Development of a Terrestrial Dynamical Core for E3SM (TDycore)

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Tale of Two Talks

Common Theme: Considerations in choosing a discretization method

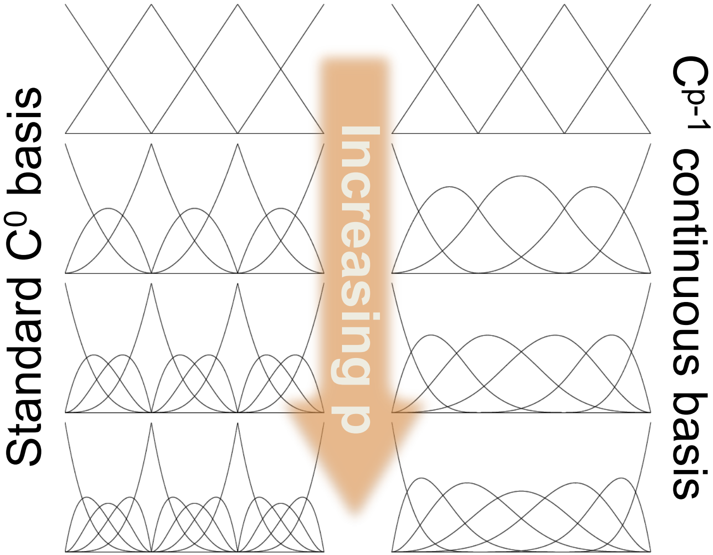
I. The Effect of a Higher Continuous Basis on Solver Performance

Victor Calo (Curtin), David Pardo (Ikerbasque), Lisandro Dalcin (KAUST), Maciej Paszynski (AGH)

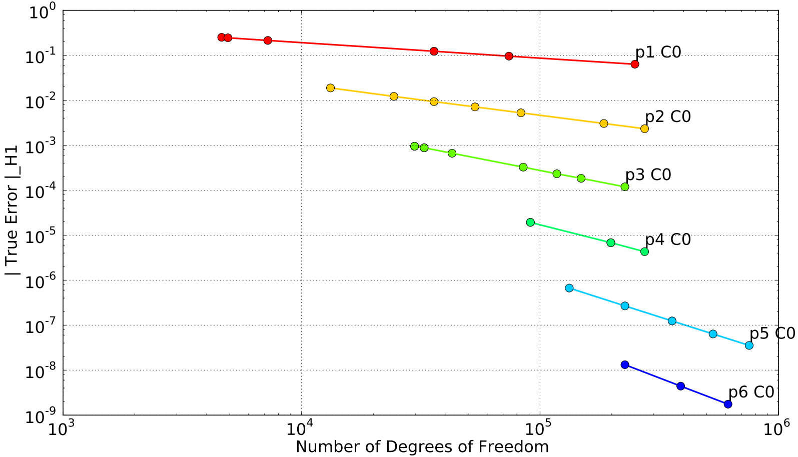
II. Selection of a Numerical Method for a Terrestrial Dynamical Core

Jed Brown (Colorado), Gautam Bisht (PNNL), Matthew Knepley (Buffalo), Jennifer Fredrick (SNL), Glenn Hammond (SNL), Satish Karra (LANL)

Higher Continuous Basis?



Poisson problem on unit cube



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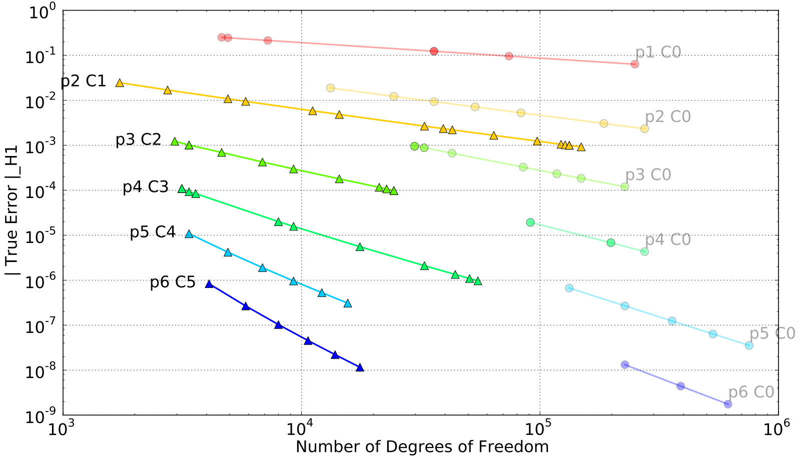


Are higher continuous spaces an efficient way to $p-$refine?

