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Block-based Algebraic Multigrid Preconditioners in Trilinos/Teko

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Motivating Example: Two-temperature model

1. Heat conduction for electron temperature T_e

$$-\nabla \cdot (k_e \nabla T_e) + g(T_e - T_l) = Q_e$$

2. Heat conduction for lattice temperature T_e

$$-\nabla \cdot (k_l \nabla T_l) + g(T_l - T_e) = Q_l$$

Discrete system:

$$\begin{bmatrix} K_e + gM & -gM \\ -gM & K_l + gM \end{bmatrix}$$

$$(K_e)_{ij} = \int_\Omega k_e \, \nabla\varphi_j \cdot \nabla\varphi_i \, dx, \quad (K_l)_{ij} = \int_\Omega k_l \, \nabla\varphi_j \cdot \nabla\varphi_i \, dx$$

$$M_{ij} = \int_\Omega \varphi_j \, \varphi_i \, dx$$

- Domain-decomposition (DD) with ILU (RCM re-ordering) (DD-ILU)

$$M_{RAS}^{-1} = \sum_{i=1}^{N} R_i^T D_i \, Q_i (\hat{L}_i \hat{U}_i)^{-1} Q_i^T \, R_i$$

- Block-based Gauss-Seidel (MueLu SA-AMG, Chebyshev smoother)

$$\mathcal{M}_{BGS}^{-1} = \begin{bmatrix} \widetilde{M}_{11}^{-1} & -\widetilde{M}_{11}^{-1} A_{12} \widetilde{M}_{22}^{-1} \\ 0 & \widetilde{M}_{22}^{-1} \end{bmatrix}$$

Define dimensionless coupling number: $\eta \equiv \frac{g\,L^2}{k}$
Coupling regimes:

- $\eta \ll 1$: Weak coupling, T_e and T_l mostly independent
- $\eta \gg 1$: Tight coupling $T_e \sim T_l$
- Consider $g = 10^4$, $\Omega = [0,1]^2$, $N_x = N_y = 1024$, $k_l = \frac{1}{2}$, $k_e = 1$, $T_e = T_l = 0$ on $\partial\Omega$

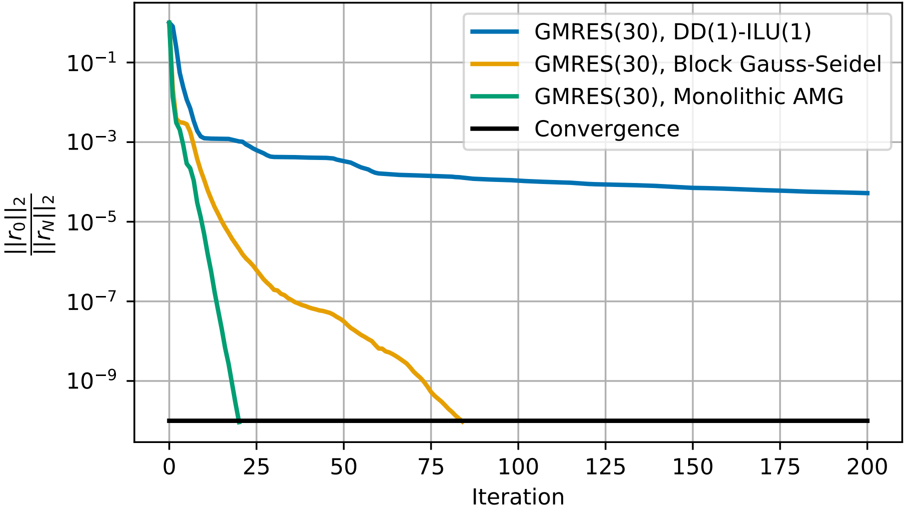

Figure: Convergence of two-temperature model solvers

Current limitations of monolithic AMG:

- Locked behind expert MueLu XML syntax
- No interoperability between blocked/non-blocked smoothers
- Difficult to incorporate per-physics:
  - Coordinates
  - Material Properties
  - Nullspaces

Desired features:

- Independent coarsening per physics
- First-class interoperability with Teko
  - Block preconditioner *within* Teko
  - Support for Teko block-based smoothers
- Support for monolithic smoothing approaches (domain-decomposition + incomplete LU)
- Easily incorporate per-physics fields coordinates, material properties, nullspaces, etc.

