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Teko Usage in Aria (UUR)

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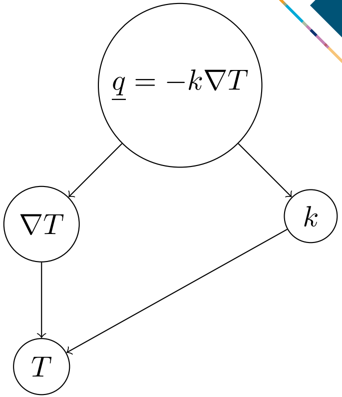
SIERRA/Aria:

- Expression-based multi-physics simulation code[1]
- Segregated and monolithic physics coupling
- Monolithic solver/preconditioner approaches:
  - KLU2/SuperLU sparse direct solvers through Amesos2
  - Domain-decomposition with incomplete LU (DD-ILU) through Ifpack2
  - *Teko physics-based preconditioners*
- Teko solvers integrate with existing Trilinos packages:
  - Amesos2, Belos, Ifpack2, MueLu



[1] Notz, Pawlowski, and Sutherland, "Graph-based software design for managing complexity and enabling concurrency in multiphysics PDE software".

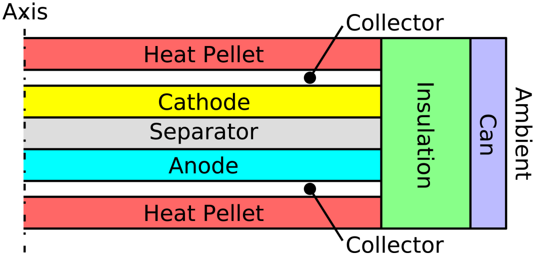
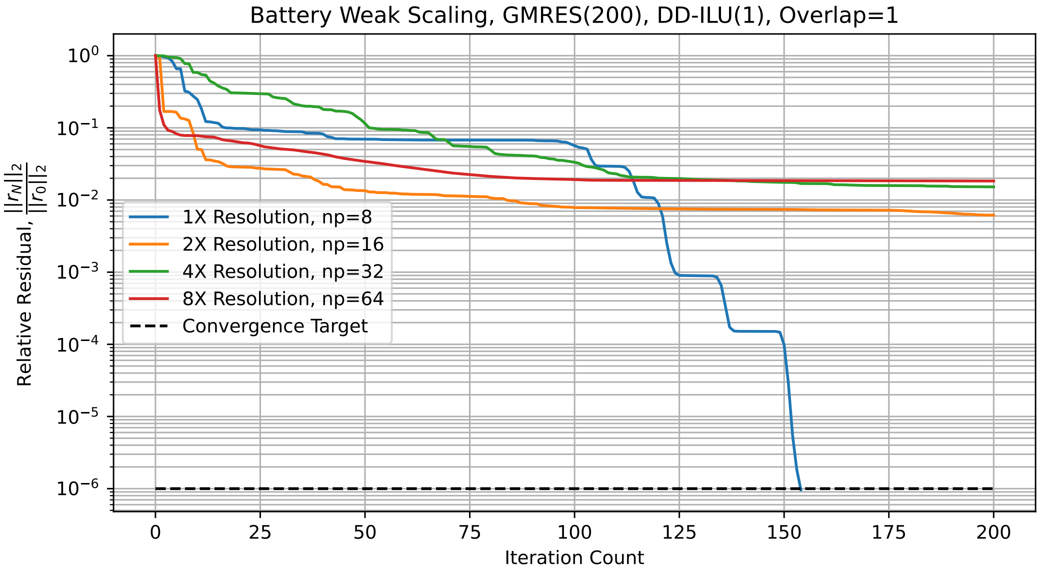


Figure: 2D axisymmetric multi-physics simulation domain[1]

- Includes several multi-physics couplings[1]:
  - Butler-Volmer
  - Stefan-Maxwell
  - Darcy's Law
  - Continuity
- DD-ILU may not converge
- Sparse direct solvers do not scale
- *Weak Scaling:* 57,640 DOFs to 461,120 DOFs
  - Solver: DD-ILU(1) preconditioned GMRES(200)

[1] Voskuilen, Moffat, Schroeder, and Roberts, "Multi-fidelity electrochemical modeling of thermally activated battery cells".