What effect does continuity have on the solver performance?

Are higher continuous spaces an efficient way to $p-$refine?

What effect does continuity have on the solver performance?

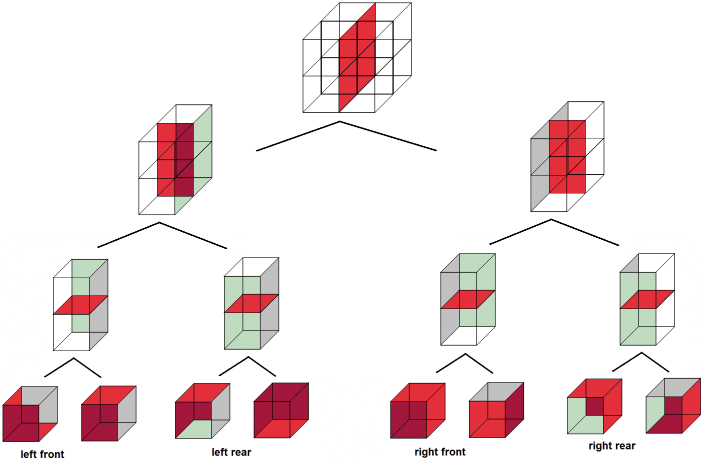
Spoiler Alert!

	C^0	C^{p-1}	C^{p-1}/C^0
Multifrontal direct solver	$\mathcal{O}(N^2 + Np^6)$	$\mathcal{O}(N^2 p^3)$	$\mathcal{O}(p^3)$
Iterative solvers*	$\mathcal{O}(Np^4)$	$\mathcal{O}(Np^6)$	$\mathcal{O}(p^2)$

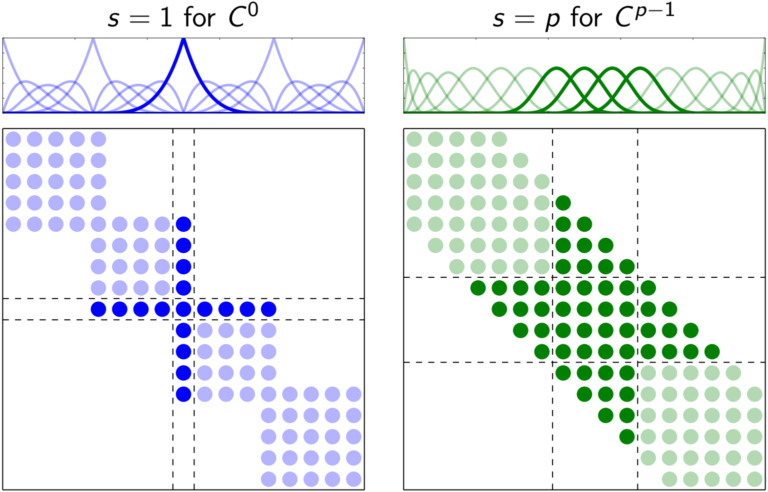
*Estimates for Matrix-Vector products

Multi-frontal direct solver

Based on the concepts of the Schur complement and nested dissection.