Monolithic Algebraic Multigrid:

$$\mathcal{A}^{(0)} = \begin{bmatrix} A_{11} & A_{12} & \cdots & A_{1N} \\ A_{21} & A_{22} & \cdots & A_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ A_{N1} & A_{N2} & \cdots & A_{NN} \end{bmatrix}, \quad \mathcal{A}^{(k+1)} = \mathcal{R}^{(k)}\mathcal{A}^{(k)}\mathcal{P}^{(k)} \text{ for levels } k = 0, \dots, \ell-1$$

Construct smoothers:

- Block-based smoothers (Block Gauss-Seidel, Block Jacobi, etc.)

$$\mathcal{S}^{(k)}_{pre} = \mathcal{S}^{(k)}_{post} = \begin{bmatrix} \widetilde{S}_{11} & A_{12} & \cdots & A_{1N} \\ & \widetilde{S}_{22} & \cdots & A_{2N} \\ & & \ddots & \vdots \\ & & & \widetilde{S}_{NN} \end{bmatrix}^{-1}$$

- Monolithic smoothers
  - Domain-decomposition with incomplete LU factorization
  - (SPD problems) Chebyshev polynomial smoothing

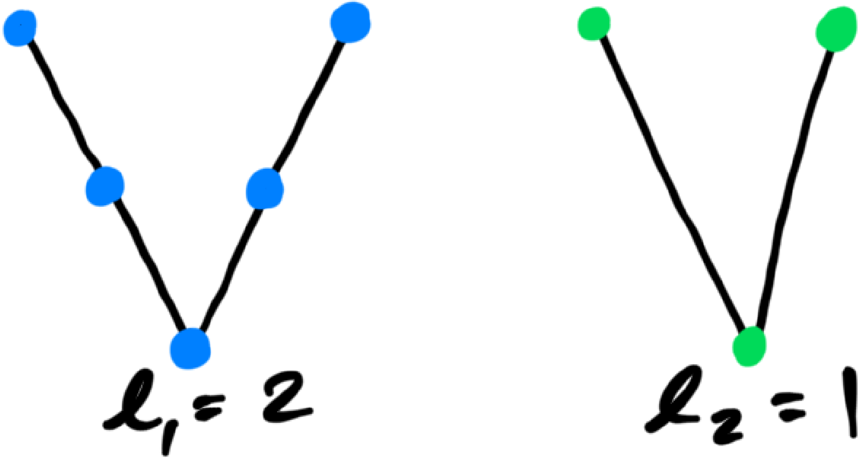

Figure: How to handle a mismatch in the number of levels?

Monolithic Algebraic Multigrid:

Generate per-subblock multigrid hierarchies (subblock $m = 1, \ldots, N$):

- For levels $i = 0, \ldots, \ell_m - 1$,

$$A_{m,m}^{(i+1)} = R_m^{(i)} \, A_{m,m}^{(i)} \, P_m^{(i)}.$$

Define the common depth

$$\ell = \max_{m=1,\ldots,N} \ell_m \quad \text{or} \quad \ell = \min_{m=1,\ldots,N} \ell_m$$

For each subblock m with $\ell_m < \ell$, pad the remaining levels $i = \ell_m, \ldots, \ell - 1$ by

- $R_m^{(i)} = I$, $P_m^{(i)} = I$, and $A_{m,m}^{(i+1)} = A_{m,m}^{(\ell_m)}$.

