Multigrid solvers for equations arising in implicit MHD simulations

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Resistive MHD equations in strong conservation form

\[
\frac{\partial U}{\partial t} + \frac{\partial F_j(U)}{\partial x_j} = \frac{\partial \tilde{F}_j(U)}{\partial x_j}
\]

Diffusive

Hyperbolic

\[
\tau_{ij} = \rho \nu \left( \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \delta_{ij} \frac{\partial u_k}{\partial x_k} \right)
\]

\[
e = \frac{p}{\gamma - 1} + \frac{1}{2} \rho u_i u_i + \frac{1}{2} B_i B_i
\]

\[
U = \{\rho, \rho u_i, B_i, e\}^T
\]

\[
F_j(U) = \begin{cases}
\rho u_j \\
\rho u_i u_j + p \delta_{ij} + \frac{1}{2} B_k B_k \delta_{ij} - B_i B_j \\
u_j B_i - B_j u_i \\
(e + p + \frac{1}{2} B_k B_k) u_j - B_i u_i B_j
\end{cases}
\]

\[
\tilde{F}_j(U) = \begin{cases}
0 \\
Re^{-1} \tau_{ij} \\
S^{-1} \eta \left( \frac{\partial B_i}{\partial x_j} + \frac{\partial B_j}{\partial x_i} \right) \\
S^{-1} \eta \left( \frac{1}{2} \frac{\partial B_i B_j}{\partial x_j} - B_i \frac{\partial B_j}{\partial x_i} \right) + Re^{-1} \tau_{ij} u_i + Pe^{-1} \kappa \frac{\partial T}{\partial x_j}
\end{cases}
\]

Reynolds no.

Lundquist no.

Peclet no.
Multigrid motivation: smoothing and coarse grid correction

The Multigrid V-cycle

Finest Grid

First Coarse Grid

Note: smaller grid

smoothing

Restriction (R)

Prolongation (P) (interpolation)
Nonlinear multigrid

- Algorithm still based on residual but now:
  - \( r = A(u) - A(x) = A(x+e) - A(x) \)
  - In multigrid, obtain solution \((x^h \sim u)\) on fine grid
  - Residual \((r^{2h})\) equation on coarse grid is:
    - \( A^{2h}(x^{2h} + e^{2h}) - A^{2h}(x^{2h}) = r^{2h} \)
    - restrict residual to coarse grid \( r^{2h} \leftarrow R (f^h - A^h(x^h)) \)
    - \( A^{2h}(R(x^h) + e^{2h}) = A^{2h}(R(x^h)) + R (f^h - A^h(x^h)) = b^{2h} \)
  - We’ve obtained coarse grid equation of the form
    - \( A^{2h}(x^{2h}) = b^{2h} \)
    - With \( e^{2h} = x^{2h} - R(x^h) \)
    - Apply correction \( x^h = x^h + P(e^{2h}) \)
(Nonlinear) Multigrid $V(v_1,v_2)$ - cycle

- **Function** $u \leftarrow \text{MGV}(A, v, f)$
  - if $A$ is coarsest grid
    - $u \leftarrow A^{-1}f$
  - else
    - $v \leftarrow S^1(f, v)$  \hspace{1cm} -- Smoother (pre)
    - $r_H \leftarrow R( f - Av )$
    - $v_H \leftarrow R( v )$
    - $c_H \leftarrow \text{MGV}( A_H, v_H, r_H + A_H(v_H) )$  \hspace{1cm} -- recursion
    - $e_H \leftarrow c_H - v_H$
    - $v \leftarrow v + Pe_H$
    - $u \leftarrow S^2(f, v)$  \hspace{1cm} -- Smoother (post)

- **F-cycles:** start on coarse grid, $V$-cycle on each grid

- **Complexity (2D), geometric sum:**
  - $1 + v_1 + v_2 + 1 + 2*(1+v_1+v_2+1)/4 + 3*(1+v_1+v_2+1)/16 \ldots$
(Pointwise) Gauss-Seidel smoothers

- Gauss-Seidel is the *ideal* multigrid smoother
  - Given \( u_{i-1} - 2u_i + u_{i+1} = f_i \):
  - Loop over all grid points (cells) \( i \)
    - \( u_i \leftarrow (u_{i-1} + u_{i+1} - f_i)/2 \)
  - We have exact G-S for 1st order upwinding & 2\(^{nd}\) order C.D.