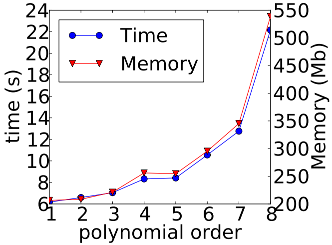


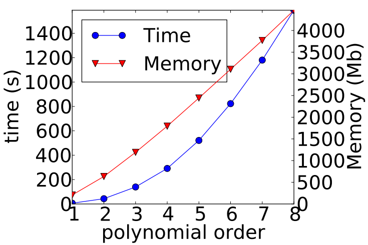
Key concept: size s of the separator



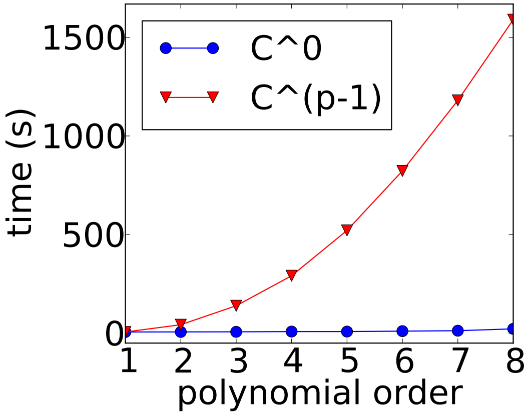
Estimates and Results ($d = 3$, $N = 30k$)

	C^0	C^{p-1}
Time	$\mathcal{O}(N^2 + Np^6)$	$\mathcal{O}(N^2 p^3)$
Memory	$\mathcal{O}(N^{4/3} + Np^3)$	$\mathcal{O}(N^{4/3} p^2)$





Solution time for C^0 vs C^{p-1} $(d = 3, N = 30k)$



Iterative solvers

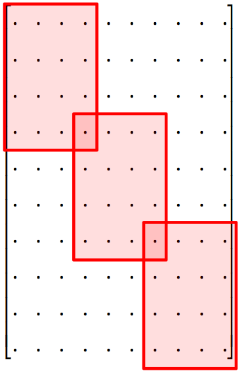
Much more complex to assess costs:

$$P\,(Ax - b) = 0$$

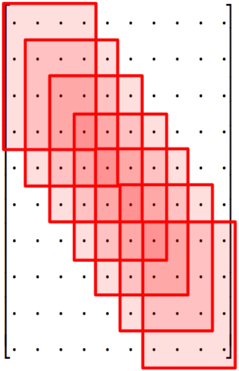
Need a model for:

- Matrix-vector multiplication
- Preconditioner (P) setup and application
- Convergence

Sample Linear Systems



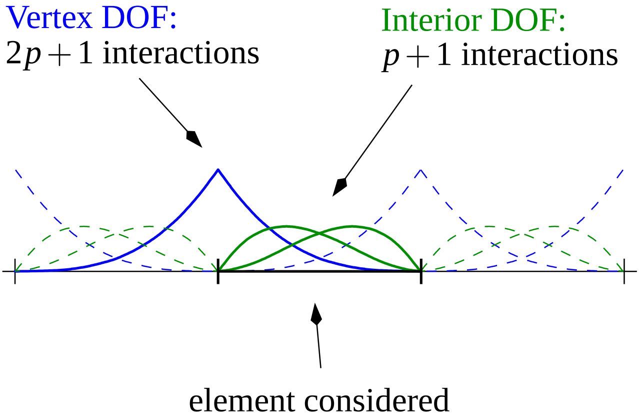
C^0 space



C^{p-1} space

Matrix-vector multiplication - C^0

The cost of a sparse matrix-vector multiply is proportional to the number of nonzero entries in the matrix.



Matrix-vector multiplication - C^0

Dimension	Entity	Number of Entities	DOFs per Entity	Number of interactions
1D	vertex	1	1	$(2p+1)$
1D	interior	1	$(p-1)$	$(p+1)$
2D	vertex	1	1	$(2p+1)^2$
2D	edge	2	$(p-1)$	$(2p+1)(p+1)$
2D	interior	1	$(p-1)^2$	$(p+1)^2$
3D	vertex	1	1	$(2p+1)^3$
3D	edge	3	$(p-1)$	$(2p+1)^2(p+1)$
3D	face	3	$(p-1)^2$	$(2p+1)(p+1)^2$
3D	interior	1	$(p-1)^3$	$(p+1)^3$

