The M3D-C^1 Implicit Solver

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$$\begin{aligned}\rho_0\dot{\mathbf{v}} + \nabla(p+\theta\delta t\dot{p}) &= \frac{1}{\mu_0}\left[(\nabla\times\mathbf{B})\times\mathbf{B}\right] \\ &+ \frac{\theta\delta t}{\mu_0}\left[\left(\nabla\times\dot{\mathbf{B}}\right)\times\mathbf{B} + (\nabla\times\mathbf{B})\times\dot{\mathbf{B}}\right]\end{aligned} \tag{20.15}$$

where we have denoted time derivatives with a dot: i.e., $\dot{\mathbf{v}} \equiv \partial\mathbf{v}/\partial t$. Next,do a similar expansion with the velocity in the magnetic field and pressure equations:

$$\dot{\mathbf{B}} = \nabla\times\left[(\mathbf{v}+\theta\delta t\dot{\mathbf{v}})\times\mathbf{B}\right] \tag{20.16}$$

$$\dot{p} = -(\mathbf{v}+\theta\delta t\dot{\mathbf{v}})\cdot\nabla p - \gamma p\nabla\cdot(\mathbf{v}+\theta\delta t\dot{\mathbf{v}}) \tag{20.17}$$

We next substitute for $\dot{\mathbf{B}}$ and $\dot{p}$ from Eqs. (20.16) and (20.17) into Eq. (20.15), multiply by δt, and finite difference the velocity forward in time so that $\delta t\dot{\mathbf{v}} \rightarrow \mathbf{v}^{n+1} - \mathbf{v}^n$. Collecting terms, we can rewrite (20.15) as:

$$\begin{aligned}\left\{\rho_0 - \theta^2(\delta t)^2\mathcal{L}\right\}\mathbf{v}^{n+1} &= \left\{\rho_0 - \theta(1-\theta)(\delta t)^2\ \mathcal{L}\right\}\mathbf{v}^n \\ &+ \delta t\left\{-\nabla p + \frac{1}{\mu_0}\left[(\nabla\times\mathbf{B})\times\mathbf{B}\right]\right\}\end{aligned} \tag{20.18}$$

Only involves velocity!

Here we have defined the operator:

$$\begin{aligned}\mathcal{L}\mathbf{v} &\equiv \frac{1}{\mu_0}\left\{\nabla\times\left[\nabla\times(\mathbf{v}\times\mathbf{B})\right]\right\}\times\mathbf{B} \\ &+ \frac{1}{\mu_0}\left\{(\nabla\times\mathbf{B})\times\nabla\times(\mathbf{v}\times\mathbf{B})\right\} \\ &+ \nabla(\mathbf{v}\cdot\nabla p + \gamma p\nabla\cdot\mathbf{v}).\end{aligned} \tag{20.19}$$

A similar technique is used on the magnetic field equations. Fully implicit Extended MHD (2-fluid) equations-- time step determined by accuracy only:

$$\begin{bmatrix} S_{11}^v & S_{12}^v & S_{13}^v \\ S_{21}^v & S_{22}^v & S_{23}^v \\ S_{31}^v & S_{32}^v & S_{33}^v \end{bmatrix} \bullet \begin{bmatrix} U \\ V_z \\ \chi \end{bmatrix}^{n+1} = \begin{bmatrix} D_{11}^v & D_{12}^v & D_{13}^v \\ D_{21}^v & D_{22}^v & D_{23}^v \\ D_{31}^v & D_{32}^v & D_{33}^v \end{bmatrix} \bullet \begin{bmatrix} U \\ V_z \\ \chi \end{bmatrix}^{n} + \begin{bmatrix} R_{11}^v & R_{12}^v & R_{13}^v \\ R_{21}^v & R_{22}^v & R_{23}^v \\ R_{31}^v & R_{32}^v & R_{33}^v \end{bmatrix} \bullet \begin{bmatrix} \psi \\ I \\ P_e \end{bmatrix}^{n}$$

$$\vec{V} = \nabla U \times \hat{z} + \nabla_\perp \chi + V_z$$
$$\vec{B} = \nabla \psi \times \hat{z} + I \hat{z}$$

