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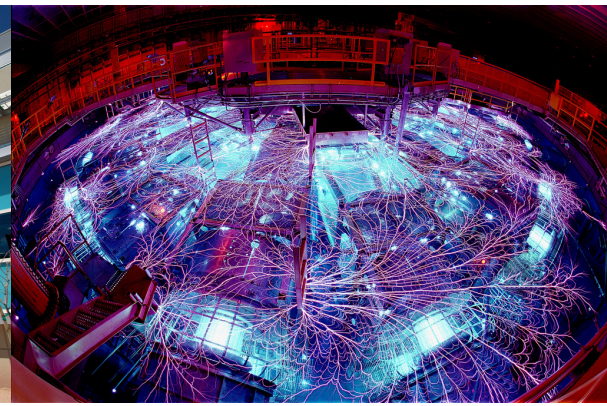

Data-Driven Approaches for Patch-Based Multigrid Smoothers

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Sandia National Laboratories

4/18/23

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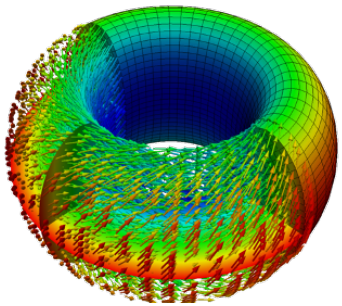
Acknowledgements

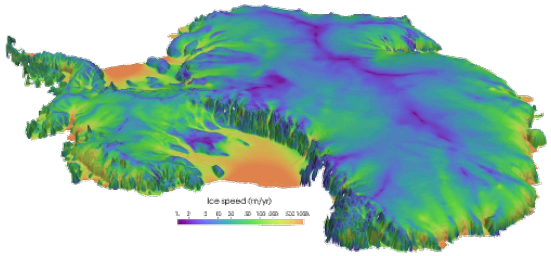
- Trilinos/MueLu/Ifpack2
- Funding: Harper's LDRD, Ridzal's LDRD, Tuminaro's ASCR
- Team: Ray Tuminaro
- Sandia National Laboratories LDRD Office, U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research

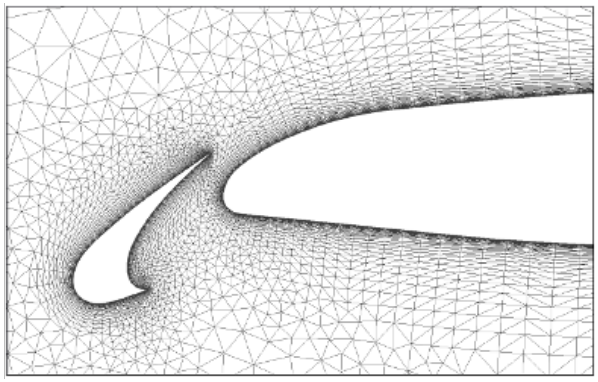
Outline

Overview for Smoothers

- Traditional simple smoothers (Jacobi) work well for low-order problems, but tend to struggle as the **polynomial degree** increases or **coupling** increases.







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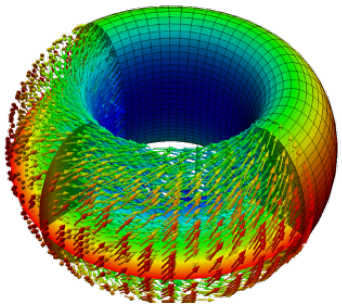