Matrix-vector multiplication - C^0

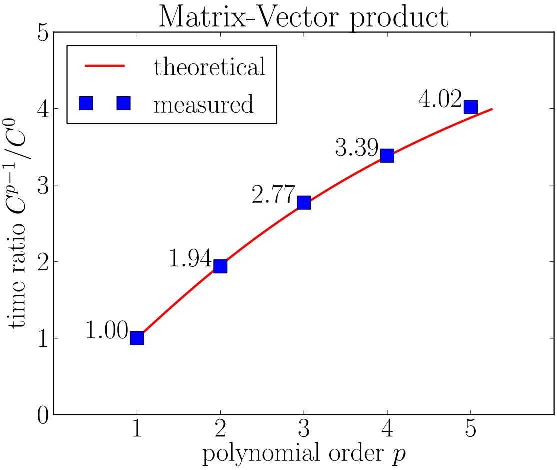
$$
\begin{aligned}
\text{nnz}^{C^0} &= \underbrace{(p-1)^3}_{\text{interior DOF}} \cdot (p+1)^3 \\
&+ \underbrace{3(p-1)^2}_{\text{face DOF}} \cdot (2p+1)(p+1)^2 \\
&+ \underbrace{3(p-1)}_{\text{edge DOF}} \cdot (2p+1)^2(p+1) \\
&+ \underbrace{1}_{\text{vertex DOF}} \cdot (2p+1)^3 \\
&= p^6 + 6p^5 + 12p^4 + 8p^3 \\
&= p^3(p+2)^3 = \mathcal{O}(p^6)
\end{aligned}
$$

Matrix-vector multiplication - C^{p-1}

The B-spline C^{p-1} basis is very regular, each DOF interacts with $2p+1$ others in 1D.

$$\text{nnz}^{C^{p-1}} = p^3(2p+1)^3 = 8p^6 + 12p^5 + 6p^4 + p^3 = \mathcal{O}(8p^6)$$

Matrix-vector multiplication



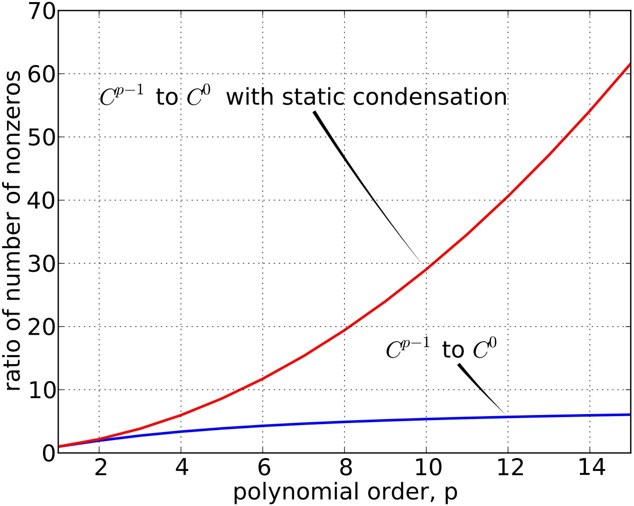
Matrix-vector multiplication

However, for C^0 spaces, we can use static condensation as in the multifrontal direct solver.

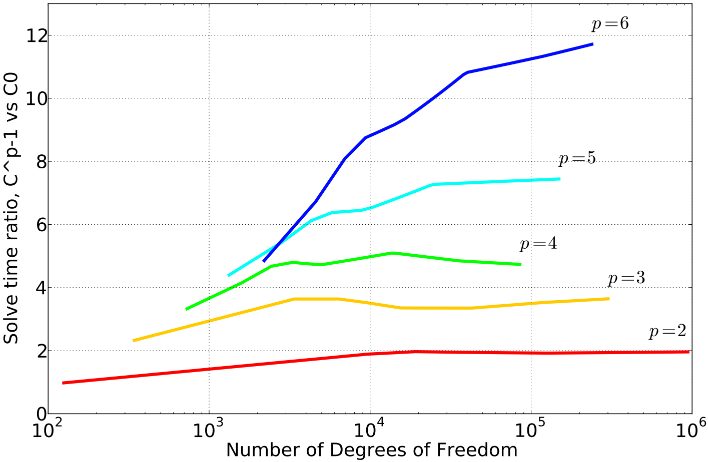
Entity	Number of Entities	DOFs per Entity	Number of interactions	Statically condensed
vertex	1	1	$(2p+1)^3$	$-8(p-1)^3$
edge	3	$(p-1)$	$(2p+1)^2(p+1)$	$-4(p-1)^3$
face	3	$(p-1)^2$	$(2p+1)(p+1)^2$	$-2(p-1)^3$