Battery Weak Scaling, GMRES(200), DD-ILU(1), Overlap=1
Relative Residual, $\frac{||r_N||_2}{||r_0||_2}$
10^0
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
0
25
50
75
100
125
150
175
200
Iteration Count
1X Resolution, np=8
2X Resolution, np=16
4X Resolution, np=32
8X Resolution, np=64
Convergence Target

- Teko block splitting (trial-and-error):
  - c: solid phase species
  - x: liquid phase mass fractions
  - p: liquid phase pressure
  - v: solid/liquid phase voltage
- Block representation of matrix:

$$\mathcal{A} = \begin{bmatrix} A_{cc} & A_{cx} & A_{cp} & A_{cv} \\ A_{xc} & A_{xx} & A_{xp} & A_{xv} \\ A_{pc} & A_{px} & A_{pp} & A_{pv} \\ A_{vc} & A_{vx} & A_{vp} & A_{vv} \end{bmatrix}$$

- Construct Block Gauss-Seidel preconditioner:

$$\tilde{\mathcal{M}}^{-1}(\mathcal{A}) = \begin{bmatrix} A_{cc} & A_{cx} & A_{cp} & A_{cv} \\ & A_{xx} & A_{xp} & A_{xv} \\ & & A_{pp} & A_{pv} \\ & & & A_{vv} \end{bmatrix}^{-1}$$

- $\tilde{\mathcal{M}}^{-1}(\mathcal{A})$ requires sub-block inverses, replace with $\mathcal{M}^{-1}(\mathcal{A})$:

$$\mathcal{M}^{-1}(\mathcal{A}) = \begin{bmatrix} M_{cc} & A_{cx} & A_{cp} & A_{cv} \\ & M_{xx} & A_{xp} & A_{xv} \\ & & M_{pp} & A_{pv} \\ & & & M_{vv} \end{bmatrix}^{-1}$$

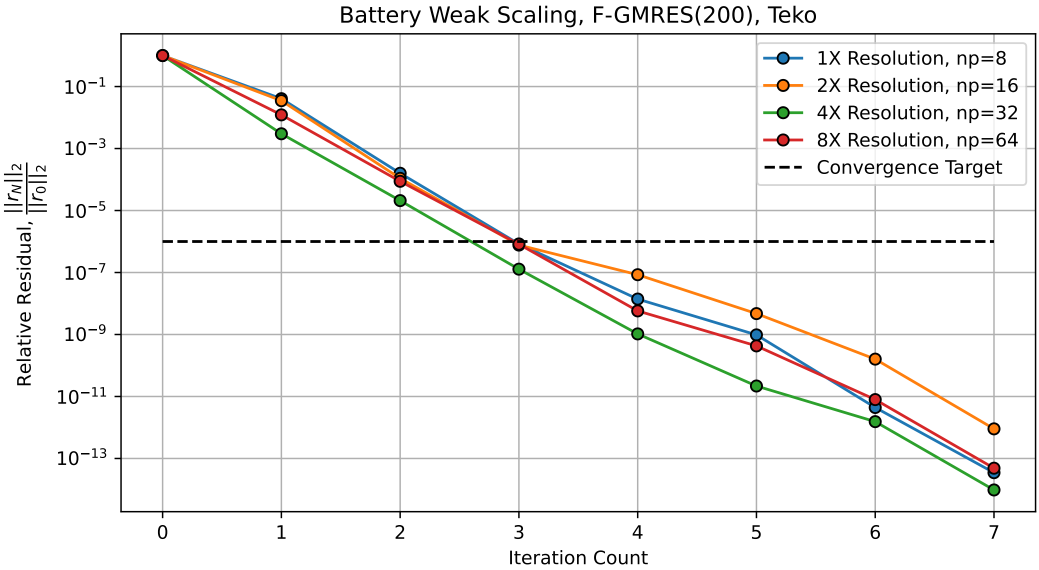
Convergence Result

A single resistant sub-block solver can derail the entire solver:

$$\begin{aligned} \kappa\left(\mathcal{M}^{-1}(\mathcal{A})\,\mathcal{A}\right) &\leq \kappa\left(\mathcal{M}^{-1}(\mathcal{A})\,\tilde{\mathcal{M}}(\mathcal{A})\right) \cdot \kappa\left(\tilde{\mathcal{M}}^{-1}(\mathcal{A})\,\mathcal{A}\right) \\ &\geq \underbrace{\max_{\forall M_{ii}^{-1} A_{ii}} \left(\kappa\left(M_{ii}^{-1} A_{ii}\right)\right)}_{\text{Sub-block Solver Conditioning}} \cdot \underbrace{\kappa\left(\tilde{\mathcal{M}}^{-1}(\mathcal{A})\,\mathcal{A}\right)}_{\text{Multi-physics Coupling}} \end{aligned}$$

- *A single resistant sub-block solver can derail the entire solver*
- Use iterative sub-block solves to ensure convergence
  - Preconditioner $\mathcal{M}^{-1}(\mathcal{A})$ *changes* per iteration
  - Requires *flexible* GMRES (F-GMRES)[2]
  - *Same orthogonalization cost*
  - *Double restart memory*
- Approximate sub-block inverses for diagonal entries:
  - M_{cc}^{-1}: Jacobi
  - M_{xx}^{-1}: GMRES + DD-ILU
  - M_{pp}^{-1}: GMRES + DD-ILU
  - $M_{vv}^{-1} = A_{vv}^{-1}$: KLU2 sparse direct solver

[2] Saad, "A flexible inner-outer preconditioned GMRES algorithm".


Battery Weak Scaling, F-GMRES(200), Teko
Relative Residual, $\frac{||r_N||_2}{||r_0||_2}$
10^{-1}
10^{-3}
10^{-5}
10^{-7}
10^{-9}
10^{-11}
10^{-13}
0
1
2
3
4
5
6
7
Iteration Count
1X Resolution, np=8
2X Resolution, np=16
4X Resolution, np=32
8X Resolution, np=64
Convergence Target

- Teko provides effective preconditioners for multi-physics problems
  - Especially useful when DD-ILU struggles

Ingredients for Teko Solver Setup

Teko solver setup requires:

1. Physics-to-sub-block mapping
2. Ordering sub-blocks
3. Solvers/preconditioners for each sub-block

- *Goal:* provide ability to *auto-magically* generate reasonable Teko settings

```
begin tpetra equation solver teko_linear_solver
  begin preset solver
    solver type = teko_multiphysics
  end preset solver
end tpetra equation solver
```

Ordering sub-blocks:

- Block Gauss-Seidel ordering matters:

$$\kappa\left(\underbrace{\begin{bmatrix} A & B \\ & D \end{bmatrix}^{-1}}_{\tilde{\mathcal{M}}^{-1}(\mathcal{A})} \underbrace{\begin{bmatrix} A & B \\ C & D \end{bmatrix}}_{\mathcal{A}}\right) \neq \kappa\left(\underbrace{\begin{bmatrix} D & C \\ & A \end{bmatrix}^{-1}}_{\tilde{\mathcal{M}}^{-1}(\mathcal{RAC})} \underbrace{\begin{bmatrix} D & C \\ B & A \end{bmatrix}}_{\mathcal{RAC}}\right)$$

Optimization Problem

Find block ordering permutation $\mathcal{R}^* (\cdot) \mathcal{C}^*$ such that:

$$(\mathcal{R}^*, \mathcal{C}^*) = \underset{\forall \mathcal{R},\mathcal{C}}{\arg\min}\, \kappa(\tilde{\mathcal{M}}^{-1} (\mathcal{RAC}) \mathcal{RAC})$$

- Naïve brute-force approach to optimal ordering is exponential in n_b
- *Collaboration with SandiaAI:* use graph-based heuristic for ordering