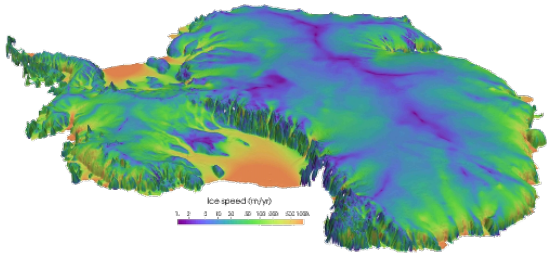

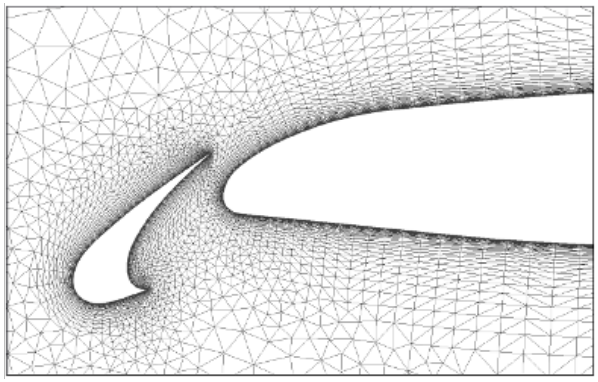

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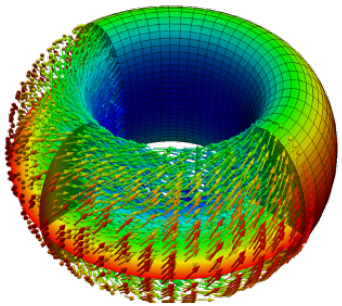
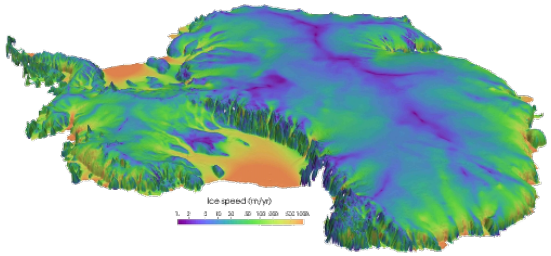
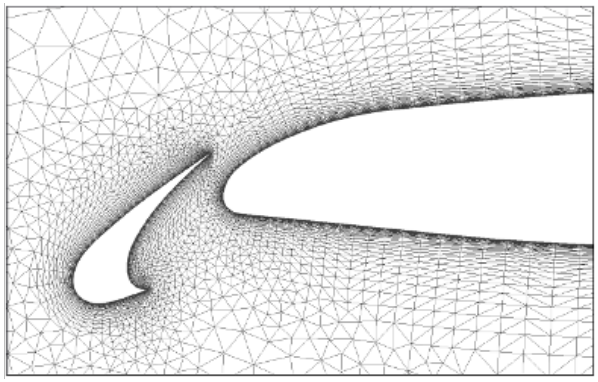






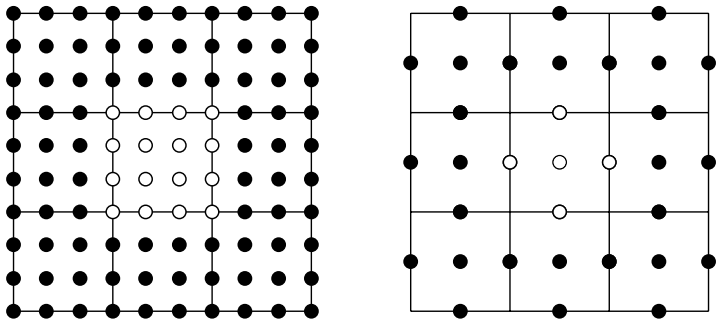
- Patch-based smoothers reduce iteration counts at the cost of storing/solving many small linear systems.
- What if we could reduce those costs?

Patch-Based Smoothers

- Recall a smoother takes the form

$$\mathbf{x} \leftarrow \mathbf{x} + \omega \tilde{M}^{-1}(A\mathbf{x} - \mathbf{b}) \tag{1}$$

- Consider an (overlapping) domain decomposition with n_p domains and boolean restriction operators R_i.



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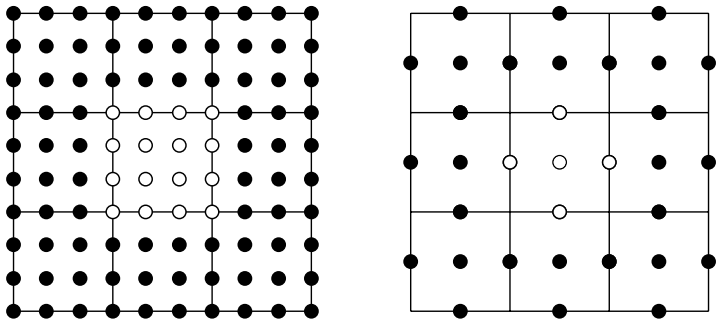

- A patch-based smoother utilizes

$$\tilde{M}^{-1} = \sum_{i=1}^{n_p} R_i^T W_i A_i^{-1} R_i \tag{2}$$

Patch-Based Smoothers

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- R_i is the boolean restriction
- W_i are the global weights, $(\text{overlap})^{-1}$
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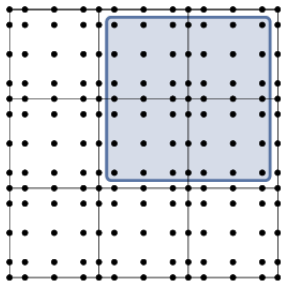
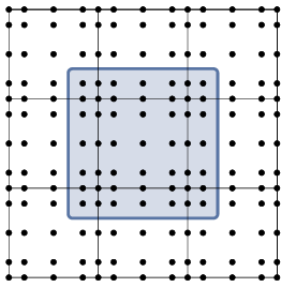
Patch methods:

- Pros: Converge more quickly, handle complex coupling more effectively
- Cons: More expensive to compute, similar storage cost to original matrix

