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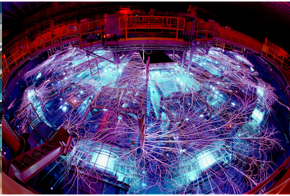

Reduced Representation and Compression Techniques for Patch-Based Relaxation

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Center for Computing Research
Sandia National Laboratories

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- Team: Ray Tuminaro
- Sandia National Laboratories LDRD Office, U.S. Department of Energy, Office of Science, Office of Advanced Scientific Computing Research

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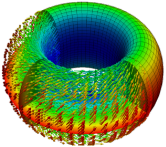
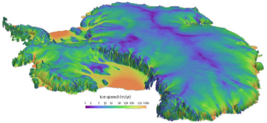
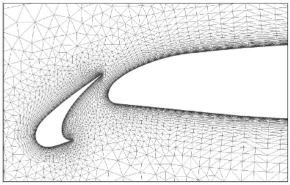
Overview for Smoothers

- 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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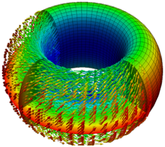

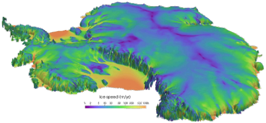

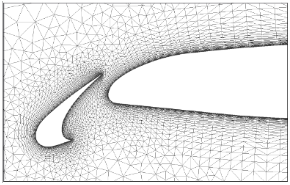

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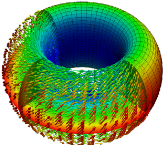
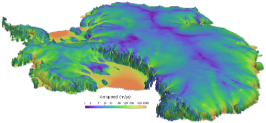
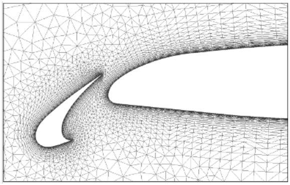




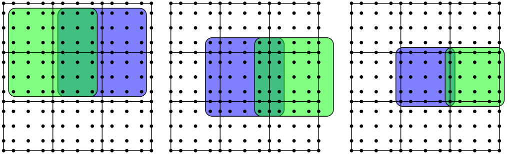
- Patch-based smoothers reduce iteration counts at the cost of storing/solving many small linear systems.
- What if we could reduce those costs?

Patch-Based Smoothers

- Recall a smoother takes the form

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

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



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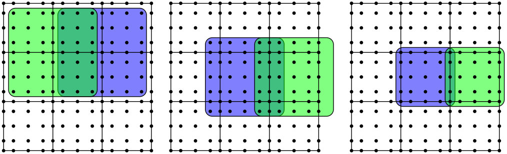

- A patch-based smoother utilizes

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

Patch-Based Smoothers

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

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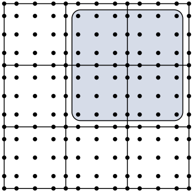
Patch methods:

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

Clarifications

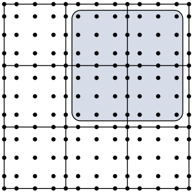


(a) Vertex-star patches

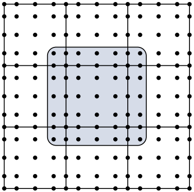
There are many kinds of patch smoothers:

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

Clarifications



(a) Vertex-star patches



(b) Cell-centered patches

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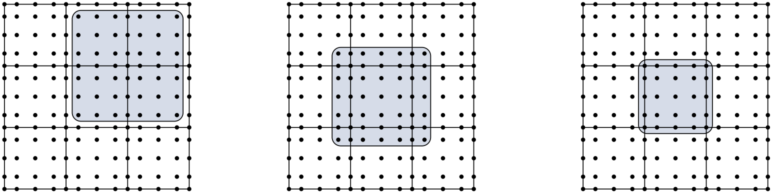


(a) Vertex-star patches (b) Cell-centered patches (c) Cell-restricted patches

There are many kinds of patch smoothers:

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

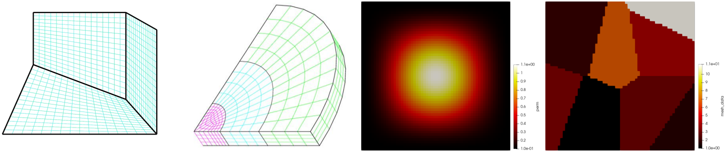
(b) Allows for structured patches, not p-robust

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

*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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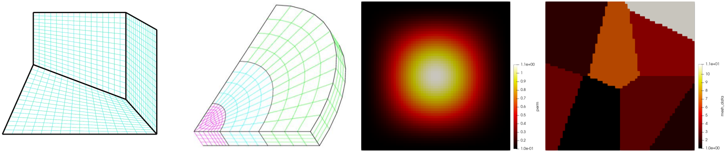

2. If patches are “similar enough,” why store and solve them multiple times?

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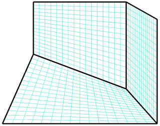
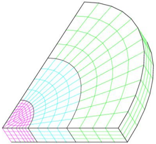
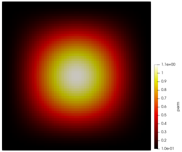
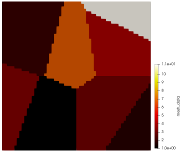

2. If patches are "similar enough," why store and solve them multiple times?

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

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- Criterion 1: $\mathcal{B}$ should approximate $\{A_i\}$ sufficiently well.
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Seek $\mathcal{B} = \{B_1, B_2, \ldots, B_{m_p}\}$ and mapping $\phi : \{1, \ldots, n_p\} \to \{1, \ldots, m_p\}$ minimizing

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

balancing efficiency and accuracy.

Also referred to as a **sparse approximation problem**.

Greedy Algorithm

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

Input: $\{A_1, A_2, \ldots, A_{n_p}\}$, ε
$\mathcal{B} := \{\}$, $\vec{\phi} = 0$
for $i = 1, \ldots, n_p$ **do**
    match:=false;
    for $j = 1, \ldots, m_p$ **do**
        if $\|I - A_i B_j^{-1}\|_2 < \varepsilon$ **then**
            match=true, $\phi(i) = j$, break;
        end if
    end for
    if match==false **then**
        append A_i to $\mathcal{B}$, $\phi(i) = |\mathcal{B}|$;
    end if
end for
Output: $\mathcal{B} = \{B_1, B_2, \ldots, B_{m_p}\}$, $\vec{\phi}$

← check patch against database

← if no matches, store patch explicitly

Greedy Local Error Bounds

Bonus: $\|I - A_i B_{\phi(i)}^{-1}\| < \varepsilon$, ensures solver quality. If

$$A_i x = v, \tag{4}$$

then approximating $B_{\phi(i)} y = v$ yields

$$\begin{aligned} \|x - y\| &= \|A_i^{-1} v - B_{\phi(i)}^{-1} v\| \\ &= \|A_i^{-1}(I - A_i B_{\phi(i)}^{-1}) v\| \\ &< \varepsilon \|A_i^{-1}\| \|v\|. \end{aligned} \tag{5}$$

*then extend to the global problem

Clustering Algorithm

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

Input: $\{A_1, A_2, \ldots, A_{n_p}\}$, m_p ← choose number of clusters
$\vec{\phi} = \text{randperm}(n_p, m_p)$;
$B_i = A_{\phi(i)}$, $i = 1, \ldots, m_p$;
while not converged **do**
  for $i = 1, \ldots, n_p$ **do**
    for $j = 1, \ldots, m_p$ **do**
      $d_{ij} = d(A_i, B_j)$; ← $d(A_i, B_j) = \|I - A_i B_j^{-1}\|_2$
    end for
    $\phi(i) = \text{argmin}_j(d_{ij})$;
  end for
  $B_i = \frac{1}{n_i} \sum_{j \text{ in cluster } i} A_j$, $i = 1, \ldots, m_p$; *treat boundaries separately!
end while
Output: $\mathcal{B} = \{B_1, B_2, \ldots, B_{m_p}\}$, $\vec{\phi}$