Ordering Heuristic

Input : $\mathcal{A}$ with n_b blocks, n maximum iterations
Output: Re-ordered $\mathcal{A}'$ more suitable for block Gauss-Seidel

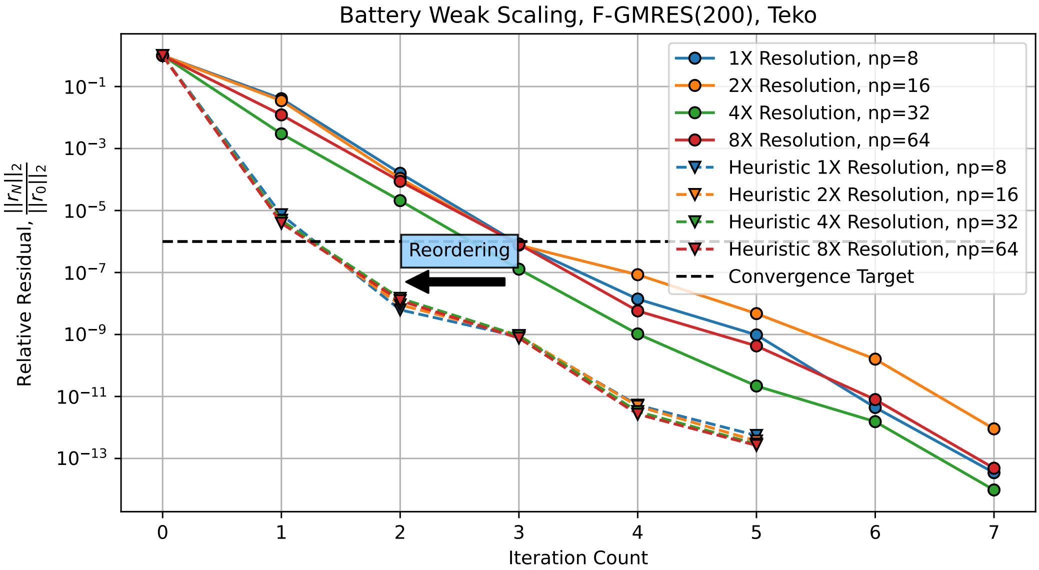
$\mathcal{A}^{(1)} = \mathcal{A}$
for $k \leftarrow 1$ **to** n **do**
  Construct undirected graph $\mathcal{G}^{(k)} \leftarrow (\mathcal{V} = \{1, \ldots, n_b\}, \mathcal{E} = (i, j) \mid \forall i \in \mathcal{V}, j \geq i)$
  Construct *symmetric* edge-weight matrix $W_{i,j}^{(k)} \leftarrow \begin{cases} \left\| \mathcal{A}_{i,j}^{(k)} \right\|_F & i > j \\ \left\| \mathcal{A}_{j,i}^{(k)} \right\|_F & j > i \\ 0 & i = j \end{cases}$
  $D^{(k)} \leftarrow \mathrm{diag}(D_1^{(k)}, \ldots, D_{n_b}^{(k)})$ with $D_i^{(k)} = \sum_{j=1}^{n_b} W_{i,j}^{(k)}$
  Form *symmetric* weighted graph Laplacian $L^{(k)} \leftarrow D^{(k)} - W^{(k)}$
  $Q^{(k)} \Lambda^{(k)} \left(Q^{(k)}\right)^T \leftarrow L^{(k)}$ with $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_{n_b}$
  Construct re-ordering from Fiedler vector $\mathcal{R}^{(k)} (\cdot) \, \mathcal{C}^{(k)} \leftarrow$ argsort(V[:,2]) `// Second smallest`
  $\mathcal{A}^{(k+1)} \leftarrow \mathcal{R}^{(k)} \mathcal{A}^{(k)} \mathcal{C}^{(k)}$
  if $\mathcal{A}^{(k+1)} = \mathcal{A}^{(k)}$ **then return** $\mathcal{A}^{(k+1)}$
end
return $\mathcal{A}^{(n+1)}$

