^{-1} L_x \partial_x(\cdot) + J_y L_y^{-1} L_y \partial_y(\cdot) + J_z L_z^{-1} L_z \partial_z(\cdot)] \\ &= I + \bar{\gamma} [J_x L_x^{-1} \partial_x(L_x(\cdot)) - J_x L_x^{-1} \partial_x(L_x)(\cdot) \\ &\quad + J_y L_y^{-1} \partial_y(L_y(\cdot)) - J_y L_y^{-1} \partial_y(L_y)(\cdot) \\ &\quad + J_z L_z^{-1} \partial_z(L_z(\cdot)) - J_z L_z^{-1} \partial_z(L_z)(\cdot)] \end{aligned}$$

where J_x is the Jacobian of the hyperbolic flux in the x-direction. L_x is the spatially local left eigenvector matrix for J_x . J_y , L_y , J_z , and L_z are similarly defined

JFNK: Resistive MHD - Preconditioner

- Directional splitting is employed to further approximate the preconditioner

$$\begin{aligned} P_h &= [I + \bar{\gamma} J_x L_x^{-1} \partial_x (L_x(\cdot))] [I + \bar{\gamma} J_y L_y^{-1} \partial_y (L_y(\cdot))] [I + \bar{\gamma} J_z L_z^{-1} \partial_z (L_z(\cdot))] \\ &\quad [I - \bar{\gamma} (J_x L_x^{-1} \partial_x (L_x) + J_y L_y^{-1} \partial_y (L_y) + J_z L_z^{-1} \partial_z (L_z))] \\ &= P_x P_y P_z P_{\text{corr}}. \end{aligned}$$

- Decoupling into 1D wave equations along characteristics

$$L_i(x) J_i(x) = \Lambda_i(x) L_i(x), \quad \Lambda_i = \text{Diag}(\lambda^1, \dots, \lambda^8)$$

$$L_i [I + \bar{\gamma} J_i L_i^{-1} \partial_i (L_i(\cdot))] \xi = L_i \beta \Leftrightarrow \zeta + \bar{\gamma} \Lambda_i \partial_i \zeta = \chi,$$

$$\text{where } \zeta = L_i \xi \text{ and } \chi = L_i \beta$$

- Thus along each direction, we get a system of linear wave equations. For each wave family, we now get a sequence of tridiagonal linear systems which can be efficiently solved. In parallel we use the method proposed by Arbenz & Gander (1994)

JFNK: Resistive MHD - Preconditioner

- For spatially varying $J(U)$ a correction solve is involved

$$P_{\text{corr}} = I - \bar{\gamma} [J_x L_x^{-1} \partial_x (L_x) + J_y L_y^{-1} \partial_y (L_y) + J_z L_z^{-1} \partial_z (L_z)] \\ = I - \bar{\gamma} [L_x^{-1} \Lambda_x \partial_x (L_x) + L_y^{-1} \Lambda_y \partial_y (L_y) + L_z^{-1} \Lambda_z \partial_z (L_z)]$$

- Since this has no spatial couplings, the resulting local block systems may be solved easily by precomputing the 8x8 block matrices P_{corr} at each location coupled with a LU factorization
- Only the fastest stiffness inducing waves need to be solved. Furthermore, accuracy may be sacrificed because this is done in the context of the preconditioner.
- It can be shown that the error bound (Reynolds, Samtaney, Woodward, 2008) q-fastest waves are preconditioned is

$$\|\chi - \hat{\chi}\|_p \leq \|L_F^{-1}\|_p \left[\sum_{l=q+1}^n \left(\frac{\|\Delta t \lambda^l \partial_x(\cdot)\|_p}{1 - \|\Delta t \lambda^l \partial_x(\cdot)\|_p} \right)^p \|(L_F b)^l\|_p^p \right]^{1/p}$$

- Error from preconditioning q-fastest waves is dominantly $\frac{|\Delta t \lambda^{q+1} / \Delta x|}{1 - |\Delta t \lambda^{q+1} / \Delta x|}$