$$33p^4 - 12p^3 + 9p^2 - 6p + 3 = \mathcal{O}(33p^4)$$

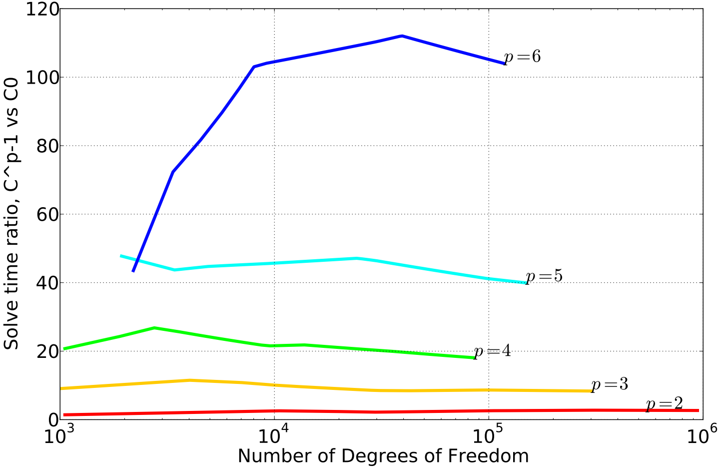
Matrix-vector multiplication



3D Poisson + CG + ILU



3D Poisson + CG + ILU + static condensation



Related Publications

- N Collier, D Pardo, L Dalcin, M Paszynski, VM Calo, The cost of continuity: A study of the performance of isogeometric finite elements using direct solvers, Computer Methods in Applied Mechanics and Engineering 213, 353-361, 2012. 10.1016/j.cma.2011.11.002
- N Collier, L Dalcin, D Pardo, VM Calo, The cost of continuity: performance of iterative solvers on isogeometric finite elements, SIAM Journal on Scientific Computing 35 (2), A767-A784, 2013. 10.1137/120881038
- N Collier, L Dalcin, VM Calo, On the computational efficiency of isogeometric methods for smooth elliptic problems using direct solvers, International Journal for Numerical Methods in Engineering 100 (8), 620-632. 10.1002/nme.4769

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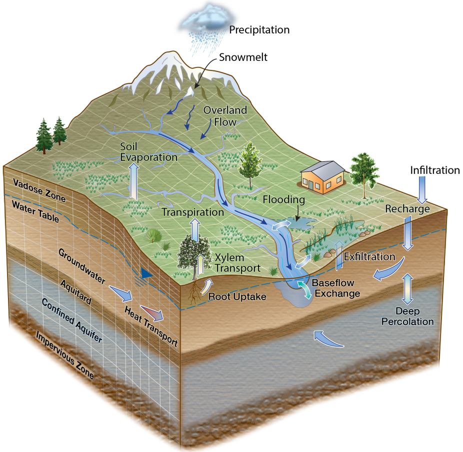
Energy Exascale Earth System Model (E3SM)

- The terrestrial water cycle is a key component of the Earth system model
- While conceptually key processes transport water laterally, the representation is 1D in current models
- Requirements: accurate velocities on distorted grids with uncertain and rough coefficients at global scale
- Naturally think of mixed finite elements



Simplified Problem Statement

Strong form Find $\mathbf{u}$ and p such that,

$$
\begin{aligned}
\mathbf{u} &= -K\nabla p && \text{in } \Omega \\
\nabla \cdot \mathbf{u} &= f && \text{in } \Omega \\
p &= g && \text{on } \Gamma_D \\
\mathbf{u} \cdot \mathbf{n} &= 0 && \text{on } \Gamma_N
\end{aligned}
$$

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Candidate approaches:

- Mixed finite elements (BDM) + FieldSplit/BDDC/hybridization
- Wheeler-Yotov (WY) + AMG
- Arnold-Boffi-Falk (ABF) + FieldSplit/BDDC/hybridization
- Multipoint flux approximation (MFPA) + AMG

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Weak form Find $\mathbf{u} \in \mathbf{V}$ and $p \in W$ such that,

$$\begin{aligned} \left(K^{-1}\mathbf{u}, \mathbf{v}\right) &= (p, \nabla\cdot\mathbf{v}) - \langle g, \mathbf{v}\cdot\mathbf{n}\rangle_{\Gamma_D}, && \mathbf{v} \in \mathbf{V} \\ (\nabla\cdot\mathbf{u}, w) &= (f, w), && w \in W \end{aligned}$$

where $\mathbf{V} = \{\mathbf{v} \in H^{\mathrm{div}}(\Omega) : \mathbf{v}\cdot\mathbf{n} = 0 \text{ on } \Gamma_N\}$, $W = L^2(\Omega)$

Problem statement

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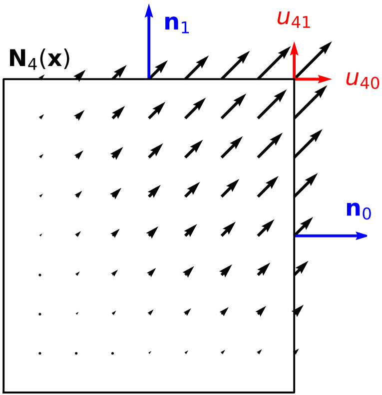
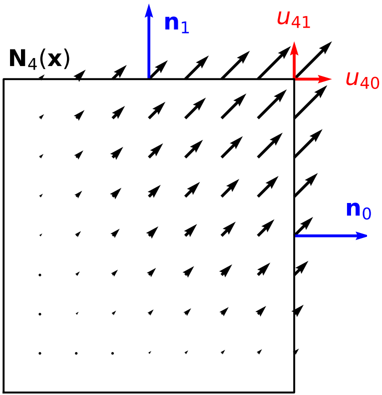
Wheeler & Yotov 2006



Ingredients:

- Brezzi–Douglas–Marini (BDM_1) velocity space
- Basis interpolatory at corners
  $\mathbf{N}_4(\mathbf{x}_4) \cdot \mathbf{n}_0 = u_{40}$
  $\mathbf{N}_4(\mathbf{x}_4) \cdot \mathbf{n}_1 = u_{41}$
- Vertex-based quadrature (under-integrated)
- Constant pressure space

Wheeler & Yotov 2006



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This means that velocity DOFs only couple to each other at vertices.

Wheeler & Yotov Assembly

for vertex v in mesh **do**
  setup vertex local problem
  $\begin{bmatrix} A & B^T \\ B & 0 \end{bmatrix} \begin{bmatrix} U \\ P \end{bmatrix} = \begin{bmatrix} G \\ F \end{bmatrix}$
  for element e connected to v **do**
    $A \leftarrow \left(K^{-1}\mathbf{u}_v, \mathbf{v}_v\right)_{\Omega_e}$
    $B^T \leftarrow -(p_e, \nabla \cdot \mathbf{v}_v)_{\Omega_e}$
    $G \leftarrow -\langle g, \mathbf{v}_v \cdot \mathbf{n}\rangle_{\Gamma_{D,e}}$
    $F \leftarrow (f_e, w_e)_{\Omega_e}$
  end for
  Assemble Schur complement
  $(BA^{-1}B^T)P = F - BA^{-1}G$
end for