Clustering Local Error Bounds

For clustering, the idea is similar. However, $d(A_i, B_{\phi(i)}) := \|(I - A_i B_{\phi(i)}^{-1}\|$ is not bounded a priori.

$$\begin{aligned} \|x - y\| &= \|A_i^{-1} v - B_{\phi(i)}^{-1} v\| \\ &= \|A_i^{-1}(I - A_i B_{\phi(i)}^{-1}) v\| \\ &< \max_i d(A_i, B_{\phi(i)}) \|A_i^{-1}\| \|v\|. \end{aligned} \tag{6}$$

may be bounded by cluster diameters.

Clustering Variations

There are a number of different ways to approach clustering.

1. **Entrywise** k**-means** $d(A_i, B_j) = \|A_i - B_j\|_{\ell_1}$,
   B_j^{-1} = inverse of entrywise cluster average.
2. **Spectral** k**-means** $d(A_i, B_j) = \|I - A_i B_j^{-1}\|_2$,
   B_j^{-1} = inverse of entrywise cluster average.
3. **Variance-minimizing clustering** $d(A_i, B_j) = \|I - A_i B_j^{-1}\|_2$,
   B_j^{-1} = inverse of member minimizing in-cluster variance.

Bootstrapped Algorithm

"But clustering is slow!"

Make it faster by bootstrapping:

1. Run Algorithm 1, obtain $\mathcal{B}$
2. Initialize Algorithm 2 clustering with $\mathcal{B}$
3. Do very few iterations of Algorithm 2

Pros:

- Better database assignments than Algorithm 1
- Faster time to result than Algorithm 2

Cons:

- More complex
- Slower than Algorithm 1

Poisson Equation

$$-\nabla \cdot (\rho(x, y)\nabla u) = f. \tag{7}$$

Dirichlet BCs, $p = 2, 3, 4, 5$ FEMs, uniform grid, solution

$$u = \sin(\pi x)\sin(\pi y)$$

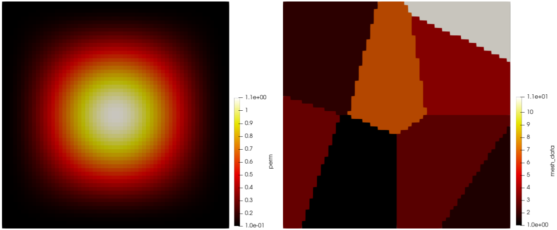

Figure: (left) smooth coefficient, (right) piecewise discontinuous coefficient.
Not pictured: constant coefficient

Timing Results

Configuration: $\rho = 1$ Poisson, $20 \times 20 \times 20$ grid, $p = 5$
GMRES with 10^{-7} tolerance, $\varepsilon = 10^{-7}$, $|\mathcal{B}| = 8000, 27$.
Implemented in **Trilinos/Ifpack2** as a preconditioner using LAPACK GETRF, GETRS. Used as additive Schwarz inner solve. Compress if $\|A_i - B_j\|_{\ell_1} < \varepsilon$. 39 iterations.

Configuration ($N = 5$) runs	Setup (s) mean$\pm$std	Apply (s) mean$\pm$std	Storage
No compression	269.52 ± 1.46	39.10 ± 0.46	2.8GB
Compression	253.12 ± 0.61	28.87 ± 0.047	9.6MB $+$ 62.5KB

Single node of Attaway supercomputer, Intel Xeon Gold 6140 Processor. Cache size is 24.75MB.

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Jacobi would cost 7.9MB.

Burgers' Equation

$$\frac{du}{dt} + \nabla \cdot \left(\frac{1}{2}\vec{\nu}u^2 - g(u)\nabla u \right) = f, \qquad (8)$$

where $\vec{\nu} = [1,1]^T$, g is nonlinear entropy-viscosity term, and SUPG stabilization is utilized in the discretization. 100×100 grid.