- Omission of waves with small speeds compared to the dynamical time scale will not significantly affect the preconditioner accuracy

JFNK: Resistive MHD - Preconditioner

- Diffusion Preconditioner P_d : This solves the subsystem $\partial_t \mathbf{U} - \nabla \cdot \mathbf{F}_v = 0$

$$P_d = J_v(\mathbf{U}) = I - \bar{\gamma} \frac{\partial}{\partial \mathbf{U}} (\nabla \cdot \mathbf{F}_v) \\ = \begin{bmatrix} I & 0 & 0 & 0 \\ 0 & I - \bar{\gamma} D_{\rho v} & 0 & 0 \\ 0 & 0 & I - \bar{\gamma} D_B & 0 \\ -\bar{\gamma} L_\rho & -\bar{\gamma} L_{\rho v} & -\bar{\gamma} L_B & I - \bar{\gamma} D_e \end{bmatrix}$$

- To solve $P_d \mathbf{y} = \mathbf{b}$ for $\mathbf{y} = [y_\rho, y_{\rho v}, y_B, y_e]^T$

1. Update $y_\rho = b_\rho$
2. Solve $(I - \bar{\gamma} D_{\rho v}) y_{\rho v} = b_{\rho v}$ for $y_{\rho v}$
3. Solve $(I - \bar{\gamma} D_B) y_B = b_B$ for y_B
4. Update $\tilde{b}_e = b_e + \bar{\gamma} (L_\rho y_\rho + L_{\rho v} y_{\rho v} + L_B y_B)$
5. Solve $(I - \bar{\gamma} D_e) y_e = \tilde{b}_e$ for y_e .

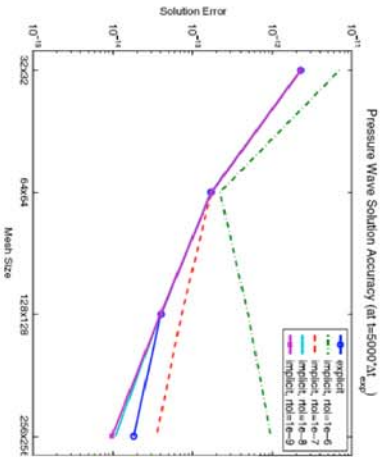
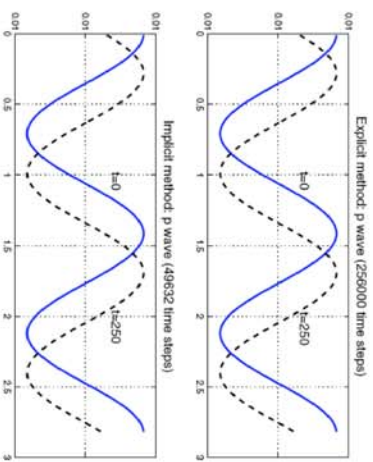
Steps 2,3 and 5 are solved using a geometric multigrid approach. Step 4 may be approximated with finite differences instead of constructing and multiplying by individual submatrices

$$L_\rho y_\rho + L_{\rho v} y_{\rho v} + L_B y_B = \frac{1}{\sigma} [\nabla \cdot \mathbf{F}_v (U + \sigma W) - \nabla \cdot \mathbf{F}_v(\mathbf{U})]_e + O(\sigma),$$