Define multiphysics (block-diagonal) transfer operators for levels $k = 0, \ldots, \ell - 1$:

$$\mathcal{P}^{(k)} = \begin{bmatrix} P_1^{(k)} & & \\ & \ddots & \\ & & P_N^{(k)} \end{bmatrix}, \qquad \mathcal{R}^{(k)} = \begin{bmatrix} R_1^{(k)} & & \\ & \ddots & \\ & & R_N^{(k)} \end{bmatrix}.$$

Monolithic AMG V-Cycle:

Algorithm Vcycle $\left(\underline{u}^{(k)}, \underline{b}^{(k)}, k\right)$

Require: Current solution $\underline{u}^{(k)}$, right-hand side $\underline{b}^{(k)}$, and level k

Ensure: Updated solution $\underline{u}^{(k)}$

if $k \neq \ell$ **then**

  $\underline{u}^{(k)} \leftarrow \mathcal{S}_{pre}^{(k)}\left(\mathcal{A}^{(k)}, \underline{u}^{(k)}, \underline{b}^{(k)}\right)$

  $\underline{r}^{(k)} \leftarrow \underline{b}^{(k)} - \mathcal{A}^{(k)}\underline{u}^{(k)}$

  $\underline{u}^{(k+1)} \leftarrow 0$

  $\underline{u}^{(k+1)} \leftarrow \mathrm{Vcycle}\left(\underline{u}^{(k+1)}, \mathcal{R}^{(k)}\underline{r}^{(k)}, k+1\right)$

  $\underline{u}^{(k)} \leftarrow \underline{u}^{(k)} + \mathcal{P}^{(k)}\underline{u}^{(k+1)}$

  $\underline{u}^{(k)} \leftarrow \mathcal{S}_{post}^{(k)}\left(\mathcal{A}^{(k)}, \underline{u}^{(k)}, \underline{b}^{(k)}\right)$

else

  $\underline{u}^{(k)} \leftarrow \left(\mathcal{A}^{(k)}\right)^{-1}\underline{b}^{(k)}$

end if

Example: Steady two-way coupled thermoelasticity with advection

1. Linear elasticity for displacement $\mathbf{u}$

$$-\nabla \cdot \boldsymbol{\sigma}(\mathbf{u}, T) = \mathbf{b}, \quad \boldsymbol{\sigma} = 2\mu\, \varepsilon(\mathbf{u}) + \lambda\, \mathrm{tr}(\varepsilon(\mathbf{u}))\mathbf{I} - \beta T \mathbf{I}$$

$$\varepsilon(\mathbf{u}) = \tfrac{1}{2}(\nabla \mathbf{u} + \nabla \mathbf{u}^T)$$

2. Advection-diffusion heat equation for temperature T

$$-\nabla \cdot (k \nabla T) + \rho c_p\, \mathbf{w} \cdot \nabla T = q + \eta\, \nabla \cdot \mathbf{u}$$

Discrete system:

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ T \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix}, \quad a_{11}(\mathbf{u}, \mathbf{v}) = \int_\Omega \left(2\mu\, \varepsilon(\mathbf{v}) : \varepsilon(\mathbf{u}) + \lambda\, (\nabla \cdot \mathbf{v})(\nabla \cdot \mathbf{u})\right)\, dx.$$

$$a_{12}(T, \mathbf{v}) = -\int_\Omega \beta\, (\nabla \cdot \mathbf{v})\, T\, dx, \quad a_{21}(\mathbf{u}, s) = -\int_\Omega \eta\, s\, \nabla \cdot \mathbf{u}\, dx$$

$$a_{22}(T, s) = \int_\Omega k\, \nabla s \cdot \nabla T\, dx + \int_\Omega \rho c_p\, s\, \mathbf{w} \cdot \nabla T\, dx$$

Consider $N_x = N_y = 256$, $\eta = 400$, $\beta = 1$, $\Omega = [0,1]^2$, $\mathbf{u} = \mathbf{0}$, $T = 0$ on $\partial\Omega$

