Superior discretizations and AMG solvers for extremely anisotropic diffusion via hyperbolic operators

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Outline

Anisotropic diffusion

Spatial discretization
  Discontinuous elements
  Continuous elements
  Structure preservation

Linear solvers
  AIR Algebraic Multigrid
  Open field lines (DG)
  Closed field lines
Anisotropic diffusion

Evolution of temperature $T$ in plasma, heat flux $q$, forcing $S$:

$$\frac{\partial T}{\partial t} - \nabla \cdot (\kappa_\parallel \nabla_\parallel + \kappa_\perp \nabla_\perp) T = S,$$

(Dirichlet BCs) $T|_{\partial \Omega} = T_{BC},$

where $b = B/|B|$ is direction of magnetic field lines, and

$$\nabla_\parallel (\cdot) := b \cdot \nabla (\cdot) b,$$

$$\nabla_\perp := \nabla - \nabla_\parallel.$$
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Many ways to skin a PDE!
Anisotropic diffusion

Evolution of temperature $T$ in plasma, heat flux $q$, forcing $S$:

$$\frac{\partial T}{\partial t} - \nabla \cdot q = S,$$

$$q = \kappa_\parallel \nabla_\parallel T + \kappa_\perp \nabla_\perp T,$$

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$$\nabla_\parallel (\cdot) := b \cdot \nabla (\cdot) b,$$

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Evolution of temperature $T$ in plasma, heat flux $\mathbf{q}$, forcing $S$:

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where $\mathbf{b} = \mathbf{B}/|\mathbf{B}|$ is direction of magnetic field lines, and

$$\nabla_{\parallel}(\cdot) := \mathbf{b} \cdot \nabla(\cdot) \mathbf{b},$$

$$\nabla_{\perp} := \nabla - \nabla_{\parallel}.$$  

- In magnetic confinement fusion, expect $\frac{\kappa_{\parallel}}{\kappa_{\perp}} \sim 10^9 - 10^{10}$.
- Parabolic equation in nature, but for non-grid-aligned $\mathbf{b}$, both discretization accuracy and implicit solve are very hard.
Directional gradient formulation

Define purely anisotropic conductivity $\kappa_\Delta := \kappa_\parallel - \kappa_\perp$.

- Diffusion isotropic if $\kappa_\Delta = 0$,
- Predominately anisotropic if $\kappa_\Delta \gg \kappa_\perp$.

Heat flux can be written as

$$q = \kappa_\Delta \nabla_\parallel T + \kappa_\perp \nabla T.$$  

Use directional derivative $\mathbf{b} \cdot \nabla T$ as auxiliary variable, reformulate

$$\frac{\partial T}{\partial t} - \sqrt{\kappa_\Delta} \nabla \cdot (\mathbf{b} \zeta) - \nabla \cdot (\kappa_\perp \nabla T) = S,$$

$$\zeta = \sqrt{\kappa_\Delta} \mathbf{b} \cdot \nabla T.$$
The steady state limit

Written in block operator form, directional gradient formulation is

\[
\begin{pmatrix}
\frac{\partial}{\partial t} + \kappa_\perp \Delta \\
-\sqrt{\kappa} \Delta \mathbf{b} \cdot \nabla \\
-\sqrt{\kappa} \Delta \nabla \cdot (\mathbf{b}(\cdot)) \\
I \cdot (\nabla \cdot (\mathbf{b}(\cdot))) \\
\end{pmatrix}
\begin{pmatrix}
T \\
\zeta \\
\end{pmatrix}
= \begin{pmatrix}
S \\
0 \\
\end{pmatrix}.
\]
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\begin{pmatrix}
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\]

Consider steady-state (no time derivative) and purely anisotropic problem ($\kappa_{\perp} = 0$). Rearranging system, we have

\[
\begin{pmatrix}
-\sqrt{\kappa_{\Delta}} b \cdot \nabla & I \\
0 & -\sqrt{\kappa_{\Delta}} \nabla \cdot (b(\cdot))
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\[\Rightarrow\] In the regime of extreme anisotropy, I claim we should treat this equation as a system of coupled hyperbolic operators rather than a parabolic operator.
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Upwind DG discretization

Discretize the transport term $\nabla \cdot (\sqrt{\kappa} \Delta b(\cdot))$, using classical DG-upwind method:

$$L_b(\theta; \phi) := -\langle \sqrt{\kappa} \Delta \theta b, \nabla \phi \rangle + \int_{\Gamma} [[\sqrt{\kappa} \Delta \phi b \cdot n]] \tilde{\theta} \, dS + \int_{\partial \Omega_{out}} \sqrt{\kappa} \Delta \phi b \cdot n \theta \, dS,$$

for $L^2$-inner product $\langle \cdot, \cdot \rangle$, and any functions $\theta, \phi \in V^\text{DG}_k(\Omega)$. $\partial \Omega_{out}$ denotes the outflow subset of boundary $\partial \Omega$ relative to $B$, $\Gamma$ denotes all interior facets, and