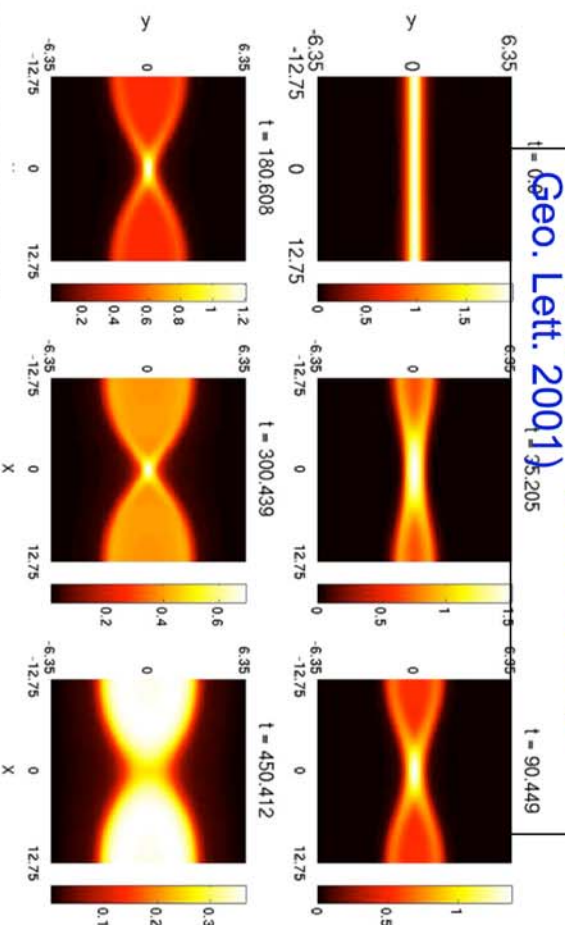
where $W = [y_\rho, y_{\rho v}, y_B, 0]^T$

Verification Tests

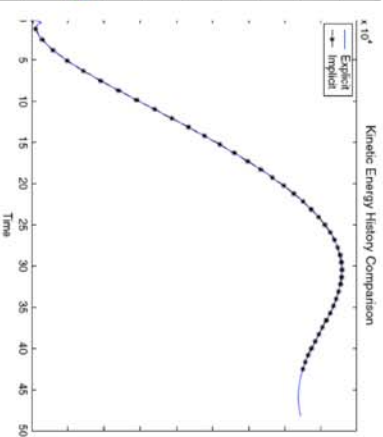
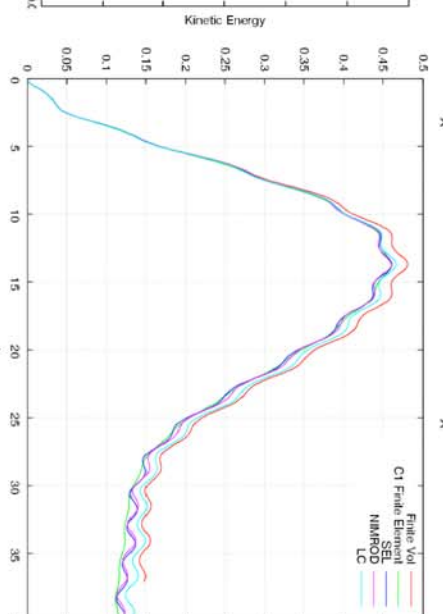
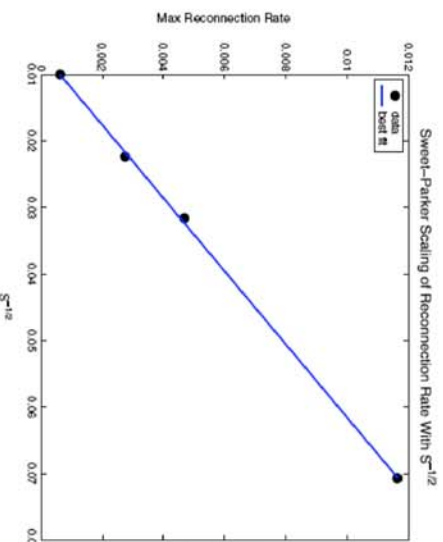
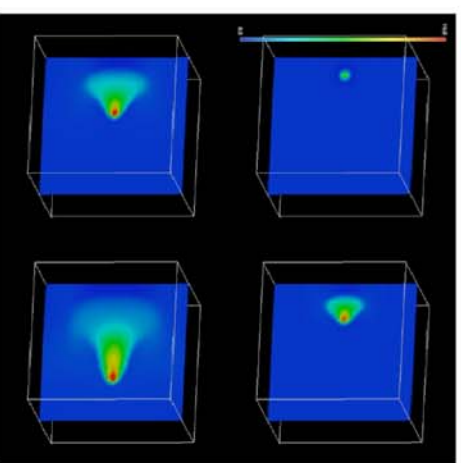
Linear wave propagation test.