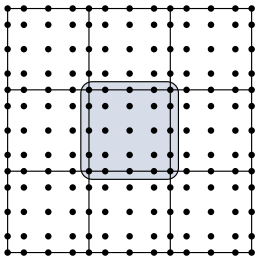
Clarifications



(a) Vertex-star patch



(b) Cell-centered patch



(c) Our cell patches

There are many kinds of patch smoothers:

(a) Scales for high values of p, difficult solves, depends on connectivity

*left figures: P. Brubeck, P. Farrell, *A Scalable and Robust Vertex-Star Relaxation for High-Order FEM*. SISC 2022

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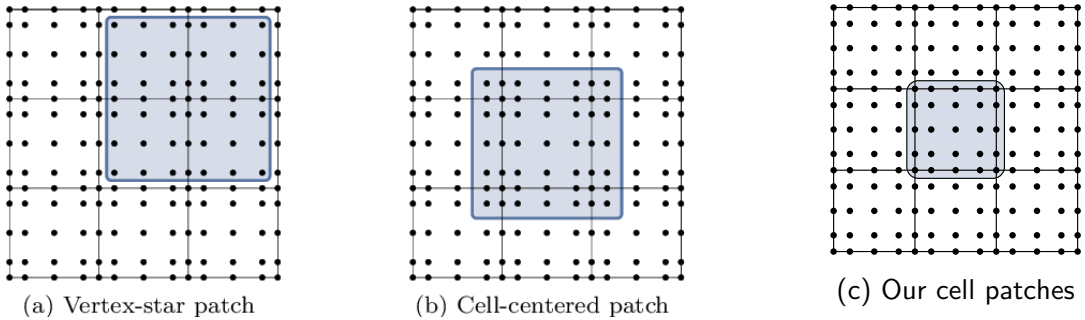

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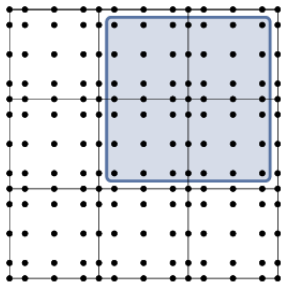

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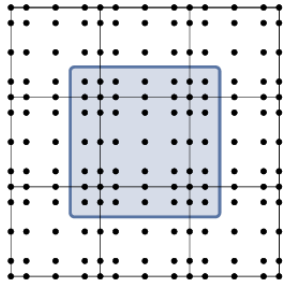

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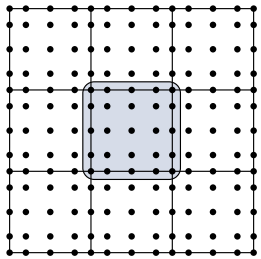


(c) Our cell patches

There are many kinds of patch smoothers:

(a) Scales for high values of p, difficult solves, depends on connectivity

(b) Allows for structured patches, not p-robust

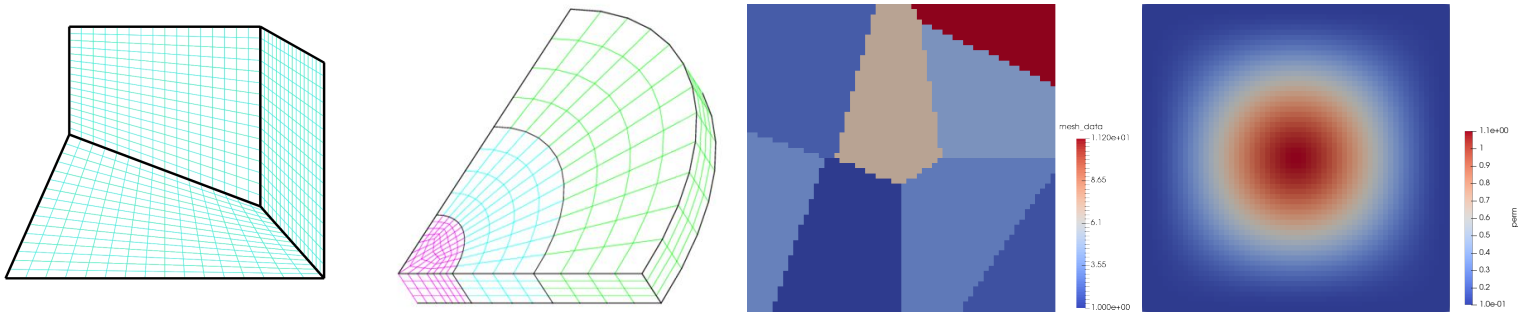
(c) Most efficient to detect, most structure to exploit

Bases with sparse patches also exist, but are not considered here.