- DD(1)-ILU(1)
- Block Gauss-Seidel
  - $\widetilde{M}_{11}^{-1}$: elasticity AMG (SA-AMG, rigid body modes as nullspace, Chebyshev smoother)
  - $\widetilde{M}_{22}^{-1}$: scalar AMG (SA-AMG, DD(1)-ILU(1) smoother)

$$\mathcal{M}_{BGS}^{-1} = \begin{bmatrix} \widetilde{M}_{11}^{-1} & 0 \\ -\widetilde{M}_{22}^{-1} A_{21} \widetilde{M}_{11}^{-1} & \widetilde{M}_{22}^{-1} \end{bmatrix}$$

- Monolithic AMG with Block Gauss-Seidel smoother (Chebyshev for $\widetilde{S}_{11}^{-1}$, DD(1)-ILU(1) for $\widetilde{S}_{22}^{-1}$)

$$\mathcal{S}_{BGS}^{-1} = \begin{bmatrix} \widetilde{S}_{11}^{-1} & 0 \\ -\widetilde{S}_{22}^{-1} A_{21} \widetilde{S}_{11}^{-1} & \widetilde{S}_{22}^{-1} \end{bmatrix}$$

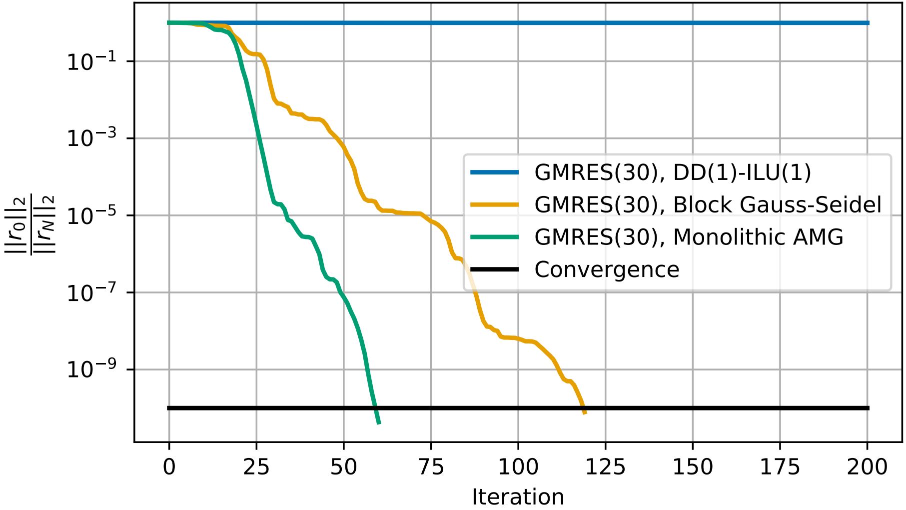

Figure: Convergence of thermo-elastic solvers

Example: Steady linear-drift Poisson–Nernst–Planck (PNP)

1. Poisson for potential ϕ

$$-\nabla \cdot (\epsilon \nabla \phi) = \rho_f + zF\, c.$$

2. Nernst-Planck (steady conservation) for concentration c

$$\nabla \cdot J = 0, \qquad J = -D\nabla c - \mu z F\, c \nabla \phi + \mathbf{u}\, c.$$

Discrete system:

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} \Phi \\ C \end{bmatrix} = \begin{bmatrix} b_\phi \\ b_c \end{bmatrix}.$$

$$(A_{11})_{ij} = \int_\Omega \epsilon\, \nabla \psi_j \cdot \nabla \psi_i \, dx, \quad (A_{12})_{ij} = -\int_\Omega zF\, \varphi_j\, \psi_i\, dx.$$

$$(A_{21})_{ij} = \int_\Omega \alpha\, \nabla \psi_j \cdot \nabla \varphi_i \, dx, \quad (A_{22})_{ij} = \int_\Omega D\, \nabla \varphi_j \cdot \nabla \varphi_i \, dx \; - \; \int_\Omega (\mathbf{u}\, \varphi_j) \cdot \nabla \varphi_i \, dx.$$