Computational time for an explicit method scales as $S^{3/2}$
Initial conditions: Perturbed Harris sheet proposed by Birn et al. (J. Geo. Lett. 2001)

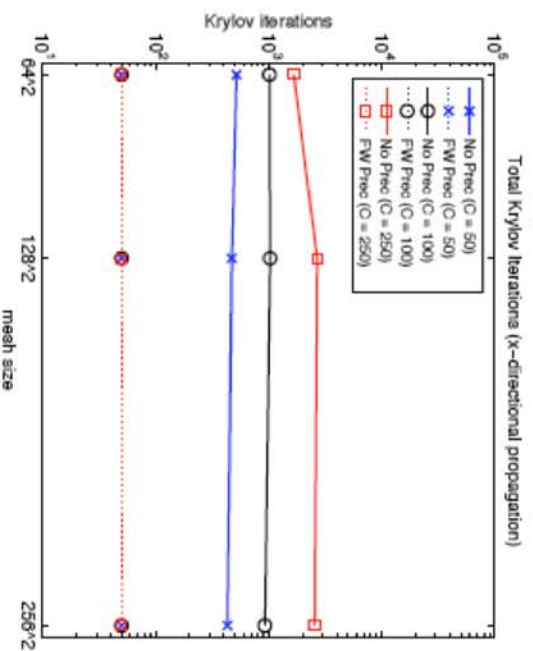


Pellet Model Problem with a similar separation of scale as the tokamak case.

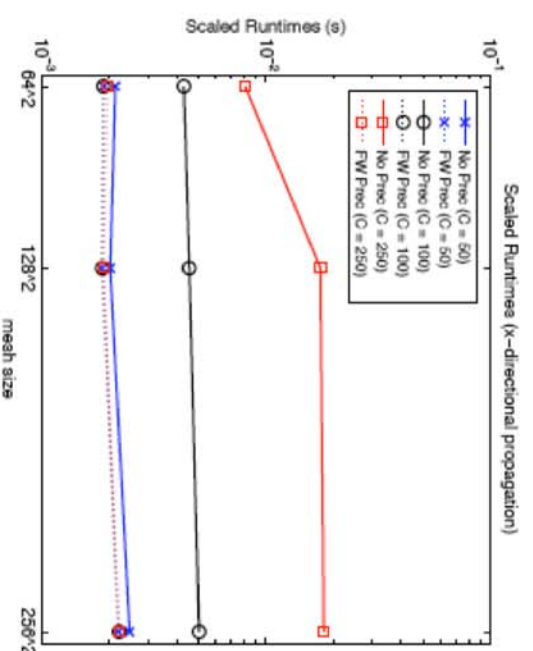


From Reynolds, Samtaney & Woodward, JCP 2006

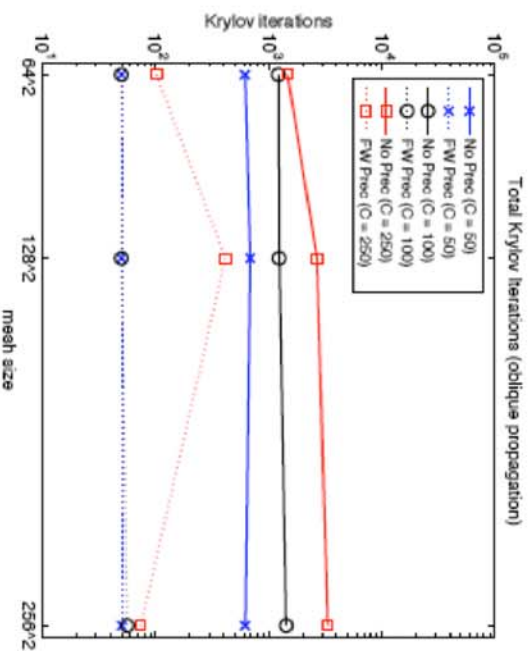
Verification Test: Linear Wave Propagation