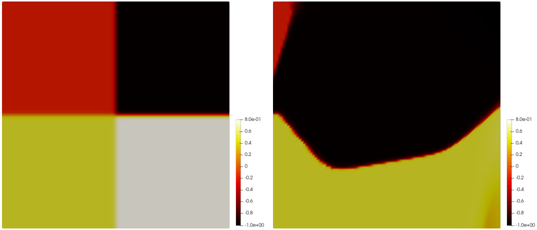
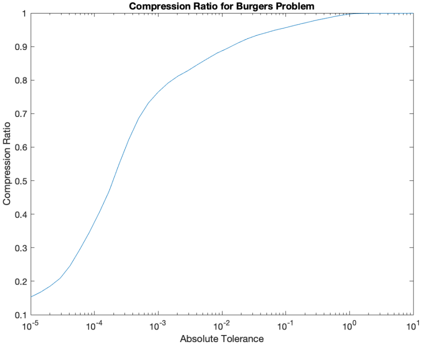


Figure: (left) $t = 0$ starting profile for Burgers' equation (right) $t = 1$ end profile for Burgers' equation

Burgers' Equation

Plotting greedy algorithm $\frac{n_p - |B|}{n_p}$ against ε shows it's compressible.



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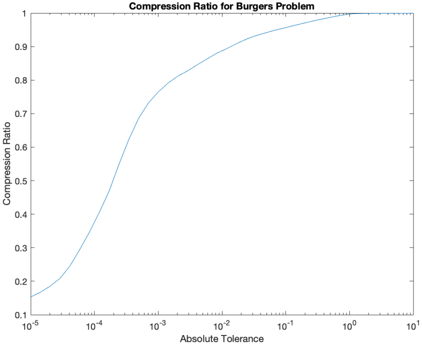
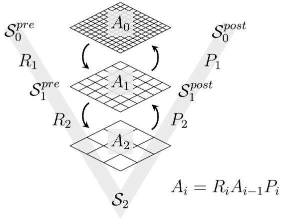


Algorithm\Database Size	10000	371	293	213	146	76	25	13
Greedy Tolerance 1	224	240	310	238	278	463	829	882
Entrywise k-means	224	342	343	377	317	353	416	420

Poisson Multigrid Method

We use the following multigrid configuration for Poisson:

- $\omega = 0.5$,
- $(\nu_1, \nu_2) = (1, 0)$,
- $N = 2$ V-cycle levels,
- Case 1: P uniform linear interp.
  Case 2: P from Ruge-Stüben AMG
- $R = P^T$, $A_c = RAP$



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

Results (Smooth Permeability, Linear P)

	Algorithm\Database Size	3600	74	35	18	15	13	7	6
$p=2$	Greedy Tolerance 1	11	12	13	14	17	26	61	68
	Spectral k-means 3	11	12	12	14	16	17	–	–
	Var-Minimizing Clustering	11	12	12	13	14	15	–	–
	Entrywise k-means	11	11	12	12	14	16	–	–
$p=3$	Algorithm\Database Size	3600	71	34	18	15	13	8	6
	Greedy Tolerance 1	12	13	13	15	18	26	58	69
	Spectral k-means 3	12	12	12	15	17	18	–	–
	Var-Minimizing Clustering	12	12	12	13	14	15	–	–
	Entrywise k-means	12	12	12	12	14	16	–	–
$p=4$	Algorithm\Database Size	3600	71	34	18	15	13	8	7
	Greedy Tolerance 1	14	14	15	17	20	29	68	67
	Spectral k-means 3	14	14	14	17	19	20	–	–
	Var-Minimizing Clustering	14	14	14	15	16	17	–	–
	Entrywise k-means	14	14	14	14	16	18	–	–
$p=5$	Algorithm\Database Size	3600	73	35	18	15	13	9	7
	Greedy Tolerance 1	15	16	17	19	22	32	78	76
	Spectral k-means 3	15	16	16	19	21	22	–	–
	Var-Minimizing Clustering	15	15	16	17	18	19	–	–
	Entrywise k-means	15	15	15	16	18	20	–	–