$$[[\psi]] := \psi^+ - \psi^-,$$

$$\tilde{\psi} := \begin{cases} 
\psi^+ & \text{if } b^+ \cdot n^+ < 0, \\
\psi^- & \text{otherwise.}
\end{cases}$$
Define two transport operators

\[ L_{b, T} (\zeta_h; \phi) := L_b(\zeta_h; \phi) + \int_{\partial \Omega_{\text{in}}} \sqrt{\kappa} \Delta \phi (b \cdot n) \zeta_{\text{in}} \, dS \quad \forall \phi \in V_{\text{DG}}^k, \]

\[ L_{b, \zeta} (\psi; T_h) := L_b(\psi; T_h) - \int_{\partial \Omega_{\text{out}}} \sqrt{\kappa} \Delta T_{BC} (b \cdot n) \psi \, dS \quad \forall \psi \in V_{\text{DG}}^k, \]

where \( \partial \Omega_{\text{in}} \) denotes inflow boundary, \( \zeta_{\text{in}} \) is known.

\[ \Rightarrow \quad \text{Known inflow boundary ensure } L_{b, T}, L_{b, \zeta} \text{ are invertible} \]
Full weak form

Define two transport operators

\[ L_{b,T}(\zeta_h; \phi) := L_b(\zeta_h; \phi) + \int_{\partial \Omega_{\text{in}}} \sqrt{\kappa} \Delta \phi(b \cdot n) \zeta_{\text{in}} \, dS \quad \forall \phi \in V_{DG}^k, \]

\[ L_{b,\zeta}(\psi; T_h) := L_b(\psi; T_h) - \int_{\partial \Omega_{\text{out}}} \sqrt{\kappa} \Delta T_{BC}(b \cdot n) \psi \, dS \quad \forall \psi \in V_{DG}^k, \]

where \( \partial \Omega_{\text{in}} \) denotes inflow boundary, \( \zeta_{\text{in}} \) is known.

\[ \implies \text{Known inflow boundary ensure } L_{b,T}, L_{b,\zeta} \text{ are invertible} \]

Two options for \( \zeta_{\text{in}} \):

1. Iterate implicit solve until \( \zeta_{\text{in}} = \zeta_h \) (within nonlinear iteration for \( T \), this is almost certainly less stiff and easier to resolve)

2. Treat auxiliary inflow \( \zeta_{\text{in}} \) explicitly; so far have found in tests it varies slowly in time.
Define two transport operators

\[ L_{b,T}(\zeta_h; \phi) := L_b(\zeta_h; \phi) + \int_{\partial \Omega_{in}} \sqrt{\kappa \Delta} \phi (b \cdot n) \zeta_{in} \, dS \quad \forall \phi \in \mathbb{V}_k^{DG}, \]

\[ L_{b,\zeta}(\psi; T_h) := L_b(\psi; T_h) - \int_{\partial \Omega_{out}} \sqrt{\kappa \Delta} T_{BC} (b \cdot n) \psi \, dS \quad \forall \psi \in \mathbb{V}_k^{DG}, \]

where \( \partial \Omega_{in} \) denotes inflow boundary, \( \zeta_{in} \) is known.

**Weak form**: find \((T_h, \zeta_h) \in (\mathbb{V}_k^{DG} \times \mathbb{V}_k^{DG})\) such that

\[ \langle \phi, \frac{\partial T_h}{\partial t} \rangle - L_{b,T}(\zeta_h; \phi) - \text{IP}(T_h; \phi) = -\int_{\partial \Omega} \kappa_{BC} \phi (T_h - T_{BC}) \, dS + \langle \phi, S \rangle, \]

\[ \langle \psi, \zeta_h \rangle + L_{b,\zeta}(\psi; T_h) = 0 \quad \forall \psi, \phi \in \mathbb{V}_k^{DG}. \]
MHD test problem

Domain $\Omega = [0, 1] \times [0, 1] \times [0, 5]$, periodic in $z$, initial $T$

$$T_0 = \sin \left( \frac{\pi x}{L_x} \right) \sin \left( \frac{\pi y}{L_x} \right),$$

with $T_{BC} = 0$ on $\partial \Omega$. $\mathbf{B}$ aligns with contours of $T_0$ in $(x, y)$ and is constant in $z$,

$$\mathbf{B} = (B_x, B_y, B_z) = (-\partial_y T, \partial_x T, 5)$$

$$\implies \text{ensures } (B_x, B_y) = \nabla \perp T_0 \text{ for 2D curl } \nabla \perp = (-\partial_y, \partial_x).$$
MHD test problem

Domain $\Omega = [0, 1] \times [0, 1] \times [0, 5]$, periodic in $z$, initial $T$

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$$B = (B_x, B_y, B_z) = (-\partial_y T, \partial_x T, 5)$$

implies $(B_x, B_y) = \nabla_\perp T_0$ for 2D curl $\nabla_\perp = (-\partial_y, \partial_x)$.