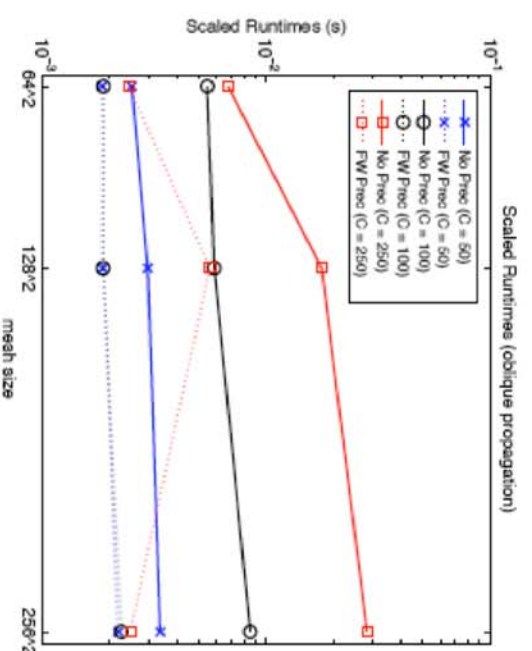
(a) Krylov iterations (*x*-dir.)



(b) scaled CPU (*x*-dir.)

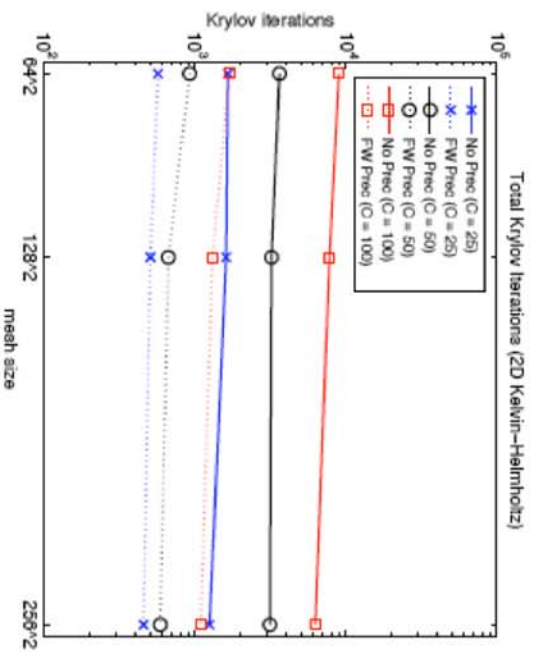


(c) Krylov iterations (oblique)

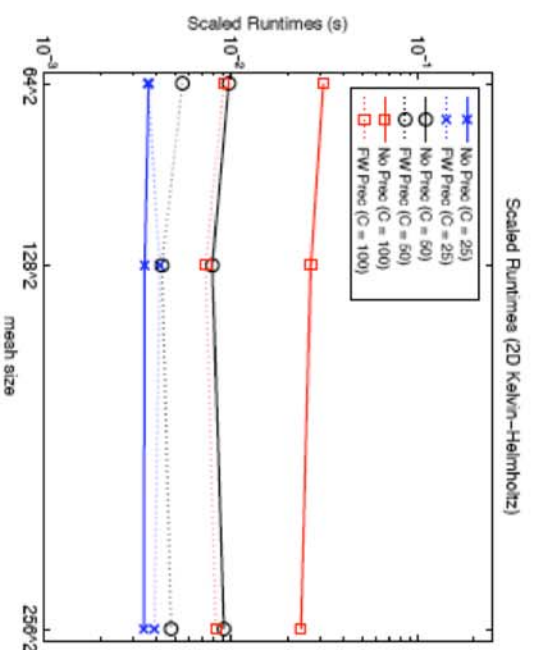


(d) scaled CPU (oblique)