*left figures: P. Brubeck, P. Farrell, *A Scalable and Robust Vertex-Star Relaxation for High-Order FEM*. SISC 2022

Observations

1. In many applications of interest, if you zoom in far enough, patterns appear.



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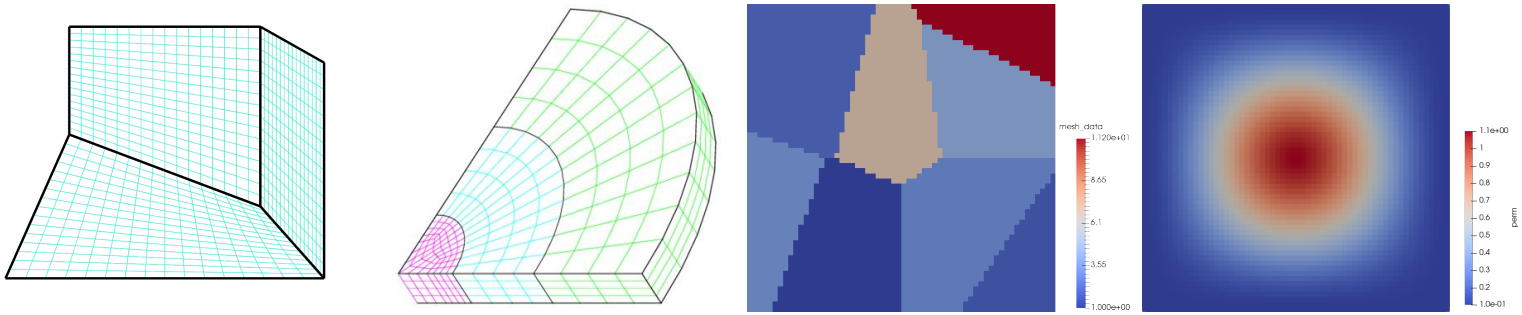

2. If patches are "similar enough," why store and solve them multiple times?

Observations

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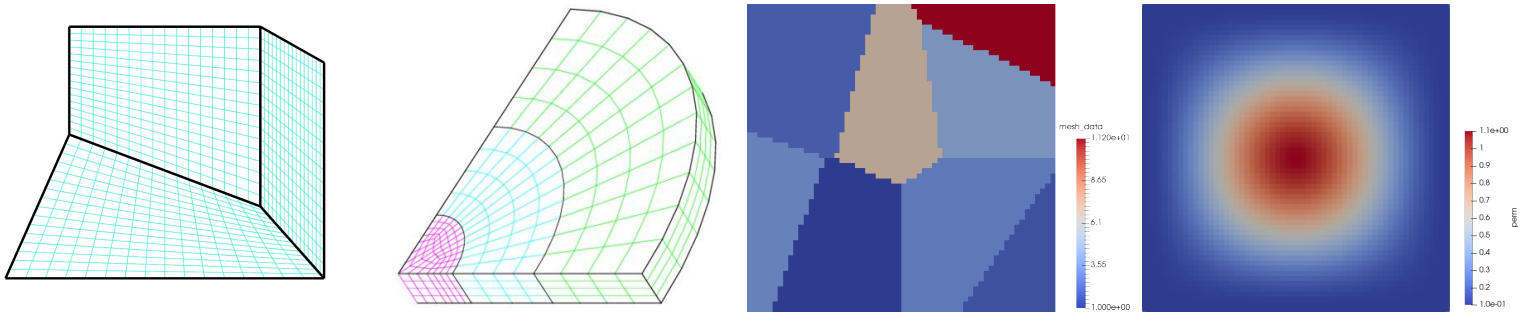


2. If patches are "similar enough," why store and solve them multiple times?

Question: How "bad" can the approximation get before the solver (smoother-only or multigrid) starts to struggle?

The Main Idea

- Construct a database of patches $\mathcal{B} = \{B_1, B_2, \ldots, B_{m_p}\}$.
- Criterion 1: $\mathcal{B}$ should approximate $\{A_i\}$ sufficiently well.
- Criterion 2: $\mathcal{B}$ should be small compared to $\{A_i\}$.

The Main Idea

- Construct a database of patches $\mathcal{B} = \{B_1, B_2, \ldots, B_{m_p}\}$.
- Criterion 1: $\mathcal{B}$ should approximate $\{A_i\}$ sufficiently well.
- Criterion 2: $\mathcal{B}$ should be small compared to $\{A_i\}$.

Seek $\mathcal{B} = \{B_1, B_2, \ldots, B_{m_p}\}$ and mapping
$\phi : \{1, \ldots, n_p\} \to \{1, \ldots, m_p\}$ minimizing

$$\mathcal{L}(\mathcal{B}, \phi) = \beta|\mathcal{B}| + \sum_{k=1}^{n_p} \|I - A_k B_{\phi(k)}^{-1}\|_2^2, \tag{3}$$

balancing efficiency and accuracy.
Also referred to as a **sparse approximation problem**.