- Problems:
  - Exact G-S is often not feasible
    - Eg, for 2\(^{nd}\) order (PLM) upwind method
  - Exact G-S may result in unstable smoother
    - Eg, central differencing

- Solutions:
  - “Defect correction” for high order (L\(_2\)) methods
    - Use low order discretization (L\(_1\)) in multigrid solver (stable)
    - Solve for \( x^{m+1} \): \( L_1x^{m+1} = f - L_2x^m + L_1x^m \)
  - “Double discretization”, similar idea
  - Develop high order methods w/ more accurate G-S smoothers
    - *Long term research*
Define

\[
E(L_h) = \frac{\min(|F(\theta)| | \theta \in T^{HIGH})}{\max(|F(\theta)| | -\pi \leq \theta < \pi)}
\]

where \(F(\theta)\) is the Fourier symbol of \(L_h\)

\(T^{HIGH} = [-\pi, \pi)^2 \setminus [-\pi/2, \pi/2)^2\) -- assumes \(H = 2h\)

**Theorem (4.7.1, Trottenberg, et. al., 2000):**

- \(E(L_h)\) bounded above 0 is necessary and sufficient for the existence of a pointwise smoother.

**Example, common stencils**

- \(\partial u/\partial x\):  
  - 1D Central differencing, \(E(L_h) = 0\)
  - 1D one sided differencing, \(E(L_h) = 1/\sqrt{2}\)
  - 2D Standard 5-point stencil of Laplacian, \(E(L_h) = .25\)

**Time derivative term increases** \(h -\) **Ellipticity**
Multigrid Approach

- **Geometric MG, Cartesian grids**
  - Piecewise constant restriction R, linear interpolation (P)
- **Red/black point Gauss-Seidel smoothers**
  - Requires inner G-S solver be coded
- **F-cycle**
  - One V-cycle at each level, starting from coarsest
  - Algebraic error < discretization error in one F-cycle iteration
    - Bank, Dupont, Math Comp. 1981
- **Matrix free - more flops less memory**
  - Memory increasingly bottleneck - Matrix free is way to go
  - Processors (cores) are cheap
    - Memory architecture is expensive and slow (relative to CPU)
- **Non-linear multigrid**
  - No linearization required
- **Defect correction for high order (L₂) methods**
  - Use low order discretization (L₁) in multigrid solver (stable)
  - Solve $L₁ x^{k+1} = f - L₂ x^k + L₁ x^k$
Magnetic reconnection problem

- **GEM reconnection test**
  - 2D Rectangular domain
  - Harris sheet equilibrium
  - Density field along axis: (fig top)
  - Magnetic (smooth) step: (fig bottom)
  - Perturb B with a “pinch”

- **Low order preconditioner**
  - Upwind - Rusanov method

- **Higher order in space: C.D.**
- **CN (2\textsuperscript{nd} order) or Backward Euler (1\textsuperscript{st} order)**

- **Solver**
  - 1 F-cycle w/ V(4,4)-cycle per time step
    - Nominally 11x explicit cost per time step
    - ~22 work units per time step

- **Viscosity:**
  - Low: $\mu=5.0\text{D-04}$, $\eta=5.0\text{D-03}$, $\kappa=2.0\text{D-02}$
  - High: $\mu=5.0\text{D-02}$, $\eta=5.0\text{D-03}$, $\kappa=2.0\text{D-02}$

- **$B_z$:** $B_z=0$ and $B_z=5.0$
  - Strong guide field $B_z$ (eg, 5.0)
  - critical for tokomak plasmas
$B_z = 0$, High viscosity

- Time = 100.0, $\Delta t = 1$
  - approximately 100x CFL on 512 X 256 grid
- 2nd order spatial convergence
- Use 2nd order Crank-Nicolson in time
- Kinetic energy compares well with other codes
Verify 2nd order convergence

- 2nd order spatial accuracy
  - Achieved with F-cycle MG solver
- $B_z = 0$, Low viscosity
- Up to 256M dof on 128 cores

GEM $B_z=0.0$, low viscosity, 2nd order convergence
**B_z = 0, Low viscosity, \( \nabla \cdot B = 0 \)**