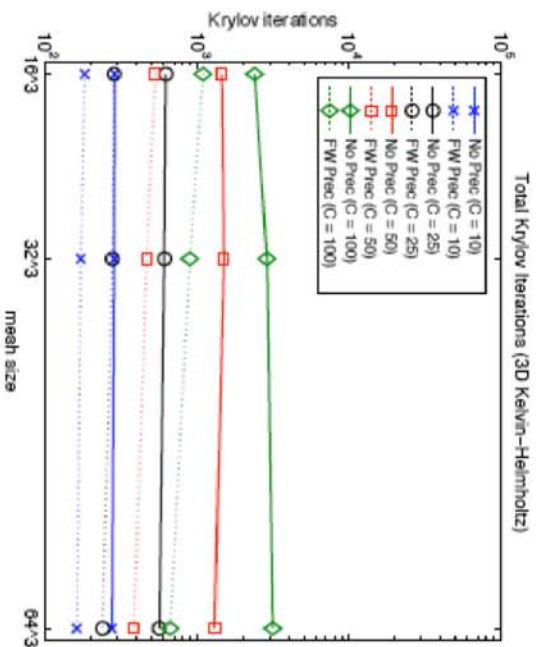
Verification Test: Kelvin-Helmholtz



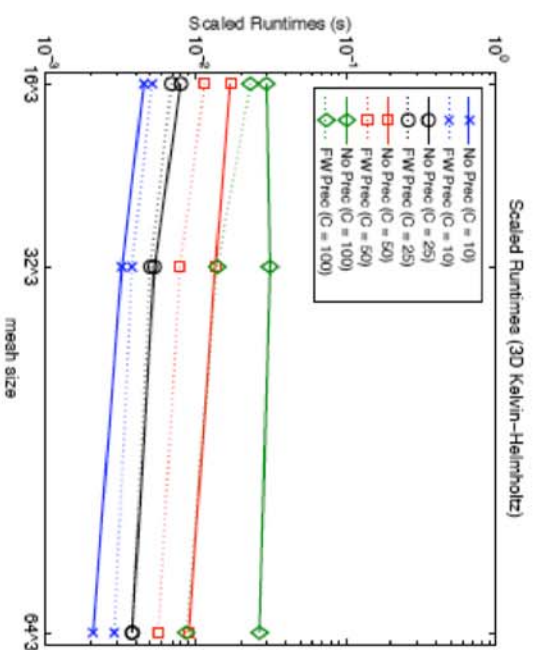
(a) Krylov iterations (2D)



(b) scaled CPU (2D)



(c) Krylov iterations (3D)



(d) scaled CPU (3D)

CSEPP Equations (from GY-FU)

- The main equation (equivalent to the perpendicular momentum equation derived from gyrokinetics)

$$\frac{d}{dt} = \frac{\partial}{\partial t} + \mathbf{V}_{\mathbf{E} \times \mathbf{B}} \cdot \nabla$$

Shear Alfvén wave term w/o ballooning term

$$\begin{aligned}
 & -\frac{d}{dt} \nabla \cdot \left(\frac{1}{V_A^2} \nabla_{\perp} \Phi \right) + \mathbf{B} \cdot \nabla \frac{\mathbf{B} \cdot \nabla \times \nabla \times \mathbf{A}}{B_0^2} + (\nabla A_{\parallel} \times \mathbf{b}) \cdot \nabla \left(\frac{\mathbf{J}_{\parallel 0}}{B_0} \right) \\
 = & \frac{1}{V_A^2} \left(\frac{3v_t^2}{4\Omega^2} \right) \nabla_{\perp}^4 \frac{d\Phi}{dt} + \mathbf{b} \times \sum_j \nabla \left(\frac{emv_t^2}{2B_0\Omega^2} \right)_j \cdot \nabla \nabla_{\perp}^2 \Phi - \sum_j \int (e\mathbf{v}_d \cdot \nabla f)_j d^3v
 \end{aligned}$$