Greedy Algorithm

Algorithm 1 Greedy Construction of $\mathcal{B}$, $\phi()$

1: **Input:** $\{A_1, A_2, \ldots, A_{n_p}\}$, ε
2: $\mathcal{B} := \{\}$, $\vec{\phi} = 0$
3: **for** $i = 1, \ldots, n_p$ **do**
4: match:=false;
5: **for** $j = 1, \ldots, m_p$ **do**
6: **if** $\|I - A_i B_j^{-1}\|_2 < \varepsilon$ **then**
7: match=true, $\phi(i) = j$, break;
8: **end if**
9: **end for**
10: **if** match==false **then**
11: append A_i to $\mathcal{B}$, $\phi(i) = |\mathcal{B}|$;
12: **end if**
13: **end for**
14: **Output:** $\mathcal{B} = \{B_1, B_2, \ldots, B_{m_p}\}$, $\vec{\phi}$

← check patch against database

← if no matches, store patch explicitly

Clustering Algorithm

Algorithm 3 Clustering Construction of $\mathcal{B}$, $\phi()$

1: **Input:** $\{A_1, A_2, \ldots, A_{n_p}\}$, m_p
2: $\vec{\phi} = \text{randperm}(n_p, m_p)$;
3: $B_i = A_{\phi(i)}$, $i = 1, \ldots, m_p$;
4: **while** not converged **do**
5: **for** $i = 1, \ldots, n_p$ **do**
6: **for** $j = 1, \ldots, m_p$ **do**
7: $d_{ij} = d(A_i, B_j)$;
8: **end for**
9: $\phi(i) = \text{argmin}_j(d_{ij})$;
10: **end for**
11: $B_i = \frac{1}{n_i} \sum_{j \text{ in cluster } i} A_j$, $i = 1, \ldots, m_p$;
12: **end while**
13: **Output:** $\mathcal{B} = \{B_1, B_2, \ldots, B_{m_p}\}$, $\vec{\phi}$

$\leftarrow$ choose number of clusters

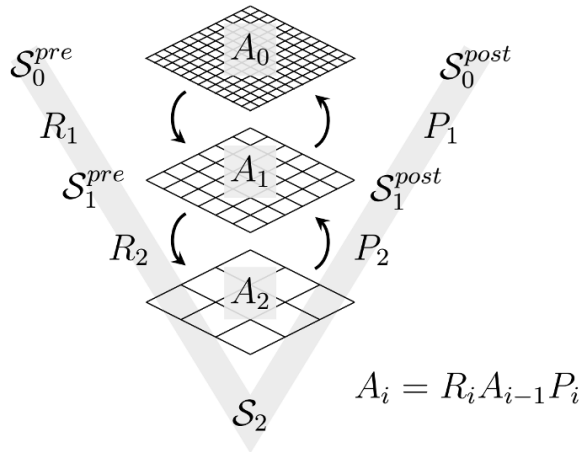
$\leftarrow d(A_i, B_j) = \|I - A_i B_j^{-1}\|_2$

*treat boundaries separately!

Multigrid Method

We use the following multigrid configuration:

- $\omega = 0.5$,
- $(\nu_1, \nu_2) = (1, 0)$,
- $N = 2$ V-cycle levels,
- P linear interpolation, $R = P^T$,
- $A_c = RAP$



With the data-driven smoother, compute $\mathcal{B}, \vec{\phi}$ during setup; use them during apply.

Example Test Cases

The following examples utilize Poisson's equation:

$$(k\nabla p_h, \nabla q_h)_{\mathcal{T}_h} = (f, q_h)_{\mathcal{T}_h}. \tag{4}$$