- Time = 100.0, \( \Delta t = .1 \)
- 2\(^{nd}\) order spatial convergence
- \( \nabla \cdot B = 0 \) converges
- Kinetic energy compares well w/ other codes

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GEM \( B_z = 0.0 \), low viscosity, convergence (space), \( \Delta t = .1 \), 1-F(4,4) cycle

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GEM Reconnection Test: Low Viscosity Case

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GEM Reconnection Test: Low Viscosity Case
Verify against M3D-C1, $B_z=5$, High viscosity

M3D-C1 – Jardin JCP 2007

Fully implicit MHD

Resistive GEM: $B_0=5$, $\eta=.005$, $\mu=.05$, $\kappa=.02$

GEM $B_z=5.0$, high viscosity, $\Delta t=.1$
$B_z = 5$, Low viscosity

- Hardest test case
- $\Delta t = 0.05$, $\sim 55 \times$ CFL
Residual history ($B_z=5$)

- F cycles achieve discretization error
- Observe “super” convergence

GEM residual history, $B_z=5$, $\Delta t = T = .1$
Conclusion (1)

- Shown that multigrid can be a viable method for solving the nonlinear equations in fully implicit MHD simulations, with potential for minimal cost
  - eg, just few “work units” per time step
- “high viscosity” and $B_z=0$ case solves very well
  - Low viscosity and/or $B_z=5$ require smaller times steps
- Challenge is getting consistent & stable G-S smoother:
  - Defect correction method useful, but not “optimal”
  - More than point-wise Gauss-Seidel - DGS
  - Additive, multistage smoothers (eg, 4\textsuperscript{th} order explicit RK)
  - Other 2nd order methods with (approximate) G-S
- Future:
  - Push back on equations: low mach number asymptotic analysis for strong guide field ($B_z$)
    - Semi-implicit to start
Hyperbolic equations $B \cdot \text{Grad}$ & distributive Gauss-Seidel

- Degenerate Hyperbolic
- Point G-S smoothing not sufficient
- Use distributive G-S
- Use backward Euler
- Right preconditioning
- Matrix free & all-at-once smoother

Model equation:

\[
\frac{\partial w}{\partial t} = \frac{1}{\rho} \left( \mathbf{B}^\perp \cdot \nabla^\perp \right) \delta_z
\]
\[
\frac{\partial \delta_z}{\partial t} = (\mathbf{B}^\perp \cdot \nabla^\perp) \delta_w
\]

\[
L(U) \equiv \begin{pmatrix}
\delta_t & -\frac{1}{\rho} \delta_t \\
-\delta & \delta_t
\end{pmatrix}
\begin{pmatrix}
u \\
v
\end{pmatrix}
= \begin{pmatrix}0 \\
0
\end{pmatrix} \equiv F
\]

where $\delta_t \equiv \frac{\partial}{\partial t}$ and $\delta \equiv B_x \cdot \frac{\partial}{\partial x} + B_y \cdot \frac{\partial}{\partial y}$. Consider the operator,

\[
C \equiv \begin{pmatrix}
\delta_t & \frac{1}{\rho} \delta_t \\
\delta & \delta_t
\end{pmatrix}
\]

and notice that

\[
LC = \begin{pmatrix}
\delta_t^2 - \frac{1}{\rho} \delta_t^2 & 0 \\
0 & \delta_t^2 - \frac{1}{\rho} \delta_t^2
\end{pmatrix}
\]

Distributed G-S w/ distributor $C$

Define $q$ by $u = Cq$:

$q \leftarrow q + B_{LC}(F - LCq)$

Pre-multiply by $C$

$Cq \leftarrow Cq + CB_{LC}(F - LCq)$

Use $u = Cq$

$u \leftarrow u + CB_{LC}(F - Lu)$
Numerical results

- **Blob (both components)**
- **“rounded square” B field** (single mode flux function)
  - $B_x = \cos(y) \cdot \sin(x)$
  - $B_y = -\cos(x) \cdot \sin(y)$
- 20 time steps
- 1 F(1,1) cycle / time step
- ~100x CFL of fast wave
- ~10x advection time scale
- 256 X 256 grid
Thank you
AllSpeed hyperbolic equations $B \cdot \nabla w = 0$ & distributed Gauss-Seidel