Consider $N_x = N_y = 1024$, $D = 5 \times 10^{-3}$, $\epsilon = 0.1$, $zF = 100$, $\alpha = 1000$
$\Omega = [0,1]^2$, $\phi = c = 0$ on $\partial\Omega$
Asymmetry in A_{22} concentration block characterized by mesh Peclet number:

$$\mathrm{Pe}_h \sim \frac{\|\boldsymbol{u}\| \, h}{D}.$$

- DD(1)-ILU(1)
- Block Gauss-Seidel
  - $\widetilde{M}_{11}^{-1}$: SA-AMG, Chebyshev smoother
  - $\widetilde{M}_{22}^{-1}$: DD(1)-ILU(1) (*Note:* no luck with Petrov-Galerkin (PG) AMG)

$$\mathcal{M}_{BGS}^{-1} = \begin{bmatrix} \widetilde{M}_{11}^{-1} & 0 \\ -\widetilde{M}_{22}^{-1} A_{21} \widetilde{M}_{11}^{-1} & \widetilde{M}_{22}^{-1} \end{bmatrix}$$

- Monolithic AMG with SA-AMG for ϕ, PG-AMG for c
  - Monolithic DD(1)-ILU(1) smoother

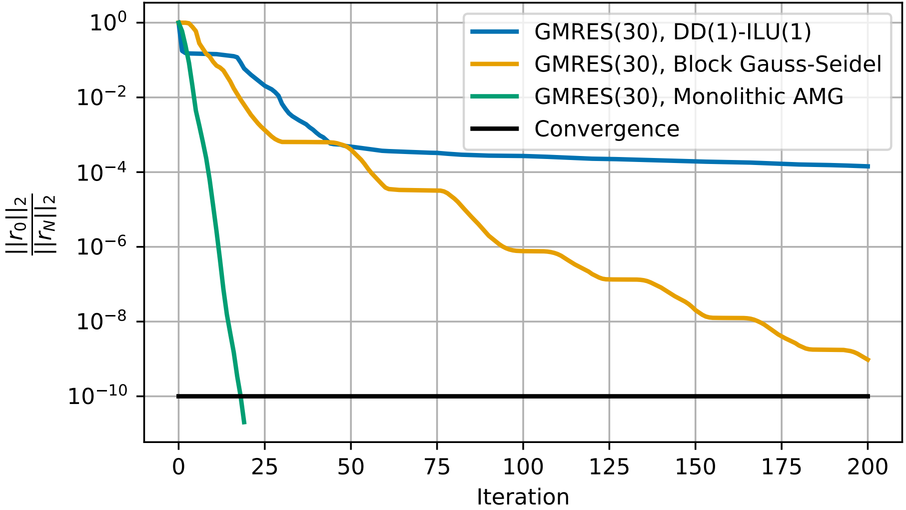

Figure: Convergence for steady linear-drift Poisson–Nernst–Planck system

Conclusions:

- Monolithic AMG approaches outperform one-level block decompositions:
  - Two-temperature electron/lattic model
  - Steady two-way coupled thermoelasticity with advection
  - Steady linear-drift Poisson–Nernst–Planck
- Extend capability in MueLu/Teko for monolithic AMG for multiphysics:
  - Utilizes existing `MueLu::MultiPhys`, `MueLu::CombinePFactory`, and `MueLu::TekoSmoother`
  - Automatically switch between `Xpetra::BlockedCrsMatrix` and `Tpetra::CrsMatrix` representations
    - Limitation: `Xpetra::BlockedCrsMatrix` requires ‘`repartition: use subcommunicators = true`’ with rebalancing
    - Cannot switch between representations mid-hierarchy
    - Explicit re-assembly `Xpetra::BlockedCrsMatrix` to `Tpetra::CrsMatrix` required on coarse-grid level with direct solvers

(a) `github.com/trilinos/Trilinos/pull/15061`

(b) `github.com/MalachiTimothyPhillips/multiphysics-examples`

- Two-temperature electron/lattice model
- Steady two-way coupled thermoelasticity with advection
- Steady linear-drift Poisson–Nernst–Planck
- Sample XML inputs for preconditioners