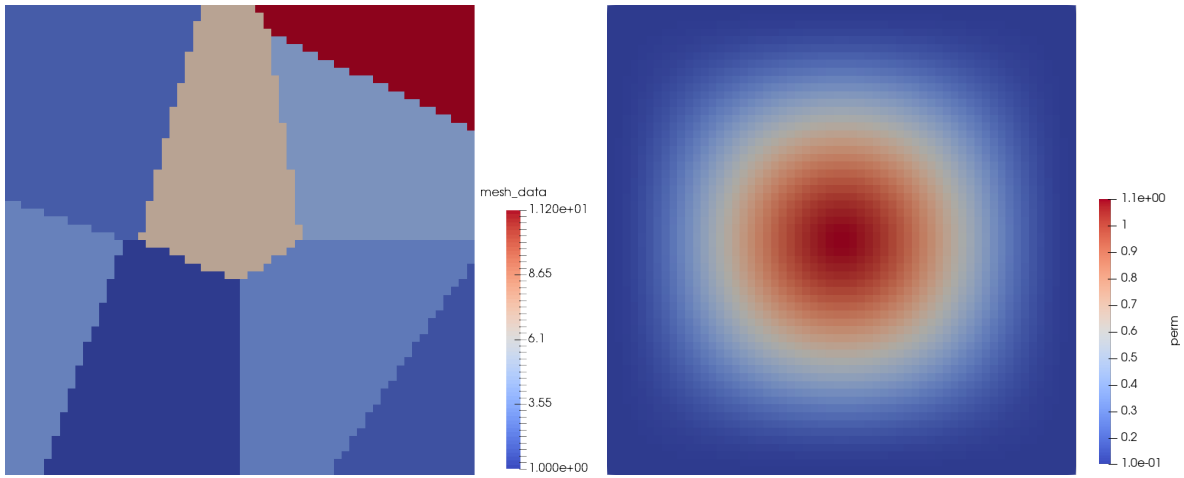
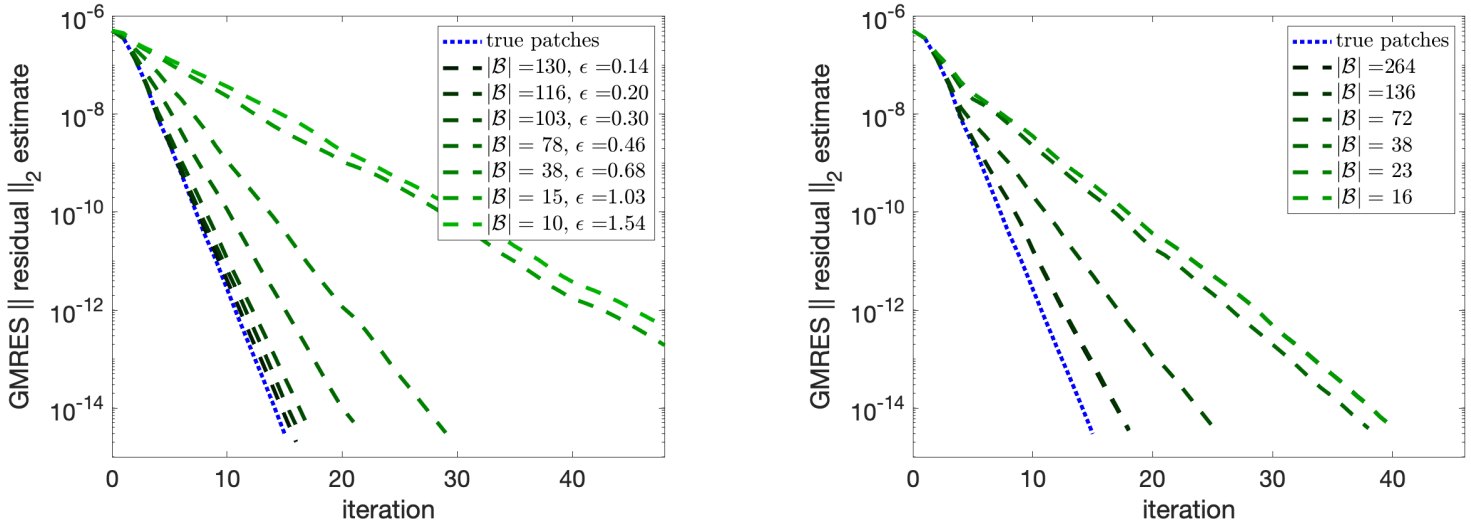


Figure: (left) piecewise discontinuous coefficient, (right) smooth varying coefficient

Results (Piecewise Constant Permeability)