- **An MHDAllspeed wave equation:**
  - Where $B$ is a given field
  - In operator form: $LU = \begin{pmatrix} 1 & -\Delta t^2 D \\ -\Delta t^2 D & 1 \end{pmatrix} \begin{pmatrix} u_{k+1} \\ w_{k+1} \end{pmatrix} = \frac{\Delta t}{\Delta x} \begin{pmatrix} u_k \\ w_k \end{pmatrix} = F$
  - Where $D = B \cdot \nabla$
  - Backward Euler time integration is used

- **Observe:** $LC = \begin{pmatrix} 1 & -\Delta t D \\ -\Delta t D & 1 \end{pmatrix} \begin{pmatrix} 1 & \Delta t D \\ \Delta t D & 1 \end{pmatrix} = \begin{pmatrix} 1 - \Delta t^2 D^2 & 0 \\ 0 & 1 - \Delta t^2 D^2 \end{pmatrix}$

  - Thus, $LC$ is an elliptic operator in limit as $\Delta t \to \infty$
  - Pointwise Gauss-Seidel is stable – needed for a smoother
  - Define $\bar{U}$ by $U = C \bar{U}$, and a pointwise smoother (eg, G-S) $B_{LC}$:
    - Defined but the iterative method: $\bar{U} = \bar{U} + B_{LC} (F - LC \bar{U})$
    - Pre multiply by $C$: $U = U + CB_{LC} (F - LU)$, using $U = C \bar{U}$
    - Stable iterative method to solve/smooth $LU = F$
The Fundamental Equations for Plasma Physics: Boltzmann+Maxwell

6D+time

\[
\frac{\partial f_\alpha}{\partial t} + \vec{u} \cdot \nabla \vec{r} f_\alpha + \frac{q_\alpha}{m_\alpha} (\vec{E} + \vec{u} \times \vec{B}) \cdot \nabla \vec{u} f_\alpha = \left( \frac{\partial f_\alpha}{\partial t} \right)_C \quad f_\alpha (\vec{r}, \vec{u}, t)
\]

\[
\frac{\partial \vec{B}}{\partial t} = -\nabla \times \vec{E} \quad \nabla \cdot \vec{B} = 0
\]

\[
\frac{1}{c^2} \frac{\partial \vec{E}}{\partial t} = \nabla \times \vec{B} - \mu_0 \vec{J} \quad \nabla \cdot \vec{E} = \frac{\sigma}{\varepsilon_0}
\]

- Complete but impractical
- Cannot solve on all time and length scales
- (MHD) Can eliminate dimensions by integrating over velocity space (with closure assumptions)
Finite Volume Discretization

- **Ideal MHD Hyperbolic system:**
  - $\frac{\partial u}{\partial t} + \frac{\partial F(u)}{\partial x} + \frac{\partial G(u)}{\partial y} + \ldots = 0$
  - $u = \{\rho, m_x, m_y, m_z, B_x, B_y, B_z, e\}$, $F(u)$ and $G(u)$ fully nonlinearly couple $u$

- **Central differencing (2nd order):**
  - $u_{i-1}---u_i---u_{i+1}---$ cells or volumes (1D), w/ length $\Delta x$
  - $F_{i-1/2} \quad F_{i+1/2}$ fluxes computed at volume faces
  - $(u_i^{k+1} - u_i^k)/\Delta t + (F(u_{i+1/2}^{k+1}) - F(u_{i-1/2}^{k+1}))/\Delta x + \ldots = 0$
    - Let $F(u_{i+1/2}) = (F(u_{i+1}) + F(u_i))/2$, and so on
  - **Backward Euler solve**, use $u^{k+1}$:
    - $u_i^{k+1} + (\Delta t/2\Delta x)(F(u_{i+1}^{k+1}) - F(u_{i-1}^{k+1})) = u_i^k$
    - At each time step

- **Upwinding (1st order Rusanov)**
  - Let $F(u_{i+1/2}) = (F(u_{i+1}) + F(u_i))/2 - |\lambda_{i+1/2}^{max}(u_{i+1} - u_i)/2$
  - $\lambda_{i+1/2}^{max}$ is a maximum wave speed of $(u_{i+1} + u_i)/2$

- **2nd order Upwinding …**
  - Piecewise linear reconstruction method (PLM)