Alfven Wave physics

$$S_{11}^n \bullet N^{n+1} = D_{11}^n \bullet N^n + \begin{bmatrix} R_{11}^n & R_{12}^n & R_{13}^n \end{bmatrix} \bullet \begin{bmatrix} U \\ V_z \\ \mathrm{X} \end{bmatrix}^{n+1} + \begin{bmatrix} Q_{11}^n & Q_{12}^n & Q_{13}^n \end{bmatrix} \bullet \begin{bmatrix} U \\ V_z \\ \mathrm{X} \end{bmatrix}^{n} + Q_{14}^n$$

density

$$S_{11}^p \bullet P^{n+1} = D_{11}^p \bullet P^n + \begin{bmatrix} R_{11}^p & R_{12}^p & R_{13}^p \end{bmatrix} \bullet \begin{bmatrix} U \\ V_z \\ \mathrm{X} \end{bmatrix}^{n+1} + \begin{bmatrix} Q_{11}^p & Q_{12}^p & Q_{13}^p \end{bmatrix} \bullet \begin{bmatrix} U \\ V_z \\ \mathrm{X} \end{bmatrix}^{n} + Q_{14}^p$$

pressure

$$\begin{bmatrix} S_{11}^p & S_{12}^p & S_{13}^p \\ S_{21}^p & S_{22}^p & S_{23}^p \\ S_{31}^p & S_{32}^p & S_{33}^p \end{bmatrix} \bullet \begin{bmatrix} \psi \\ I \\ P_e \end{bmatrix}^{n+1} = \begin{bmatrix} D_{11}^p & D_{12}^p & D_{13}^p \\ D_{21}^p & D_{22}^p & D_{23}^p \\ D_{31}^p & D_{32}^p & D_{33}^p \end{bmatrix} \bullet \begin{bmatrix} \psi \\ I \\ P_e \end{bmatrix}^{n} + \begin{bmatrix} R_{11}^p & R_{12}^p & R_{13}^p \\ R_{21}^p & R_{22}^p & R_{23}^p \\ R_{31}^p & R_{32}^p & R_{33}^p \end{bmatrix} \bullet \begin{bmatrix} U \\ V_z \\ \chi \end{bmatrix}^{n+1} + \begin{bmatrix} Q_{11}^p & Q_{12}^p & Q_{13}^p \\ Q_{21}^p & Q_{22}^p & Q_{23}^p \\ Q_{31}^p & Q_{32}^p & Q_{33}^p \end{bmatrix} \bullet \begin{bmatrix} U \\ V_z \\ \chi \end{bmatrix}^{n}$$

Whistler, KAW, field diffusion physics

- 4 sequential matrix solves per time step
- 3 non-trivial subsets with 6,4,2 variables

In 2D, Implicit equations are solved using SuperLU_Dist

Details for bassi.nersc.gov:

Mesh points	180 x 180
Matrix Rank	5.9×10^5
# Non-zeros	9.5×10^7
# NZ in L/U	8.8×10^8

# processors	8	32	128
Factor (s)	69.5	38.1	16.9
Gflop/s	27.2	50.1	112.8*

Total problem time (8 processors) for typical high resolution GEM reconnection problem = 208 s x 400 cycles x 8p = 185 p-hrs

Note that for linear problem, Matrix need only be factored once. For semi-implicit method, matrix needs to be factored only occasionally.

*NOTE: if we had 100 planes with simultaneous instances of SuperLU, this would be 12,800 p and 11.2 Tflop/s actual!

How to take this to 3D ?

Consider (1,1) component in 3D: Strauss Equations

$$\nabla_\perp^2 \dot{U} + \left[\nabla_\perp^2 U, U\right] = \left[\nabla_\perp^2 \psi, \psi\right] + B\frac{\partial}{\partial z}\nabla_\perp^2 \psi$$

$$\dot{\psi} + \left[\psi, U\right] = B\frac{\partial}{\partial z}U$$

Taylor expand in time:

$$\nabla_\perp^2 \dot{U} + \left[\nabla_\perp^2 U + \theta\delta t \nabla_\perp^2 \dot{U}, U + \theta\delta t \dot{U}\right] = \left[\nabla_\perp^2 \psi + \theta\delta t \nabla_\perp^2 \dot{\psi}, \psi + \theta\delta t \dot{\psi}\right]$$
$$+ B\frac{\partial}{\partial z}\nabla_\perp^2 \psi + \theta\delta t B\frac{\partial}{\partial z}\nabla_\perp^2 \dot{\psi}$$

$$\dot{\psi} + \left[\psi, U + \theta\delta t \dot{U}\right] = B\frac{\partial}{\partial z}U + \theta\delta t B\frac{\partial}{\partial z}\dot{U}$$