Wheeler & Yotov Assembly

for vertex v in mesh **do**
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  end for
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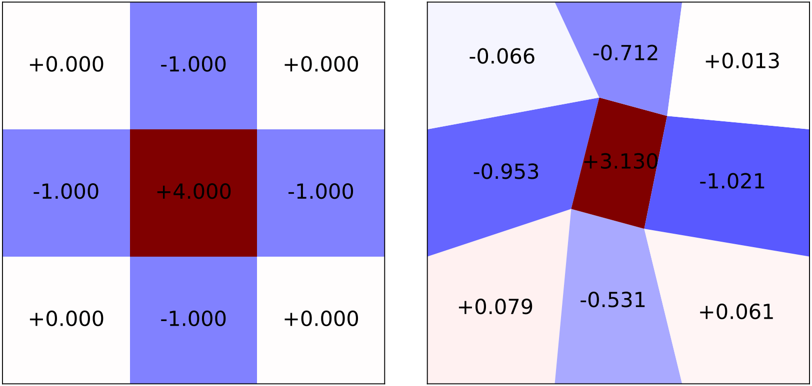
  $(BA^{-1}B^T)P = F - BA^{-1}G$
end for

Global cell-centered pressure system which is SPD

Sample Wheeler-Yotov Stencils

$$K = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



Sample Wheeler-Yotov Stencils

$$K = \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix}$$

+0.000	-1.000	+0.000
-3.000	+8.000	-3.000
+0.000	-1.000	+0.000

$$R_{10}\ K\ R_{10}^T$$

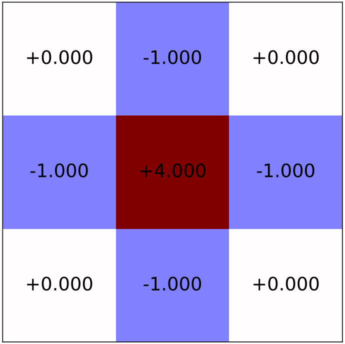
+0.133	-0.985	-0.209
-2.865	+7.850	-2.865
-0.209	-0.985	+0.133

$$R_{45}\ K\ R_{45}^T$$

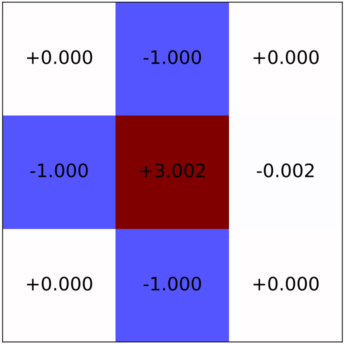
+0.250	-1.500	-0.750
-1.500	+7.000	-1.500
-0.750	-1.500	+0.250

Sample Wheeler-Yotov Stencils

$$K = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$



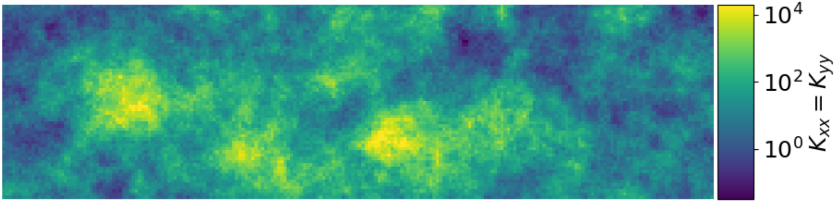
$$K \cdot (10^{-3} \text{ if } x > 2/3)$$



SPE10 Test Problem

We use the permeabilities from the SPE10 problem:

- $60 \times 220 \times 85 = 1{,}122{,}000$ cells
- Diagonal permeability $K_{xx} = K_{yy} \neq K_{zz}$
- We induce flow by Dirichlet conditions
- Solve on original permeabilities and also rotate around two axes



Sample slice of the permeability field

Solver Options

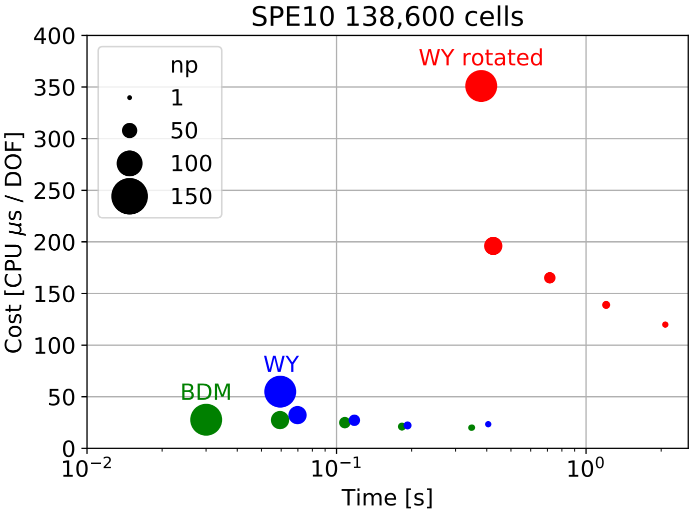
WY Options

```
-ksp_type cg
-pc_type hypre
```