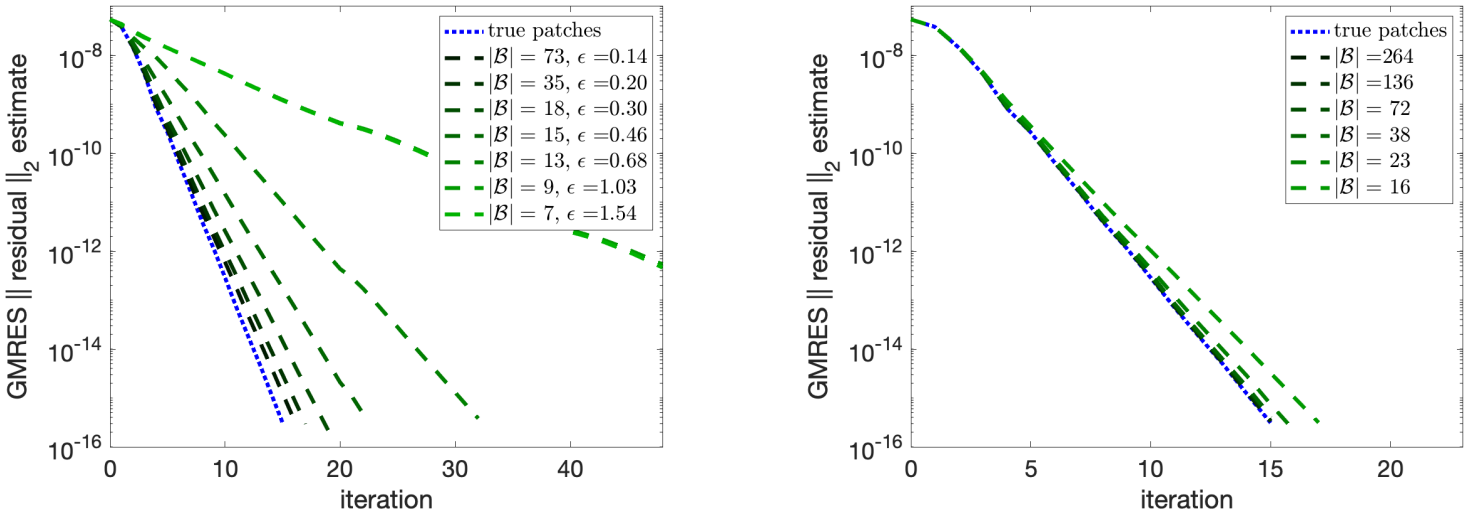


(a) greedy algorithm

(b) clustering algorithm

Figure: Multigrid residual histories on 60×60 mesh with $p = 5$** for piecewise constant problem, varying database sizes $\mathcal{B}$.

Results (Smooth Permeability)



(a) greedy algorithm

(b) clustering algorithm

Figure: Multigrid residual histories on 60×60 mesh with $p = 5$ for smooth problem, varying database sizes $\mathcal{B}$.

Results (Database Mappings)