Add counter forcing $S = -\kappa_\perp \Delta T_0$, to ensure a steady state test case. Error can be measured relative to the initial condition,

$$e_T(t) = \frac{\|T_h(t) - T_0\|_2}{\|T_0\|_2}.$$
Accuracy and results

Compare with:

- **CG-primal system**: (i.e. without auxiliary heat flux) for $T$ in second order CG, $\nabla_2^{CG}$.

- **DG-primal system**: for $T$ in $\nabla_2^{DG}$ (similar to recent papers Green et al, Vogl et al.).

- **Mixed CG**: original directional gradient formulation in $\nabla_2^{CG} - \nabla_1^{DG}$ from Gunter et al (does not use transport disc. techniques).
Figure: Relative $L^2$ error for anisotropy ratios from left to right $10^3$, $10^6$, and $10^9$. Orange circles denote novel mixed DG scheme, green diamonds mixed CG, red triangles primal DG, and purple triangles primal CG.
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Continuous Galerkin

Let $\mathbb{V}_T := \text{CG}(\Omega)_k$ denote $k^{th}$ order continuous Galerkin space, and

$\mathbb{V}_{T_{bc}} := \{ \eta \in \text{CG}(\Omega)_k : \eta|_{\partial\Omega} = T_{bc} \}$, \quad $\mathbb{\hat{V}}_T := \{ \eta \in \text{CG}(\Omega)_k : \eta|_{\partial\Omega} = 0 \}$.

**Weak form:** find $(T \in \mathbb{V}_{T_{bc}}, \zeta \in \mathbb{V}_\zeta)$ such that

\begin{align*}
\langle \eta, \frac{\partial T}{\partial t} \rangle + \langle \kappa || b \cdot \nabla \eta, \zeta \rangle &= F \quad \forall \eta \in \mathbb{\hat{V}}_T, \quad (1) \\
\langle \eta, \zeta - b \cdot \nabla T \rangle &= 0 \quad \forall \phi \in \mathbb{V}_\zeta. \quad (2)
\end{align*}

for CG or DG auxiliary space $\mathbb{V}_\zeta$ w/o any associated BCs.

- Analogous to DG case, we set auxiliary space equal to temperature space (ensures square advective blocks).
Transport stabilization (it works!)

Define velocity field $\mathbf{s} := \sqrt{\kappa \parallel \mathbf{b}}$. For stabilization parameter $\tau$, define advective and flux based SUPG operators

$$S_a(\eta) = \eta + \tau \mathbf{s} \cdot \nabla \eta, \quad S_f(\eta) = \eta + \mathbf{s} \cdot \nabla (\tau \eta).$$

Mixed CG, SUPG stabilized discretization given by

$$\left\langle S_a(\eta), \frac{\partial T}{\partial t} \right\rangle + \left\langle \mathbf{s} \cdot \nabla \eta, S_f(\zeta) \right\rangle = \left\langle S_a(\eta), F \right\rangle +$$

$$\int_{\partial \Omega} \tau (\mathbf{s} \cdot \nabla \eta)(\mathbf{s} \cdot \mathbf{n})(\mathbf{s} \cdot \nabla T) dS \quad \forall \eta \in \hat{V}_T,$$

$$\left\langle \eta, S_f(\zeta) \right\rangle - \left\langle \mathbf{s} \cdot \nabla T, S_f(\eta) \right\rangle = 0 \quad \forall \eta \in V_T.$$
**Transport stabilization (it works!)**

- A boundary integral appears because while \( \eta \) vanishes along Dirichlet boundary, SUPG-modification \( s \cdot \nabla \eta \) need not (gradient first computed within cells neighboring \( \partial \Omega \), then evaluated along \( \partial \Omega \)).

- Averaged stabilization parameter for tuning parameter \( \lambda \in [0, 1] \):
  \[
  \tau = \left( \lambda \frac{2}{\Delta t} + \frac{\sqrt{\kappa}}{2\Delta x} \right)^{-1}
  \]

- Specific form of \( S_f(\eta) \) and \( S_a(\eta) \) derived for structure preservation and consistency.

- In practice, we use weak BCs for CG formulation. Recall we swap the algebraic system’s block rows. In Firedrake, non-trivial to form the correct block row-swapped system with strong BCs.
Figure: Magnetic surface test case: plasma trapped in series of concentric tori. We “unfold” concentric tori with rational winding number and temperature perturbation spreading on surface. $\kappa_\perp = 0, \kappa_\parallel = 100$, integrate to one Alfven time.
Figure: Magnetic surface test case; “unfolded” concentric tori with rational winding number and temperature perturbation spreading on surface. \( \kappa_\perp = 0, \kappa_{\parallel} = 100 \), integrate to one Alfven time.
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**Consistency**

**Proposition:** The CG and DG space discretizations are consistent, i.e. a solution satisfying the continuous equation also satisfies the discretizations with sufficiently regular test functions $\eta$.