- Apply ordering heuristic to battery problem
  - c: solid phase species
  - x: liquid phase mass fractions
  - p: liquid phase pressure
  - v: solid/liquid phase voltage
- Previous ordering:

$$\mathcal{A} = \begin{bmatrix} A_{cc} & A_{cx} & A_{cp} & A_{cv} \\ A_{xc} & A_{xx} & A_{xp} & A_{xv} \\ A_{pc} & A_{px} & A_{pp} & A_{pv} \\ A_{vc} & A_{vx} & A_{vp} & A_{vv} \end{bmatrix}, \mathcal{M}^{-1}\left(\mathcal{A}\right) = \begin{bmatrix} M_{cc} & A_{cx} & A_{cp} & A_{cv} \\ & M_{xx} & A_{xp} & A_{xv} \\ & & M_{pp} & A_{pv} \\ & & & M_{vv} \end{bmatrix}^{-1}$$

- New ordering:

$$\mathcal{A}' = \begin{bmatrix} A_{vv} & A_{vp} & A_{vc} & A_{vx} \\ A_{pv} & A_{pp} & A_{pc} & A_{px} \\ A_{cv} & A_{cp} & A_{cc} & A_{cx} \\ A_{xv} & A_{xp} & A_{xc} & A_{xx} \end{bmatrix}, \mathcal{M}^{-1}\left(\mathcal{A}'\right) = \begin{bmatrix} M_{vv} & A_{vp} & A_{vc} & A_{vx} \\ & M_{pp} & A_{pc} & A_{px} \\ & & M_{cc} & A_{cx} \\ & & & M_{xx} \end{bmatrix}^{-1}$$



Battery Weak Scaling, F-GMRES(200), Teko
Relative Residual, $\frac{||r_N||_2}{||r_0||_2}$
10^{-1}
10^{-3}
10^{-5}
10^{-7}
10^{-9}
10^{-11}
10^{-13}
0
1
2
3
4
5
6
7
Iteration Count
Reordering
1X Resolution, np=8
2X Resolution, np=16
4X Resolution, np=32
8X Resolution, np=64
Heuristic 1X Resolution, np=8
Heuristic 2X Resolution, np=16
Heuristic 4X Resolution, np=32
Heuristic 8X Resolution, np=64
Convergence Target

Physics-to-sub-block mapping:

- Strongly coupled physics may require monolithic approach:

$$\kappa\left(\underbrace{\begin{bmatrix} A & B & C \\ & E & F \\ & & J \end{bmatrix}^{-1}}_{\tilde{\mathcal{M}}^{-1}(\mathcal{A})}\underbrace{\begin{bmatrix} A & B & C \\ D & E & F \\ G & H & J \end{bmatrix}}_{\mathcal{A}}\right) \neq \kappa\left(\underbrace{\begin{bmatrix} \begin{bmatrix} A & B \\ D & E \end{bmatrix} & \begin{bmatrix} C \\ F \end{bmatrix} \\ & J \end{bmatrix}^{-1}}_{\tilde{\mathcal{M}}^{-1}(\mathcal{A}')}\underbrace{\begin{bmatrix} \begin{bmatrix} A & B \\ D & E \end{bmatrix} & \begin{bmatrix} C \\ F \end{bmatrix} \\ \begin{bmatrix} G & H \end{bmatrix} & J \end{bmatrix}}_{\mathcal{A}'}\right)$$

- Monolithically treat combined block with DD-ILU
  - Alternative: sub-iterate via *Hierarchical Block Gauss-Seidel*
- Simple greedy heuristic for grouping (next slide)
- At every step, reduce $n_b \times n_b$ block system to $(n_b - 1) \times (n_b - 1)$:

$$\mathcal{A}^*_{(n_b-1)\times(n_b-1)} \leftarrow \underset{\mathcal{A}'_{(n_b-1)\times(n_b-1)}}{\arg\min} \; \max_{\forall i,j\in\{1,\ldots,n_b-1\}, j\neq i} \left\| \left(\mathcal{A}'_{i,j}\right)_{(n_b-1)\times(n_b-1)} \right\|_F$$