Results (Piecewise Constant Permeability, Linear P)

	Algorithm\Database Size	3600	131	113	96	52	25	5	3
$p=2$	Greedy Tolerance 1	11	12	12	14	17	22	47	52
	Spectral k-means 3	11	17	19	19	26	27	–	–
	Var-Minimizing Clustering	11	20	20	20	29	31	–	–
	Entrywise k-means	11	12	17	17	26	31	–	–
	Algorithm\Database Size	3600	131	114	100	59	32	8	5
$p=3$	Greedy Tolerance 1	12	12	13	14	17	26	48	50
	Spectral k-means 3	12	20	26	26	34	35	–	–
	Var-Minimizing Clustering	12	24	24	24	32	32	–	–
	Entrywise k-means	12	13	19	19	29	33	–	–
	Algorithm\Database Size	3600	130	114	103	70	36	12	9
$p=4$	Greedy Tolerance 1	14	14	15	15	19	28	51	53
	Spectral k-means 3	14	23	32	32	33	38	36	–
	Var-Minimizing Clustering	14	27	27	27	27	38	37	–
	Entrywise k-means	14	16	22	22	22	35	37	–
	Algorithm\Database Size	3600	130	116	103	78	38	15	10
$p=5$	Greedy Tolerance 1	15	16	16	17	21	29	60	64
	Spectral k-means 3	15	25	35	30	35	40	43	39
	Var-Minimizing Clustering	15	28	28	54	47	40	40	44
	Bootstrapped Var-Minimizing	15	16	16	17	22	26	44	39
	Entrywise k-means	15	18	25	25	25	38	40	38

Maxwell's Equations, Distorted Mesh

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$$-\nabla \times \nabla \times \mathbf{u} - \sigma \mathbf{u} = \mathbf{f}. \tag{9}$$

where $\sigma = 10^{-4}$. Arnold-Falk-Winther patches are utilized. $30 \times 30 \times 30$ grid, $29^3 = 24389$ patches. Perturbed structured grid

$$\begin{aligned} x &= \hat{x} + 0.6\sin(\pi\hat{x}/2)\sin(\pi\hat{y}/2)\sin(\pi\hat{z}/2), \\ y &= \hat{y} + 0.6\cos(\pi\hat{x}/2)\cos(\pi\hat{y}/2)\cos(\pi\hat{z}/2), \\ z &= \hat{z} + 0.6\cos(\pi\hat{x}/2)\cos(\pi\hat{y}/2). \end{aligned} \tag{10}$$

Solution

$$\mathbf{u} = \begin{bmatrix} \sin(\pi x)\sin(\pi y) \\ y \\ z \end{bmatrix}.$$

Results (Maxwell's Equations, Distorted Mesh)

Unrestarted GMRES, relative tolerance 10^{-6}, initial guess $10^2 x + 10y + z$.
2-level MG, two sweeps as a pre-smoother with a damping parameter $\omega = 0.7$.

Case 1: linear interp. P (ignoring distortion)

Algorithm\Database Size	24389	361	129	43	16
Greedy Tolerance 1	33	34	34	35	DNC
Spectral k-means 3	33	33	DNC	DNC	DNC

Case 2: Ruge-Stüben AMG

Algorithm\Database Size	24389	361	129	43	16
Greedy Tolerance 1	56	57	58	60	DNC
Spectral k-means 3	56	57	DNC	DNC	DNC

Results (Database Mappings)