Substitute field derivatives into velocity equation to get implicit equation:

Finite Difference in Z: $\dot{U}_z = \frac{1}{\delta z}\left[\dot{U}_{j+1} - \dot{U}_{j-1}\right]$ $\dot{U}_{zz} = \frac{1}{(\delta z)^2}\left[\dot{U}_{j+1} - 2\dot{U}_j + \dot{U}_{j-1}\right]$

We get a block tridiagonal equation, with the matrix blocks being 2D matrices:

$$B_j^0 U_j^{n+1} + D_j^0 + \varepsilon(A_j^1 U_{j+1}^{n+1} + B_j^1 U_j^{n+1} + C_j^1 U_{j-1}^{n+1} + D_j^1) = 0$$

$$B_j^0 U_j^{n+1} = \nu_i \nabla_\perp^2 \dot{U}_j - (\theta\delta t)^2 \left[+\nabla_\perp^2 \psi \left[\nu_i, \left[\psi, U_j^{n+1} \right]\right] - \left(\left[\psi, U_j^{n+1} \right], \left[\nu_i, \psi \right] \right) + B\left(\nu_i, \left[\psi_z, U_j^{n+1} \right] \right) \right]$$

$$B_j^1 U_j^{n+1} = \nu_i \nabla_\perp^2 \dot{U}_j - (\theta\delta t)^2 \left[-\frac{2B^2}{(\delta z)^2} \nu_i \nabla_\perp^2 U_j^{n+1} \right]$$

$$A_j U_{j+1}^{n+1} = -(\theta\delta t)^2 \left[\begin{array}{l} -\frac{B}{\delta z} \nabla_\perp^2 \psi \left[\nu_i, U_{j+1}^{n+1} \right] - \frac{B}{\delta z} \nabla_\perp^2 U_{j+1}^{n+1} \left[\nu_i, \psi \right] \\ + \frac{B^2}{(\delta z)^2} \nu_i \nabla_\perp^2 U_{j+1}^{n+1} + \frac{B}{\delta z} \left(\nu_i, \left[\psi, U_{j+1}^{n+1} \right] \right) \end{array} \right]$$

$$C_j U_{j-1}^{n+1} = -(\theta\delta t)^2 \left[\begin{array}{l} \frac{B}{\delta z} \nabla_\perp^2 \psi \left[\nu_i, U_{j-1}^{n+1} \right] + \frac{B}{\delta z} \nabla_\perp^2 U_{j-1}^{n+1} \left[\nu_i, \psi \right] \\ + \frac{B^2}{(\delta z)^2} \nu_i \nabla_\perp^2 U_{j-1}^{n+1} - \frac{B}{\delta z} \left(\nu_i, \left[\psi, U_{j-1}^{n+1} \right] \right) \end{array} \right]$$

Can this structure be used to define an efficient iteration scheme where the 2D direct solves serve as a preconditioner ?

Summary

$$B_j^0 U_j^{n+1} + D_j^0 + \varepsilon(A_j^1 U_{j+1}^{n+1} + B_j^1 U_j^{n+1} + C_j^1 U_{j-1}^{n+1} + D_j^1) = 0$$

U_j^{n+1} is vector of all unknown velocities on plane j at new time

$B_j^0, A_j^1, B_j^1, C_j^1$ are 2D sparse matrices at plane j

D_j^0, D_j^1 are 2D vectors at plane j

Possible iteration scheme:

$$U_j^{i+1} = -\left[B_j^0\right]^{-1} \bullet \left[D_j^0 + \varepsilon(A_j^1 U_{j+1}^{i} + B_j^1 U_j^{i} + C_j^1 U_{j-1}^{i} + D_j^1)\right]$$

Note that B_j^0 matrices only need to be factored once per timestep