Block Grouping Heuristic

Input : Matrix $\mathcal{A}$ with n_b blocks, maximum iterations $n < n_b$, threshold τ

Output: Re-grouped matrix $\mathcal{A}'$ with $n_b' < n_b$ blocks

/* Note: $\left\| \begin{bmatrix} A & B \\ C & D \end{bmatrix} \right\|_F = \sqrt{\|A\|_F^2 + \|B\|_F^2 + \|C\|_F^2 + \|D\|_F^2}$. */

$\mathcal{A}^{(0)} \leftarrow \mathcal{A}$

$r_0 \leftarrow \max_{i,j,i \neq j} \|\mathcal{A}_{i,j}^{(0)}\|_F$

for $k \leftarrow 0$ **to** $n - 1$ **do**

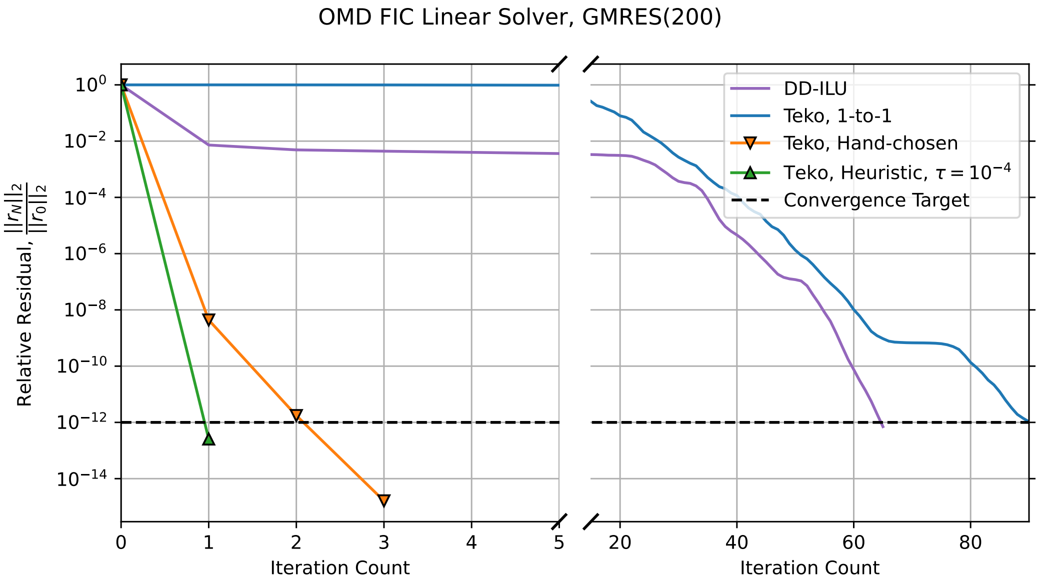
- $(i^*, j^*) \leftarrow \arg\max_{i,j,i \neq j} \left\| \mathcal{A}_{i,j}^{(k)} \right\|_F$
- $\mathcal{A}^{(k+1)} \leftarrow \text{combine}(\mathcal{A}^{(k)}, i^*, j^*)$ // $\mathcal{A}^{(k+1)}$ is a $n_b - (k+1)$ block system
- $r_{k+1} \leftarrow \max_{i,j,i \neq j} \|\mathcal{A}_{i,j}^{(k+1)}\|_F$
- **if** $\frac{r_{k+1}}{r_0} \leq \tau$ **then return** $\mathcal{A}^{(k+1)}$

end

return $\mathcal{A}^{(n)}$

OMD FIC multi-physics example:

- 14 coupled PDEs:
  - Solid conduction
  - Porous-fluid coupled flow
  - Enthalpy
  - Species transport
- Comparison between four preconditioners with $\frac{\|\underline{r}_N\|_2}{\|\underline{r}_0\|_2} = 10^{-12}$
  - Monolithic DD-ILU
  - One-to-one physics-to-block mapping, using heuristic order
  - Hand-chosen grouping/order
  - Heuristic grouping/ordering, target reduction $\tau = 10^{-4}$
- KLU2 sparse direct solver for sub-blocks