Ion FLR term

Diamagnetic drift

All other kinetic terms from both thermal and fast ions

Model Equations

- Model assumes isothermal electrons
- If first and third terms in V_e can be neglected, we don't have to solve an equation for $V_{\parallel,i}$
- The equations can then be rewritten as:

$$\frac{\partial L(\Phi)}{\partial t} = R_{\Phi}(A_{\parallel}, \Phi) + S(f)$$

$$\frac{\partial A_{\parallel}}{\partial t} = R_A(\Phi, n_e)$$

$$\frac{\partial \delta n_e}{\partial t} = R_{n_e}(A_{\parallel}, n_e)$$

$$L = \frac{1}{V_A^2} \left[\nabla_{\perp}^2 + \left(\frac{3v_t^2}{4\Omega^2} \right) \nabla_{\perp}^4 \right]$$

$$\frac{\partial A_{\parallel}}{\partial t} = \nabla_{\parallel} \Phi - E_{\parallel}$$

$$\frac{\partial \delta n_e}{\partial t} = \nabla \cdot (V_e n_e)$$

$$E_{\parallel} = -\frac{1}{en_e} \nabla_{\parallel} \delta p_e = -\frac{T_e}{en_e} \nabla_{\parallel} \delta n_e$$

$$V_e = \frac{E \times B}{B_0^2} - \frac{\delta J_{\parallel}}{en_e} + v_{\parallel,i} \mathbf{b} \approx -\frac{\delta J_{\parallel}}{en_e}$$

$$\mathbf{J} \approx \nabla_{\perp}^2 \mathbf{A}_{\parallel}$$

Implicit Solve for Model

- Define $\Psi = L(\Phi)$
- If we use backward Euler
 - *Unknowns are $\Psi, \Phi, \mathbf{A}_{\parallel}, \delta n_e$*

$$\begin{aligned}\Psi^{n+1} - \Delta t R_{\Phi}^n + 1 - L(\Phi^n) - \Delta t S^n(f) &= 0 \\ \mathbf{A}_{\parallel}^{n+1} - \Delta t R_{\mathbf{A}}^n + 1 - \mathbf{A}^n &= 0 \\ \delta n_e^{n+1} - \Delta t R_{n_e}^n + 1 - \delta n_e^n &= 0 \\ \Phi^{n+1} - L^{-1}(\Psi^{n+1}) &= 0\end{aligned}$$

- This can be cast into the JFNK framework
- It will require an elliptic solve for Ψ
 - *Has been done in the context of reduced MHD where a Poisson operator was inverted during each Newton step (Chacon, Knoll & Finn, JCP 2002)*

Implicit Solve for Model - Issues

- The operator L includes a fourth order operator
 - Will require an additional auxiliary variable if C0 continuous finite or spectral elements are employed
 - A solver to invert L will have to be developed
- As mentioned earlier Krylov methods can have convergence problems
 - Especially true if the linear system is ill-conditioned
 - Physics-based preconditioners will have to be developed for the linear Krylov phase of the solver
 - Such preconditioners are a subject of ongoing research

Summary & Future Work

- Presented a primer on Jacobian-Free Newton-Krylov methods for nonlinearly implicit solution of PDEs
- Preconditioning is the key to have an effective JFNK method
 - *Presented an example of wave-structure based preconditioner for MHD*
- Discussed a set of model equations relevant to CSEPP
- Future Directions
 - *Recommend developing a code to test the JFNK ideas in a simple geometry*
 - *Develop physics-based preconditioners for the model system*

Acknowledgement

- Phillip Colella, the Applied Numerical Algorithms Group, and the Applied Partial Differential Equations Center (APDEC) at Lawrence Berkeley National Laboratory
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