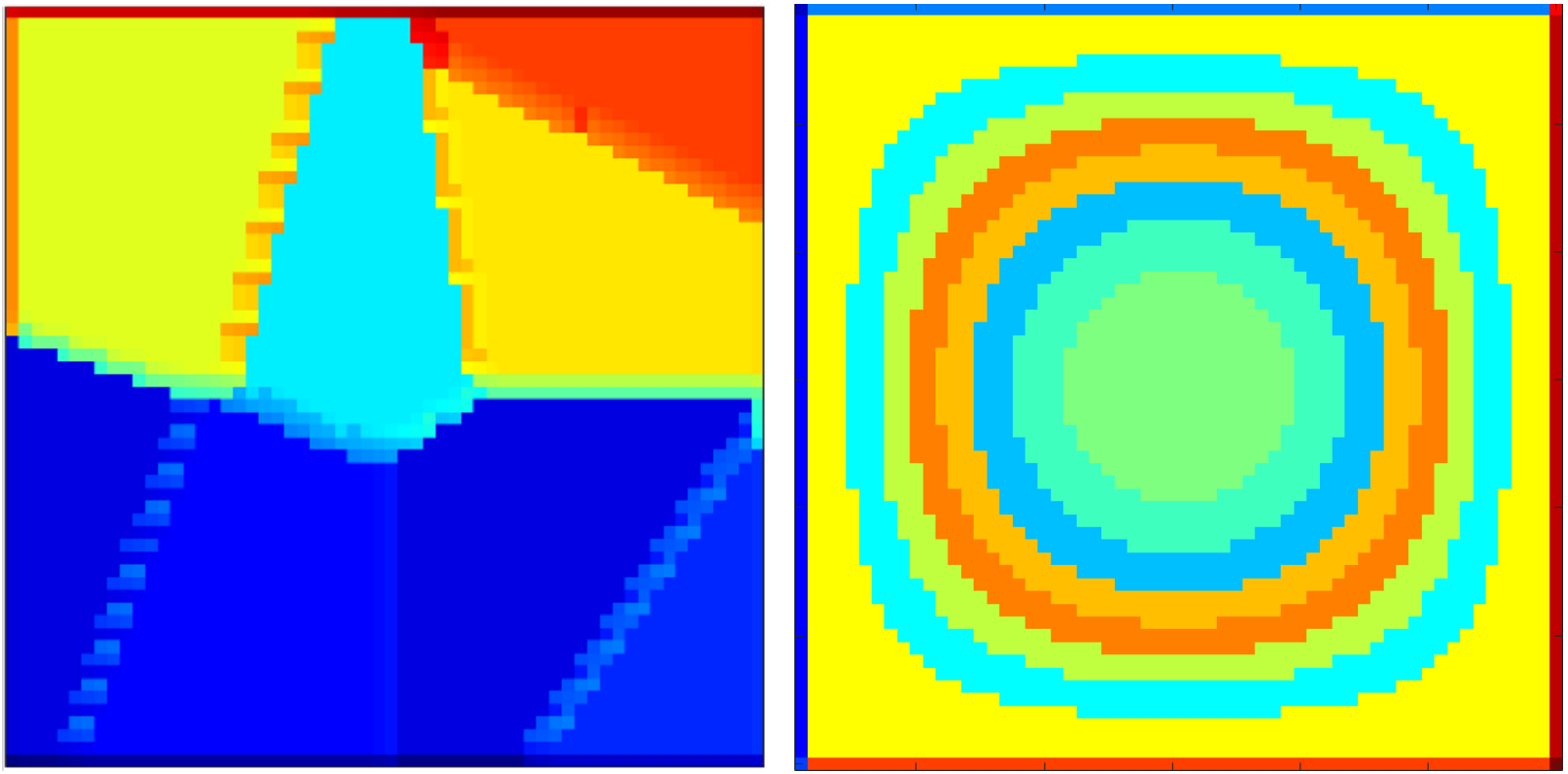


Figure: Visualization of database ϕ mapping. (left) greedy algorithm on piecewise constant permeability, (right) clustering algorithm on smooth permeability

Results (Compressibility Profile)

For Burgers' equation with a shock on a 100×100 mesh:

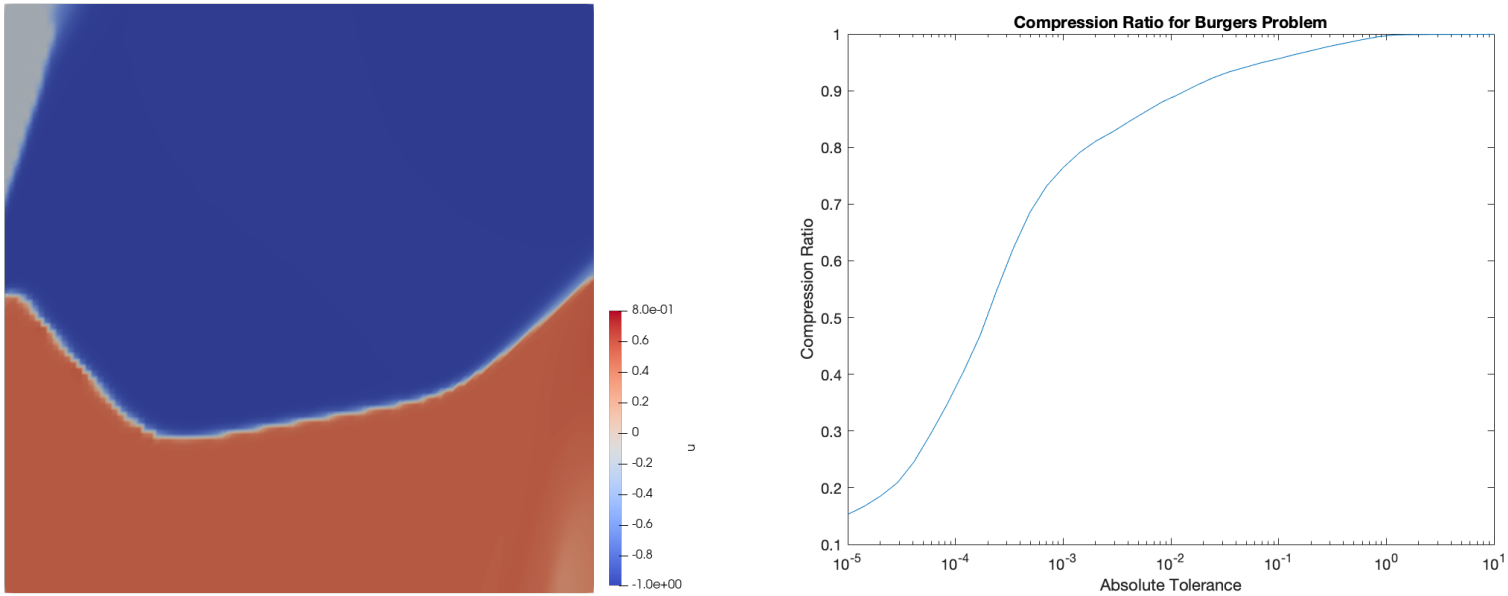


Figure: (left) Burgers' equation profile with a shock, (right) the compressibility profile associated with the problem

Timing Results

Implemented in **Trilinos/Ifpack2** as a preconditioner. Used as additive Schwarz inner solve.

Configuration	m_p	$p_s \times p_s$	Setup (s)	Apply (s)
No database	3600	36×36	2.274	0.4157
Database	9	36×36	2.442	0.2624

Apply speedup of 30% on small test problem on an Intel Xeon workstation. *Expected to extend well.

Interested in trying it?
`https://github.com/trilinos/Trilinos/pull/11517`

Conclusion

Takeaways:

- Memory cost $= \mathcal{O}(\text{Jacobi})$
- Faster apply than without database
- Generalizes for any structure detection method

Current/Future Work:

- Performance improvements
- Time-dependent problems
- Ridzal's LDRD: R-adaptivity to detect and enhance compressibility
- Summer student looking into clustering on eigenvalues
- Unsupervised deep learning

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Thank You

- Questions?