Note, most discretizations would be consistent, but using stabilization techniques like hyper-diffusion are not.
Diffusion

Continuous system is dissipative up to forcing and total in- and outflux:

\[
\frac{1}{2} \frac{d}{dt} \| T \|_2^2 = \langle T, F \rangle - \| \sqrt{\kappa} \| b \cdot \nabla T \|_2^2 + \int_{\partial \Omega} T \kappa \| (b \cdot n)(b \cdot \nabla T) dS.
\]

- DG discretization satisfies this weakly, in the sense that the diffusion property is satisfied up to a weak BC penalty, and if a strong solution satisfies the BCs, we satisfy the diffusion property.
- CG discretization with Neumann or weak Dirichlet BCs satisfies this weakly.
Continuous system conserves total temperature up to forcing and total in- and outflux:

\[
\frac{d}{dt} \int_{\Omega} T \, dx = \int_{\Omega} F \, dx + \int_{\partial\Omega} \kappa_{\parallel} (\mathbf{b} \cdot \mathbf{n}) (\mathbf{b} \cdot \nabla T) \, dS.
\]

- DG discretization satisfies this weakly up to normal continuity \(\mathbf{b}\) (strong solution will satisfy).
- CG discretization with Neumann BCs satisfies this automatically.
- CG discretization with weak Dirichlet BCs satisfies this weakly (multiple extra terms in weak form, but eliminated with strong solution).
Spurious heat loss

Movie!
Spurious heat loss

- $\kappa_\perp = 0$, physical $\kappa_\parallel$ taken from Braginski model, fixed Dirichlet BCs.
- Time step of 1 Alfven time.
- Periodic domain in angle, CG disc. has 11K DOFs, DG disc. 47K DOFs.
Spurious heat loss

Figure: Spurious temperature loss for different discretizations. Final losses: CG2: -44%; DG2: -39%; CG2-DG1: -33%; DG1-DG1: -13%; DG2-DG2: -4.9%; CG2-CG2: -2.8%.
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Algebraic multigrid (AMG)

One of fastest methods (when applicable) to solve large, sparse systems $Ax = b$.

⇒ Two parts: *Relaxation* and *coarse-grid correction*:

\[ x_{k+1} = x_k + M^{-1}(b - Ax_k), \]
\[ x_{k+1} = x_k + P(RAP)^{-1} R(b - Ax_k). \]
Algebraic multigrid (AMG)

One of fastest methods (when applicable) to solve large, sparse systems $Ax = b$.

$\implies$ Two parts: *Relaxation* and *coarse-grid correction*:

$$
e_{k+1} = (I - M^{-1}A)e_k,
\quad e_{k+1} = (I - P(RAP)^{-1}RA)e_k
\quad = (I - \Pi)e_k.
$$
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\end{align*}
\]

AMG is typically for symmetric positive definite (SPD) matrices.

- If $A$ is SPD, $\|x\|^2_A = \langle Ax, x \rangle$ defines norm.
- $R := P^T \implies \|\Pi\|_A = 1$. 

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AMG is typically for symmetric positive definite (SPD) matrices.

- If \(A\) is SPD, \(\|x\|_A^2 = \langle Ax, x \rangle\) defines norm.
- \(R := P^T \implies \|\Pi\|_A = 1.\)
- Non-orthogonal projection can increase error 😞
Notation

CF-Splitting:
• Assume DOFs partitioned into coarse points (C) and fine points (F)
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• Assume DOFs partitioned into coarse points (C) and fine points (F)

Write vectors and matrices in block form:

\[ A = \begin{pmatrix} A_{ff} & A_{fc} \\ A_{cf} & A_{cc} \end{pmatrix}, \quad P = \begin{pmatrix} W \\ I \end{pmatrix}, \]

\[ R = \begin{pmatrix} Z & I \end{pmatrix}, \quad \mathcal{K} := RAP. \]
Coarse-grid correction and $R_{\text{ideal}}$

Decompose F-point error $e_f = We_c + \delta e_f$:

$$e^{(i+1)} = \begin{pmatrix} e_f^{(i)} \\ e_c^{(i)} \end{pmatrix} - P(RAP)^{-1} RA \left[ \begin{pmatrix} We_c^{(i)} \\ e_c^{(i)} \end{pmatrix} + \begin{pmatrix} \delta e_f^{(i)} \\ 0 \end{pmatrix} \right]$$
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$$= \begin{pmatrix} e_f^{(i)} - W e_c^{(i)} \\ 0 \end{pmatrix} - P(RAP)^{-1} RA \begin{pmatrix} \delta e_f^{(i)} \\ 0 \end{pmatrix}.$$
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$$= \begin{pmatrix} e_f^{(i)} - We_c^{(i)} \\ 0 \end{pmatrix} - P(RAP)^{-1} RA \begin{pmatrix} \delta e_f^{(i)} \\ 0 \end{pmatrix}.$$ 