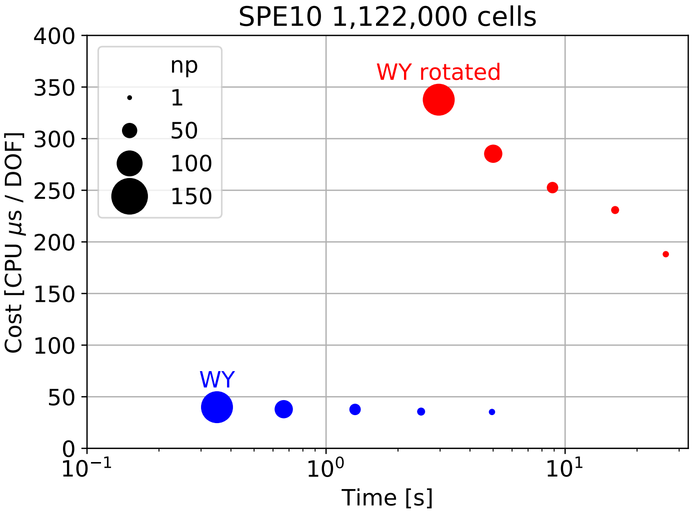
BDM Options

```
-ksp_type gmres
-pc_type fieldsplit
-pc_fieldsplit_type schur
-pc_fieldsplit_schur_fact_type full
-pc_fieldsplit_schur_precondition selfp
-fieldsplit_0_ksp_type cg
-fieldsplit_0_pc_type jacobi
-fieldsplit_1_ksp_type cg
-fieldsplit_1_pc_type hypre
```

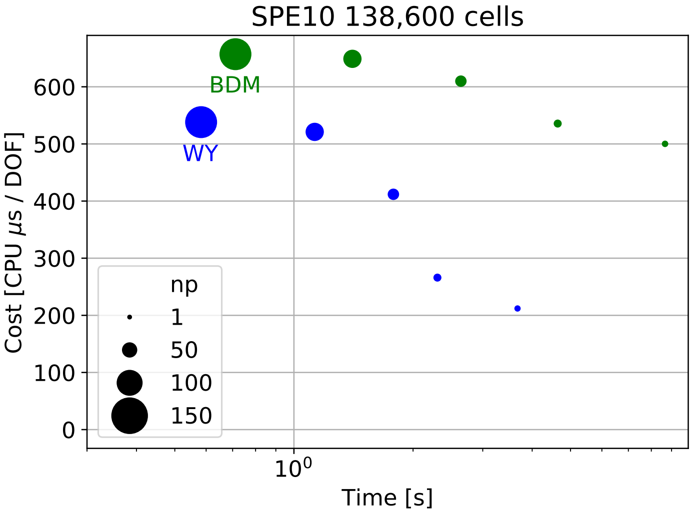
Solver Performance



Solver Performance



Assembly Performance (not optimized)



Concluding Remarks

TDycore:

- From limited results, WY approach is at least competitive although it appears to hit the strong scaling limit before BDM/fieldsplit
- BDM appears to use more memory than WY ($\approx$ 10 times)
- WY assembly is competitive although BDM lends itself to easier vectorization
- Experimentation is key: `-tdy_method {wy|bdm|...}`

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- WY assembly is competitive although BDM lends itself to easier vectorization
- Experimentation is key: `-tdy_method {wy|bdm|...}`

Talk/Meeting:

- All of the presented work uses PETSc (PetIGA + DMPlex/Section)
- Using DMPlex/Section opens doors for solver approaches
- Most of my exposure to solvers comes from using PETSc
- Originally exposed to PETSc ≈ 11 years ago at DOE ACTS workshops