OMD FIC Linear Solver, GMRES(200)
Relative Residual, $\frac{||r_N||_2}{||r_0||_2}$
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
10^{-14}
0
1
2
3
4
5
20
40
60
80
Iteration Count
Iteration Count
DD-ILU
Teko, 1-to-1
Teko, Hand-chosen
Teko, Heuristic, $\tau = 10^{-4}$
Convergence Target

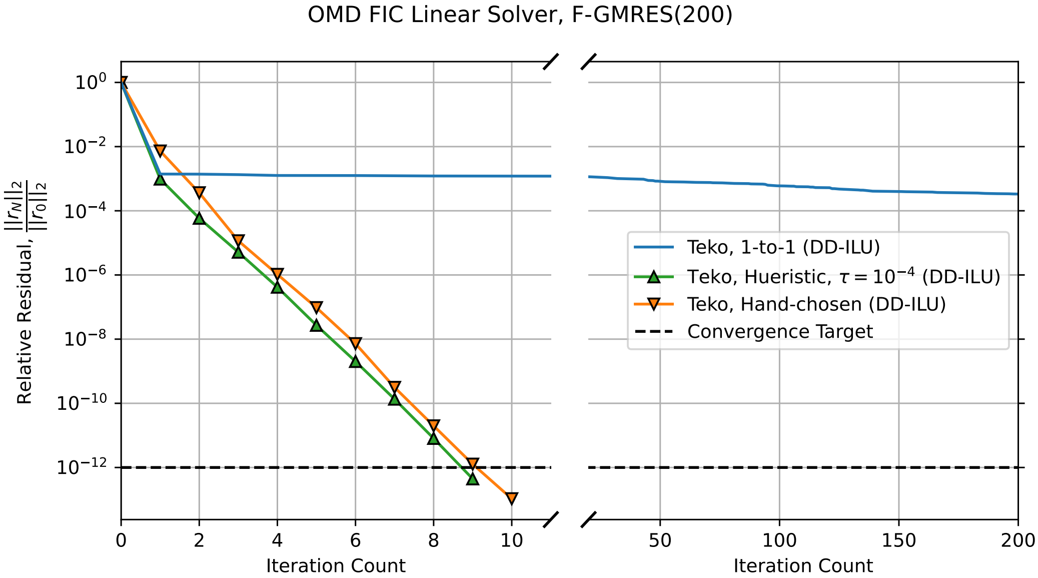
Solvers/preconditioners for each sub-block:

- *Many* sub-blocks will incorporate several physics

Poor man's solution

- DD-ILU preconditioned GMRES(30)
- Target one order-of-magnitude residual reduction
- F-GMRES(200) as outer solver

- Repeat OMD FIC example:
  - One-to-one physics-to-block mapping, using heuristic order
  - Hand-chosen grouping/order
  - Heuristic grouping/ordering, target reduction $\tau = 10^{-4}$


OMD FIC Linear Solver, F-GMRES(200)
Relative Residual, $\frac{||r_N||_2}{||r_0||_2}$
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{-12}
0
2
4
6
8
10
50
100
150
200
Iteration Count
Iteration Count
Teko, 1-to-1 (DD-ILU)
Teko, Hueristic, $\tau = 10^{-4}$ (DD-ILU)
Teko, Hand-chosen (DD-ILU)
Convergence Target

Concluding remarks:

- DD-ILU is a great work-horse preconditioner
  - *It can fail to converge*
- Teko provides diversification to multi-physics solver portfolio
- Relies on existing preconditioners/solvers at sub-block level:
  - DD-ILU
  - MueLu
- Flexible, extensible package with many options
- Large landscape of solver settings difficult for users to navigate
  - *WIP: Provide users with guidance through heuristics*

Questions?

- e-mail: `malphil@sandia.gov`