Ideal restriction:

$$RA \begin{pmatrix} \delta e_f^{(i)} \\ 0 \end{pmatrix} = (ZA_{ff} + A_{cf}) \delta e_f = 0$$

$$\implies R_{\text{ideal}} = \begin{pmatrix} -A_{cf}A_{ff}^{-1} & I \end{pmatrix}$$
Coarse-grid correction and $R_{\text{ideal}}$

Decompose F-point error $e_f = We_c + \delta e_f$:

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e^{(i+1)} = \begin{pmatrix} e_f^{(i)} \\ e_c^{(i)} \end{pmatrix} - P(RAP)^{-1} RA \left[ \begin{pmatrix} We_c^{(i)} \\ e_c^{(i)} \end{pmatrix} + \begin{pmatrix} \delta e_f^{(i)} \\ 0 \end{pmatrix} \right]$$

$$= \begin{pmatrix} e_f^{(i)} - We_c^{(i)} \\ 0 \end{pmatrix} - P(RAP)^{-1} RA \begin{pmatrix} \delta e_f^{(i)} \\ 0 \end{pmatrix}.$$ 

**Lemma 1 (Orthogonal coarse-grid correction).**

Coarse-grid correction with

$$R_{\text{ideal}} = \begin{pmatrix} -A_{cf} A_{ff}^{-1} & I \end{pmatrix}, \quad P = \begin{pmatrix} 0 \\ I \end{pmatrix}$$

is an $\ell^2$-orthogonal projection.
Reduction based AMG as block LDU

Partition (discontinuous) elements into C-elements and F-elements. Then in matrix form,

\[
\begin{bmatrix}
A_{ff} & A_{fc} \\
A_{cf} & A_{cc}
\end{bmatrix}^{-1} = \begin{bmatrix}
I & -A_{ff}^{-1}A_{fc} \\
0 & I
\end{bmatrix} \begin{bmatrix}
A_{ff}^{-1} & 0 \\
0 & S^{-1}
\end{bmatrix} \begin{bmatrix}
-I & 0 \\
-A_{cf}A_{ff}^{-1} & I
\end{bmatrix}.
\]

Reduction based AMG preconditioner \(M^{-1}\) looks like:

\[
M^{-1} = \begin{bmatrix}
I & \hat{W} \\
0 & I
\end{bmatrix} \begin{bmatrix}
\Delta_F & 0 \\
0 & \mathcal{K}^{-1}
\end{bmatrix} \begin{bmatrix}
Z & I \\
I & 0
\end{bmatrix},
\]

where \(\hat{W} = (I - \Delta_F A_{ff})W - \Delta A_{fc}\). Want \(\Delta_F \approx A_{ff}^{-1}, Z \approx -A_{cf}A_{ff}^{-1}\).
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I & 0 \\
Z & I
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\]

where \(\hat{W} = (I - \Delta_F A_{ff})W - \Delta A_{fc}\). Want \(\Delta_F \approx A_{ff}^{-1}\), \(Z \approx -A_{cf}A_{ff}^{-1}\).

\(\implies\) Can we approximate \(A_{ff}^{-1}\) well?
Approximate ideal restriction

For $i$th C-point ($i$th row of $R$), choose restriction neighborhood $\mathcal{R}_i = \{\ell_1, \ldots, \ell_{S_i}\}$ of some “nearby” F-points. Solve

$$a_{ij} + \sum_{k \in \mathcal{R}_i} z_{ik} a_{kj} = 0.$$

Sets $RA$ equal to zero within F-point sparsity pattern.
Approximate ideal restriction

For \( i \)th C-point (\( i \)th row of \( R \)), choose restriction neighborhood \( \mathcal{R}_i = \{ \ell_1, \ldots, \ell_{S_i} \} \) of some “nearby” F-points. Solve

\[
 a_{ij} + \sum_{k \in \mathcal{R}_i} z_{ik} a_{kj} = 0.
\]

Sets \( RA \) equal to zero within F-point sparsity pattern.
Approximate ideal restriction

For \( i \)th C-point (\( i \)th row of \( R \)), choose restriction neighborhood \( \mathcal{R}_i = \{l_1, \ldots, l_{S_i}\} \) of some “nearby” F-points. Solve

\[
a_{ij} + \sum_{k \in \mathcal{R}_i} z_{ik} a_{kj} = 0.
\]

Sets \( RA \) equal to zero within F-point sparsity pattern.