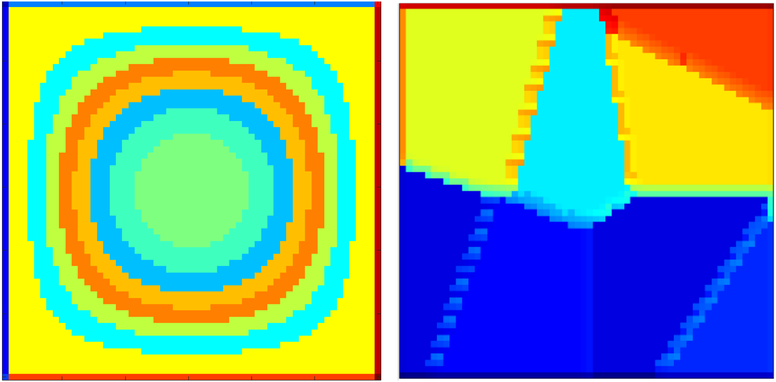


Figure: Visualization of database ϕ mapping. (left) clustering algorithm on smooth permeability, (right) greedy algorithm on piecewise constant permeability

Results (Other Visualization)

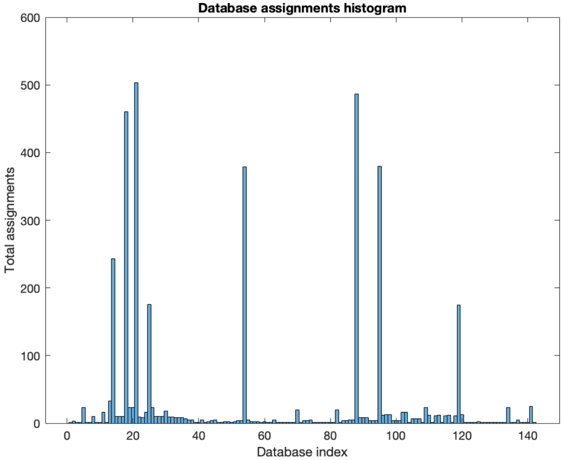


Figure: Database assignments for piecewise discontinuous problem, $\varepsilon = 10^{-7}$

Conclusion

Takeaways:

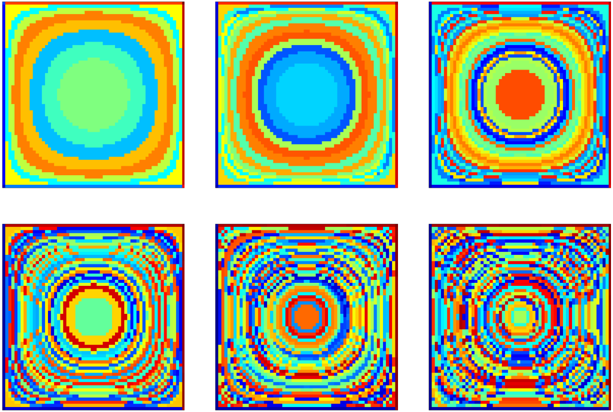
- Memory cost $= \mathcal{O}(\text{Jacobi})$
- Faster apply than without database
- Generalizes for any structure detection method

Current/Future Work:

- Utilize Kokkos, not LAPACK
- Time-dependent problems
- Ridzal's LDRD: R-adaptivity to detect and enhance compressibility
- Unsupervised deep learning

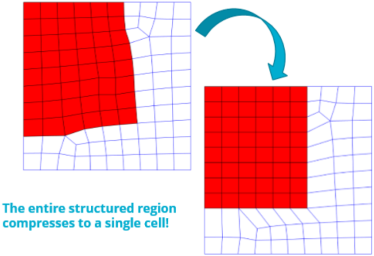
Thank You

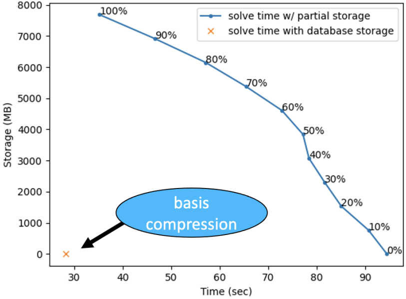
- Questions?



Supplemental Slides

R-adaptivity refers to moving mesh nodes.
We're interested in the following scenario:





for finite element basis reuse. This also results in patch reuse.

Supplemental Slides

Preliminary investigations by summer students Nichole Etienne (Emory) and Eugene Agyei-Kodie (Michigan State) on different clustering approaches