**Goal:**

1. Use AIR to achieve accurate solution at C-points.
2. Follow with F-relaxation to distribute accuracy to F-points.
Consider transport on structured 2d grid and partition elements into C-elements and F-elements.
AIR for upwind transport

Notice that there are no C-C or F-F connections

\[ A_{ff} = A_{cc} = I. \]
If $A_{ff} = I$, AMG coarse grid given by $A_{cc} - A_{cf}A_{fc} \iff$ all C-F-C connections.
AIR for upwind transport

If $A_{ff} = I$, AMG coarse grid given by $A_{cc} - A_{cf}A_{fc} \iff$ all C-F-C connections. One of these connections is weak!
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Reorder discrete $2 \times 2$ block system

$$
\begin{pmatrix}
-\sqrt{\kappa \Delta} G_b \\
\frac{1}{\Delta t} (M + \tilde{\kappa}_{BC} M_{BC}, h_e) + \kappa_{\perp} L
\end{pmatrix}
\begin{pmatrix}
M \\
\sqrt{\kappa \Delta} G_b^T
\end{pmatrix}
\begin{pmatrix}
T^{n+1} \\
\zeta^{n+1}
\end{pmatrix}
= 
\begin{pmatrix}
F_{\zeta} \\
F_T
\end{pmatrix}.
$$

Assume $\tilde{\kappa}_{BC} \sim O(1)$, so that $M + \tilde{\kappa}_{BC} M_{BC}, h_e \approx M$ in spectral analysis. Apply block triangular preconditioner,

$$
\begin{pmatrix}
-\sqrt{\kappa \Delta} G_b \\
\frac{1}{\Delta t} (M + \tilde{\kappa}_{BC} M_{BC}) + \kappa_{\perp} L
\end{pmatrix}
\begin{pmatrix}
0 \\
\sqrt{\kappa \Delta} G_b^T
\end{pmatrix}^{-1}.
$$
2 × 2 DG system

Reorder discrete 2 × 2 block system

\[
\begin{pmatrix}
-\sqrt{\kappa \Delta} G_b \\
\frac{1}{\Delta t}(M + \tilde{\kappa}_BC M_{BC,h_e}) + \kappa \perp L
\end{pmatrix}
\begin{pmatrix}
M \\
\sqrt{\kappa \Delta} G_b^T
\end{pmatrix}
\begin{pmatrix}
T^{n+1} \\
\zeta^{n+1}
\end{pmatrix}
= \begin{pmatrix} F\zeta \\ F_T \end{pmatrix}.
\]

Assume \( \tilde{\kappa}_{BC} \sim O(1) \), so that \( M + \tilde{\kappa}_{BC} M_{BC,h_e} \approx M \) in spectral analysis. Apply block triangular preconditioner,

\[
\begin{pmatrix}
-\sqrt{\kappa \Delta} G_b \\
\frac{1}{\Delta t}(M + \tilde{\kappa}_BC M_{BC}) + \kappa \perp L
\end{pmatrix}
\begin{pmatrix}
0 \\
\sqrt{\kappa \Delta} G_b^T
\end{pmatrix}^{-1}.
\]

Convergence of fixed-point / Krylov fully defined by approximating Schur complement:

\[
S_{22} := \sqrt{\kappa \Delta} G_b^T + \left( \frac{1}{\Delta t} M + \kappa \perp L \right) (\sqrt{\kappa \Delta} G_b)^{-1} M.
\]
Spectral analysis of Schur complement

Preconditioned $S_{22}$ similar to SPD operator:

\[
(\sqrt{\kappa \Delta} G_b^T)^{-1} S_{22} = I + \frac{1}{\Delta t \kappa \Delta} G_b^T M G_b^{-1} M + \frac{\kappa \perp}{\kappa \Delta} G_b^T L G_b^{-1} M \\
\sim I + \frac{1}{\Delta t \kappa \Delta} M^{1/2} G_b^T M G_b^{-1} M^{1/2} + \frac{\kappa \perp}{\kappa \Delta} M^{1/2} G_b^T L G_b^{-1} M^{1/2}.
\]
Spectral analysis of Schur complement

Preconditioned $S_{22}$ similar to SPD operator:

\[
(\sqrt{\kappa \Delta} G_b^T)^{-1} S_{22} = I + \frac{1}{\Delta t \kappa \Delta} G_b^T M G_b^{-1} M + \frac{\kappa}{\kappa \Delta} G_b^T L G_b^{-1} M
\]

\[
\sim I + \frac{1}{\Delta t \kappa \Delta} M^{1/2} G_b^T M G_b^{-1} M^{1/2} + \frac{\kappa}{\kappa \Delta} M^{1/2} G_b^T L G_b^{-1} M^{1/2}.
\]

First (anisotropic) term: for mesh $h$ and constants $c_1, c_2$:

\[
\sigma \left( \frac{1}{\Delta t \kappa \Delta} M^{1/2} G_b^T M G_b^{-1} M^{1/2} \right) \subset \frac{1}{\Delta t \kappa \Delta} [c_1 h^2, c_2].
\]
Spectral analysis of Schur complement

Preconditioned $S_{22}$ similar to SPD operator:

$$(\sqrt{\kappa_{\Delta}} G_b^T)^{-1} S_{22} = I + \frac{1}{\Delta t \kappa_{\Delta}} G_b^{-T} M G_b^{-1} M + \frac{\kappa_{\perp}}{\kappa_{\Delta}} G_b^{-T} L G_b^{-1} M$$

$$\sim I + \frac{1}{\Delta t \kappa_{\Delta}} M^{1/2} G_b^{-T} M G_b^{-1} M^{1/2} + \frac{\kappa_{\perp}}{\kappa_{\Delta}} M^{1/2} G_b^{-T} L G_b^{-1} M^{1/2}.$$

First (anisotropic) term: for mesh $h$ and constants $c_1, c_2$:

$$\sigma \left( \frac{1}{\Delta t \kappa_{\Delta}} M^{1/2} G_b^{-T} M G_b^{-1} M^{1/2} \right) \subset \frac{1}{\Delta t \kappa_{\Delta}} [c_1 h^2, c_2].$$

Second (isotropic) term: 2D and $b$ aligned in $x$. Second term

$$\sim \partial_{\times x}^{-1} (\partial_{\times x} + \partial_{\times y}) = 1 + \partial_{\times x}^{-1} \partial_{\times y}.$$ On unit domain, Laplacian eigendecomposition $\{u_{jk}, \pi^2 (j^2 + k^2)\}$, $u_{jk} = 2 \sin(j \pi x) \sin(k \pi y)$; similar for $\partial_{\times x}$ in $(j, x)$. $\implies$ Highest frequency in $y$, $k = 1 / h$, and smoothest in $x$, $j = 1$, yields eigenpair

$$(1 + \partial_{\times x}^{-1} \partial_{\times y}) 2 \sin(\pi x) \sin\left(\frac{1}{h} \pi y\right) = \left(1 + \frac{1}{h^2}\right) 2 \sin(\pi x) \sin\left(\frac{1}{h} \pi y\right).$$
Spectral analysis of Schur complement

Preconditioned $S_{22}$ similar to SPD operator:

$$(\sqrt{\kappa \Delta} G_b^T)^{-1} S_{22} = I + \frac{1}{\Delta t \kappa \Delta} G_b^{-T} M G_b^{-1} M + \frac{\kappa}{\kappa \Delta} G_b^{-T} L G_b^{-1} M$$

$\sim I + \frac{1}{\Delta t \kappa \Delta} M^{1/2} G_b^{-T} M G_b^{-1} M^{1/2} + \frac{\kappa}{\kappa \Delta} M^{1/2} G_b^{-T} L G_b^{-1} M^{1/2}.$

**First (anisotropic) term**: for mesh $h$ and constants $c_1, c_2$:

$$\sigma \left( \frac{1}{\Delta t \kappa \Delta} M^{1/2} G_b^{-T} M G_b^{-1} M^{1/2} \right) \subset \frac{1}{\Delta t \kappa \Delta} [c_1 h^2, c_2].$$

**Second (isotropic) term**:

$$\sigma \left( \frac{\kappa}{\kappa \Delta} M^{1/2} G_b^{-T} L G_b^{-1} M^{1/2} \right) \subset \left( 0, \frac{\kappa}{\kappa \Delta} h^2 \right].$$
Spectral analysis of Schur complement

Preconditioned $S_{22}$ similar to SPD operator:

$$(\sqrt{\kappa_{\Delta}} G_b^T)^{-1} S_{22} = I + \frac{1}{\Delta t \kappa_{\Delta}} G_b^{-T} M G_b^{-1} M + \frac{\kappa_{\perp}}{\kappa_{\Delta}} G_b^{-T} L G_b^{-1} M$$

$$\sim I + \frac{1}{\Delta t \kappa_{\Delta}} M^{1/2} G_b^{-T} M G_b^{-1} M^{1/2} + \frac{\kappa_{\perp}}{\kappa_{\Delta}} M^{1/2} G_b^{-T} L G_b^{-1} M^{1/2}.$$ 

First (anisotropic) term: for mesh $h$ and constants $c_1, c_2$:

$$\sigma \left( \frac{1}{\Delta t \kappa_{\Delta}} M^{1/2} G_b^{-T} M G_b^{-1} M^{1/2} \right) \subset \frac{1}{\Delta t \kappa_{\Delta}} [c_1 h^2, c_2].$$

Second (isotropic) term:

$$\sigma \left( \frac{\kappa_{\perp}}{\kappa_{\Delta}} M^{1/2} G_b^{-T} L G_b^{-1} M^{1/2} \right) \subset \left( 0, \frac{\kappa_{\perp} c_3}{\kappa_{\Delta} h^2} \right),$$

$$\sigma \left( (\sqrt{\kappa_{\Delta}} G_b^T)^{-1} S_{22} \right) \subset \left( 1, 1 + \frac{\kappa_{\perp} c_3}{\kappa_{\Delta} h^2} + \frac{c_2}{\Delta t \kappa_{\Delta}} \right).$$
Eigenvectors computed in practice via Lanczos:

<table>
<thead>
<tr>
<th>$\Delta t$</th>
<th>$\kappa_\parallel / \kappa_\perp$</th>
<th>2D</th>
<th>3D</th>
</tr>
</thead>
<tbody>
<tr>
<td>$10^{-3}$</td>
<td>$10^3$</td>
<td>7.8e0</td>
<td>6.6e2</td>
</tr>
<tr>
<td></td>
<td>$10^6$</td>
<td>7.8e-3</td>
<td>4.0e2</td>
</tr>
<tr>
<td></td>
<td>$10^9$</td>
<td>7.8e-6</td>
<td>3.4e2</td>
</tr>
<tr>
<td>$10^{-2}$</td>
<td>$10^3$</td>
<td>8.0e-1</td>
<td>6.6e1</td>
</tr>
<tr>
<td></td>
<td>$10^6$</td>
<td>8.0e-4</td>
<td>1.1e2</td>
</tr>
<tr>
<td></td>
<td>$10^9$</td>
<td>8.0e-7</td>
<td>2.8e2</td>
</tr>
</tbody>
</table>

Table: Largest eigenvalues of error propagation, $(\sqrt{\kappa_\Delta} G_b^T)^{-1} S_{22} - I$. The three values for each given anisotropy ratio correspond to three successive spatial refinement levels.
Results

- Analagous problem as DG convergence study, with open field lines so advection is invertible.
- Block preconditioned FGMRES, outer relative tolerance $10^{-8}$.
- Inner AIR tolerance $\min\{10^{-3}, 10^{-3}/\|b\|\}$, where $b$ is current right-hand side.
  - Effectively absolute \textit{and} relative tolerance.
  - If $(\Delta t \kappa_\Delta)^{-1}$ or $\kappa_\perp / \kappa_\Delta$ is not $\ll 1$, right-hand side provided to second AIR solve can be very large, e.g., $O(10^4)$. Then, relative tolerance $10^{-3}$ doesn’t even lead to residual $< 1$ in norm, and outer iteration fails to converge.
Results

Figure: Average total inner iteration counts per time step. Left column: mixed CG, classical AMG. Center column: mixed DG, classical AMG. Right column: mixed DG, AIR.
Results

Figure: Average wall-clock times in seconds per time step. Left column: mixed CG, classical AMG. Center column: mixed DG, classical AMG. Right column: mixed DG, AIR.
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Difficulties with closed field lines

- Advection operators are no longer invertible (recall, no time derivative on advection term) \(\implies\) cannot use open field lines approach directly.
- In one step, information traverses a closed field line *many* times.
- Will have closed field lines in most/all realistic problems.
Difficulties with closed field lines

- Advection operators are no longer invertible (recall, no time derivative on advection term) \(\implies\) cannot use open field lines approach directly.
- In one step, information traverses a closed field line *many* times.
- Will have closed field lines in most/all realistic problems.

**Idea:** keep reordered system

\[
\begin{pmatrix}
-\sqrt{\kappa} \Delta G_b \\
\frac{1}{\Delta t} M + \kappa \perp L
\end{pmatrix}
\begin{pmatrix}
M \\
\sqrt{\kappa} \Delta G_b^T
\end{pmatrix}
\begin{pmatrix}
T^{n+1} \\
\zeta^{n+1}
\end{pmatrix}
=
\begin{pmatrix}
F_\zeta \\
F_T
\end{pmatrix}.
\]

and apply AIR all at once to this system.
DG Tokamak test case

<table>
<thead>
<tr>
<th>ref level</th>
<th>AMG iters</th>
<th>Rel accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CG2/DG1</td>
<td>DG2-DG2</td>
</tr>
<tr>
<td>0</td>
<td>438</td>
<td>145</td>
</tr>
<tr>
<td>1</td>
<td>2263</td>
<td>265</td>
</tr>
<tr>
<td>2</td>
<td>6312</td>
<td>380</td>
</tr>
</tbody>
</table>

Table: Two toroidal planes and physical $\kappa$ values, AMG iters and accuracy shown for three poloidal ref levels.
Conclusions

Review:

- Diffusion in magnetic confinement fusion is extremely anisotropic in the direction of field lines.
- Rewrote diffusion system based on directional gradients, apply discretization and solver techniques developed for advection.
- Orders of magnitude decrease in error and solve wallclock time vs. traditional/existing methods.
Conclusions

Review:

• Diffusion in magnetic confinement fusion is extremely anisotropic in the direction of field lines.
• Rewrote diffusion system based on directional gradients, apply discretization and solver techniques developed for advection.
• Orders of magnitude decrease in error and solve wallclock time vs. traditional/existing methods.

Next steps:

• Incorporate into larger MHD simulations.
• Better solvers for closed field lines or mixed regimes.
• Other extremely anisotropic equations??
Thank you!

Papers:


