A Scalable Parallel Implementation of Double Porosity/Permeability Model

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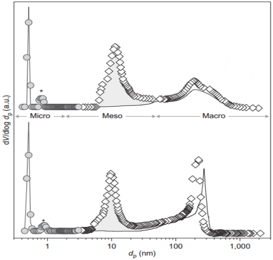
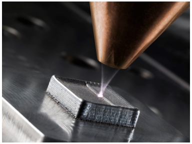
Motivation and insights
Materials with complex pore-networks

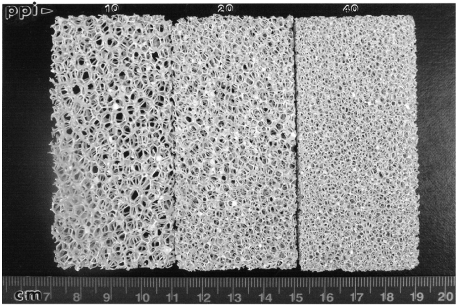
Flow in fissured rocks



[Mitchell et al., Nature Chemistry, 4:825-831, 2012]



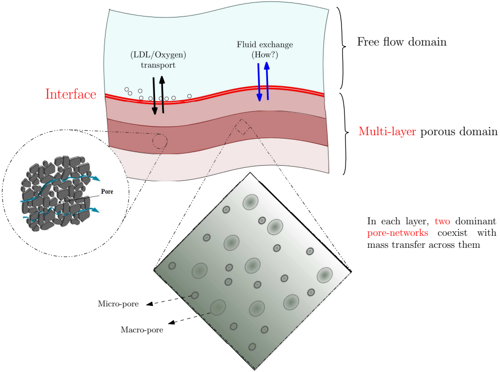
Additive manufacturing

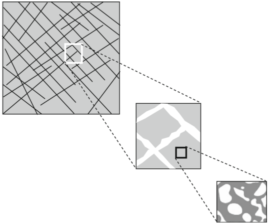


Next-generation biomedical implants

Complex physics of problem

Double porosity/permeability model





Microstructure of double porosity media

- Layered heterogeneity + coupled multi-pore networks
- system of coupled flow + transport

Scientific questions

- What **stabilized frameworks** are available for DPP?
- When you **scaled up the size** of problem, Which FEs to use?
- How to **precondition** large system of equations arises from DPP?

What flow model governs the domain?

Double porosity/permeability model (DPP)

- Formulated flow of a fluid through a porous medium for the first time.
- Barenblatt proposed the first DPP with a simple mass transfer model between networks.

Henry Darcy (1803–1858)

Macro-pore network

Balance of Linear Momentum

$$\mu \mathbf{K}_1^{-1}\mathbf{u}_1(\mathbf{x}) + \mathrm{grad}[p_1] = \gamma \mathbf{b}(\mathbf{x}) \quad \text{in } \Omega$$

Balance of Mass

$$\mathrm{div}[\mathbf{u}_1] = +\chi(\mathbf{x}) \quad \text{in } \Omega$$

Boundary conditions

$$\mathbf{u}_1(\mathbf{x}) \cdot \widehat{\mathbf{n}}(\mathbf{x}) = u_{n1}(\mathbf{x}) \quad \text{on } \Gamma_1^u$$

$$p_1(\mathbf{x}) = p_{01}(\mathbf{x}) \quad \text{on } \Gamma_1^p$$

Mass transfer

$$\chi(\mathbf{x}) = -\frac{\beta}{\mu}(p_1(\mathbf{x}) - p_2(\mathbf{x}))$$

Micro-pore network

Balance of Linear Momentum

$$\mu \mathbf{K}_2^{-1}\mathbf{u}_2(\mathbf{x}) + \mathrm{grad}[p_2] = \gamma \mathbf{b}(\mathbf{x}) \quad \text{in } \Omega$$

Balance of Mass

$$\mathrm{div}[\mathbf{u}_2] = -\chi(\mathbf{x}) \quad \text{in } \Omega$$

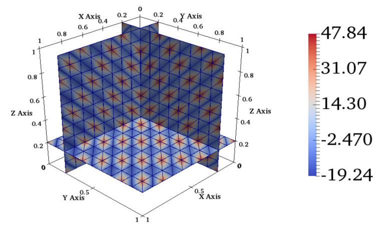
Boundary conditions

$$\mathbf{u}_2(\mathbf{x}) \cdot \widehat{\mathbf{n}}(\mathbf{x}) = u_{n2}(\mathbf{x}) \quad \text{on } \Gamma_2^u$$

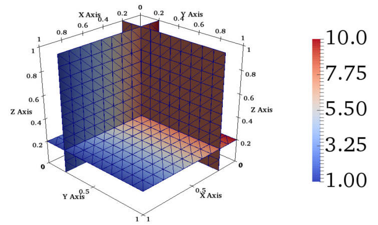
$$p_2(\mathbf{x}) = p_{02}(\mathbf{x}) \quad \text{on } \Gamma_2^p$$

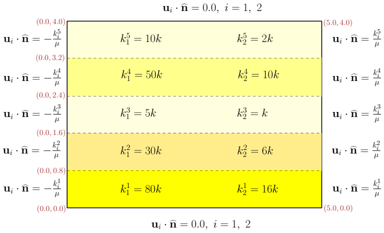
Numerical hurdles

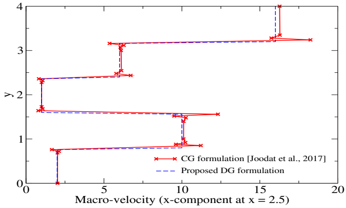
LBB violation and Gibbs phenomenon



Galerkin formulation with equal order interpolation, results in spurious oscillations in the pressure profile







Under the Galerkin formulation, Gibbs phenomenon is observed along the interfaces of the layers

Stabilized mixed DG formulation for DPP

$$\mathcal{B}_{\mathrm{DG}}^{\mathrm{stab}}(\mathbf{w_1}, \mathbf{w_2}, q_1, q_2; \mathbf{u_1}, \mathbf{u_2}, p_1, p_2) = \mathcal{L}_{\mathrm{DG}}^{\mathrm{stab}}(\mathbf{w_1}, \mathbf{w_2}, q_1, q_2)$$

The bilinear form:

$$\mathcal{B}_{\mathrm{DG}}^{\mathrm{stab}} := \mathcal{B}_{\mathrm{DG}} \boxed{- \frac{1}{2}\left(\mu k_1^{-1}\mathbf{w_1} - \mathrm{grad}[q_1]; \mu^{-1} k_1(\mu k_1^{-1}\mathbf{u_1} + \mathrm{grad}[p_1])\right) - \frac{1}{2}\left(\mu k_2^{-1}\mathbf{w_2} - \mathrm{grad}[q_2]; \mu^{-1} k_2(\mu k_2^{-1}\mathbf{u_2} + \mathrm{grad}[p_2])\right)}$$
$$\boxed{+ \eta_u h\left(\{\{\mu k_1^{-1}\}\}[\![\mathbf{w_1}]\!]; [\![\mathbf{u_1}]\!]\right)_{\Gamma^{\mathrm{int}}} + \eta_u h\left(\{\{\mu k_2^{-1}\}\}[\![\mathbf{w_2}]\!]; [\![\mathbf{u_2}]\!]\right)_{\Gamma^{\mathrm{int}}} + \frac{\eta_p}{h}\left(\{\{\mu^{-1} k_1\}\}[\![q_1]\!]; [\![p_1]\!]\right)_{\Gamma^{\mathrm{int}}} + \frac{\eta_p}{h}\left(\{\{\mu^{-1} k_2\}\}[\![q_2]\!]; [\![p_2]\!]\right)_{\Gamma^{\mathrm{int}}}}$$

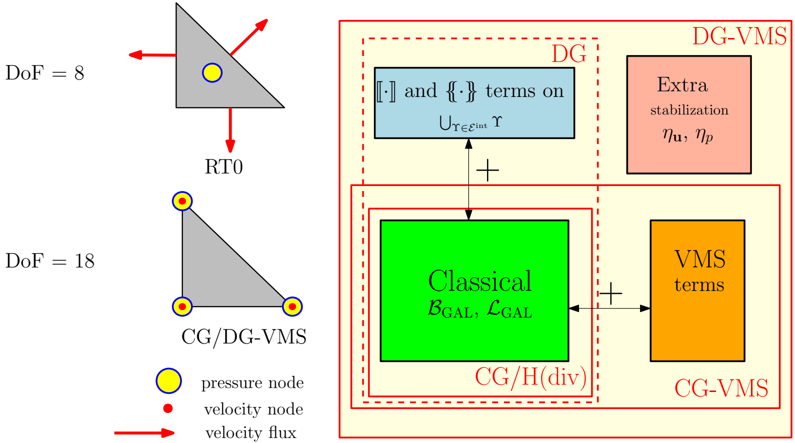
The linear functional:

$$\mathcal{L}_{\mathrm{DG}}^{\mathrm{stab}} := \mathcal{L}_{\mathrm{DG}} \boxed{- \frac{1}{2}\left(\mu k_1^{-1}\mathbf{w_1} - \mathrm{grad}[q_1]; \mu^{-1} k_1 \gamma \mathbf{b_1}\right) - \frac{1}{2}\left(\mu k_2^{-1}\mathbf{w_2} - \mathrm{grad}[q_2]; \mu^{-1} k_2 \gamma \mathbf{b_2}\right)}$$

$\mathcal{B}_{\mathrm{DG}}$ and $\mathcal{L}_{\mathrm{DG}}$: bilinear form and linear functional under conventional DG.

What are the available enriched FEs for DPP?

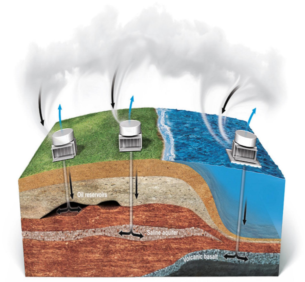
H(div) vs CG-VMS vs DG-VMS



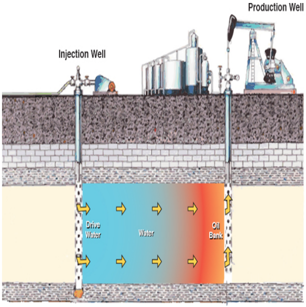
What is the best FEMs (H(div) or CG-VMS or DG-VMS) for DPP?

Real-life, large-scale problems

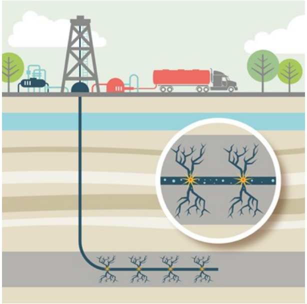
in subsurface flow and geophysical simulations



CO2 sequestration



Enhanced oil recovery



Hydraulic fracturing

- Large domains ($\sim$ 1km – $\sim$100km), multiscale, multiphysics couplings.
- High performance parallel processing are required for solving these problems.
- **Specialized iterative block solver methodologies are required.**

Composable block solvers I

Two approaches to effectively precondition large system of equations

Method 1: splitting by scales

$$\mathbf{K} = \begin{bmatrix} \mathbf{K}^1_{uu} & \mathbf{K}^1_{up} & 0 & 0 \\ \mathbf{K}^1_{pu} & \mathbf{K}^1_{pp} & 0 & \mathbf{K}^{12}_{pp} \\ 0 & 0 & \mathbf{K}^2_{uu} & \mathbf{K}^2_{up} \\ 0 & \mathbf{K}^{21}_{pp} & \mathbf{K}^2_{pu} & \mathbf{K}^2_{pp} \end{bmatrix} \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{p}_1 \\ \mathbf{u}_2 \\ \mathbf{p}_2 \end{pmatrix} = \begin{pmatrix} \mathbf{f}^1_u \\ \mathbf{f}^1_p \\ \mathbf{f}^2_u \\ \mathbf{f}^2_p \end{pmatrix}$$

$$\mathbf{A} := \begin{bmatrix} \mathbf{K}^1_{uu} & \mathbf{K}^1_{up} \\ \mathbf{K}^1_{pu} & \mathbf{K}^1_{pp} \end{bmatrix}, \quad \mathbf{B} := \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{K}^{12}_{pp} \end{bmatrix},$$

$$\mathbf{C} := \begin{bmatrix} 0 & 0 \\ 0 & \mathbf{K}^{21}_{pp} \end{bmatrix}, \quad \mathbf{D} := \begin{bmatrix} \mathbf{K}^2_{uu} & \mathbf{K}^2_{up} \\ \mathbf{K}^2_{pu} & \mathbf{K}^2_{pp} \end{bmatrix}$$

- **A** and **D** have similar compositions to classical mixed Poisson → Schur complement approach.
- Individually precondition the decoupled **A** and **D** blocks.

$$\mathbf{A}^{-1} = \begin{bmatrix} \mathbf{I} & -\left(\mathbf{K}^1_{uu}\right)^{-1}\mathbf{K}^1_{up} \\ 0 & \mathbf{I} \end{bmatrix} \begin{bmatrix} \left(\mathbf{K}^1_{uu}\right)^{-1} & 0 \\ 0 & \left(\mathbf{S}^1\right)^{-1} \end{bmatrix} \begin{bmatrix} \mathbf{I} & 0 \\ -\mathbf{K}^1_{pu}\left(\mathbf{K}^1_{uu}\right)^{-1} & \mathbf{I} \end{bmatrix}$$

$$\mathbf{D}^{-1} = \begin{bmatrix} \mathbf{I} & -\left(\mathbf{K}^2_{uu}\right)^{-1}\mathbf{K}^2_{up} \\ 0 & \mathbf{I} \end{bmatrix} \begin{bmatrix} \left(\mathbf{K}^2_{uu}\right)^{-1} & 0 \\ 0 & \left(\mathbf{S}^2\right)^{-1} \end{bmatrix} \begin{bmatrix} \mathbf{I} & 0 \\ -\mathbf{K}^2_{pu}\left(\mathbf{K}^2_{uu}\right)^{-1} & \mathbf{I} \end{bmatrix}$$

1. $\mathbf{K}^1_{uu}$, $\mathbf{K}^2_{uu}$ are mass matrices → ILU(0) to invert.
2. Precondition $\mathbf{S}^1$, and $\mathbf{S}^2$:

$$\mathbf{S}^1_p = \mathbf{K}^1_{pp} - \mathbf{K}^1_{pu}\mathrm{diag}\left(\mathbf{K}^1_{uu}\right)^{-1}\mathbf{K}^1_{up}$$

$$\mathbf{S}^2_p = \mathbf{K}^2_{pp} - \mathbf{K}^2_{pu}\mathrm{diag}\left(\mathbf{K}^2_{uu}\right)^{-1}\mathbf{K}^2_{up}$$

3. Apply multigrid V-cycle on $\mathbf{S}^1_p$ and $\mathbf{S}^2_p$ from the HYPRE BoomerAMG.
4. Single sweep of flexible GMRES to obtain the solution of full 4×4 block system.

Composable block solvers II

Method 2: splitting by fields

$$K = \begin{bmatrix} K^1_{uu} & 0 & K^1_{up} & 0 \\ 0 & K^2_{uu} & 0 & K^2_{up} \\ K^1_{pu} & 0 & K^1_{pp} & K^{12}_{pp} \\ 0 & K^2_{pu} & K^{21}_{pp} & K^2_{pp} \end{bmatrix} \begin{pmatrix} u_1 \\ u_2 \\ p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} f^1_u \\ f^2_u \\ f^1_p \\ f^2_p \end{pmatrix}$$

$$A := \begin{bmatrix} K^1_{uu} & 0 \\ 0 & K^2_{uu} \end{bmatrix}, \quad B := \begin{bmatrix} K^1_{up} & 0 \\ 0 & K^2_{up} \end{bmatrix},$$

$$C := \begin{bmatrix} K^1_{pu} & 0 \\ 0 & K^2_{pu} \end{bmatrix}, \quad D := \begin{bmatrix} K^1_{pp} & K^{12}_{pp} \\ K^{21}_{pp} & K^2_{pp} \end{bmatrix}$$

- The inverse of K is:

$$K^{-1} = \begin{bmatrix} I & -A^{-1}B \\ 0 & I \end{bmatrix} \begin{bmatrix} A^{-1} & 0 \\ 0 & S^{-1} \end{bmatrix} \begin{bmatrix} I & 0 \\ -CA^{-1} & I \end{bmatrix}.$$

1. A is mass matrix → use ILU(0).
2. Precondition S^{-1} by employing diagonal mass-lumping of A:

$$\begin{aligned} S_p &= D - C\mathrm{diag}(A)^{-1} B \\ &= \begin{bmatrix} K^1_{pp} - K^1_{pu}\mathrm{diag}(K^1_{uu}) K^1_{up} & K^{12}_{pp} \\ K^{21}_{pp} & K^2_{pp} - K^2_{pu}\mathrm{diag}(K^2_{uu}) K^2_{up} \end{bmatrix} \end{aligned}$$

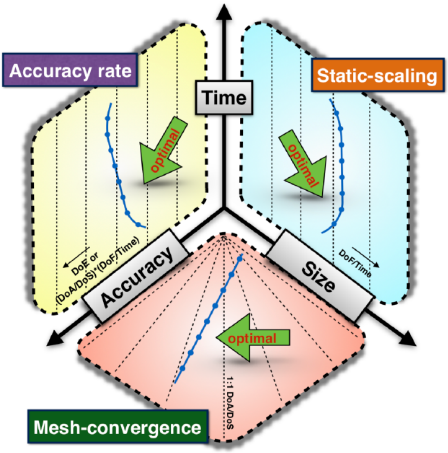
3. Apply V-cycle on each diagonal block.
4. Single sweep of flexible GMRES to obtain the solution of full system.

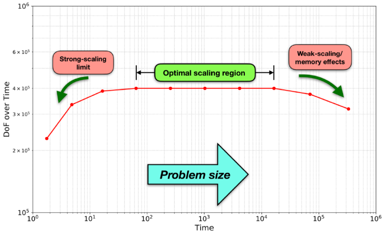
Which method performs better?

How to gauge parallel performance and scalability?

Performance spectrum modeling

(Time-Accuracy-Size) TAS model





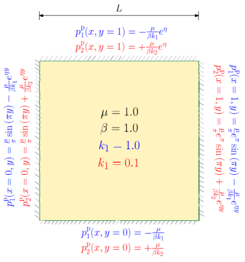
METRICS:

- Parallel efficiency $= \frac{Time_1}{Time_p \times \# MPIprocessors}\%$
- *Digits of Accuracy* DoA$:=-\log_{10}(L_2^{\mathrm{norm}})$
  Digits of Size DoS$:=-\log_{10}(DoF)$
- *Digits of Efficacy*
  DoE$:=-\log_{10}(L_2^{\mathrm{norm}} \times Time)$

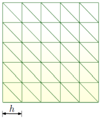
Numerical results
2D/3D DPP problems with analytical solution

We used the composable solvers feature in *PETSc* and the FE libraries under the *Firedrake Project*.

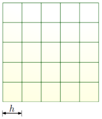
Method of manufactured solutions:



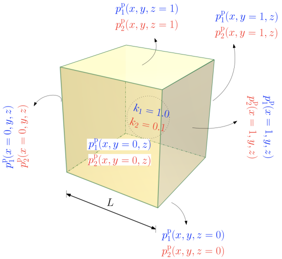
(a) Schematic



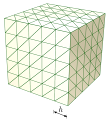
(b) TRI mesh



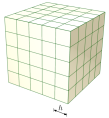
(c) QUAD mesh



(a) Schematic



(b) TET mesh

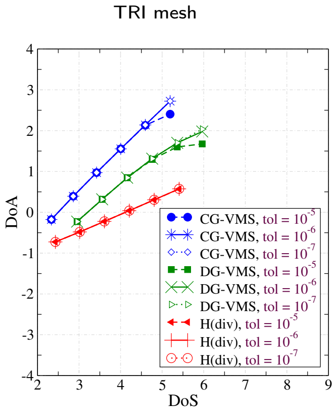


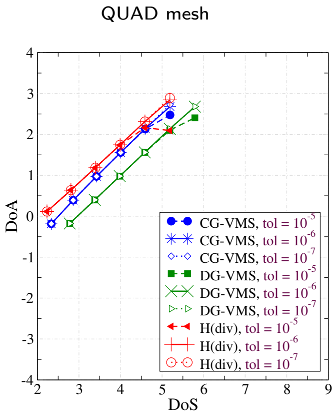
(c) HEX mesh

What is the best FEMs (H(div) or CG-VMS or DG-VMS)?
We use TAS model

FEs comparison (mesh convergence)

Macro-velocity field





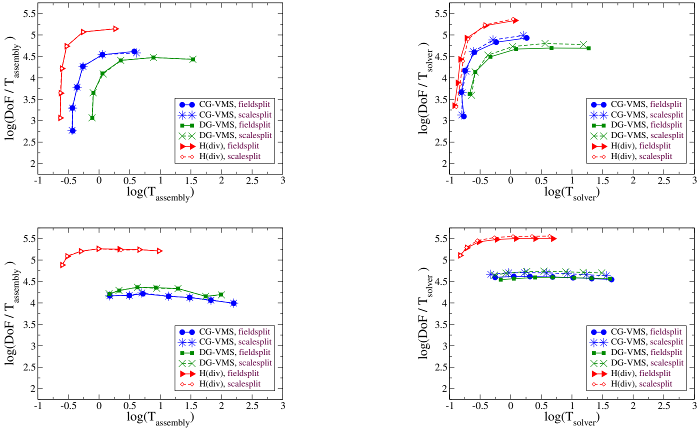
- VMS slope ≈ 1. H(div) slop ≈ 0.5
- Numerical accuracy: VMS > H(div)

- VMS slope ≈ 1.
- H(div) shows super. conv. close ≈ 1.
- Numerical accuracy: VMS $\gtrapprox$ H(div).

- Tight solver tol is needed to avoid flattening out.
- Same pattern obsereved for $\mathbf{u_2}$,p_1, and p_2.

FEs comparisons (static scaling results)

2D vs 3D for simplicial elements



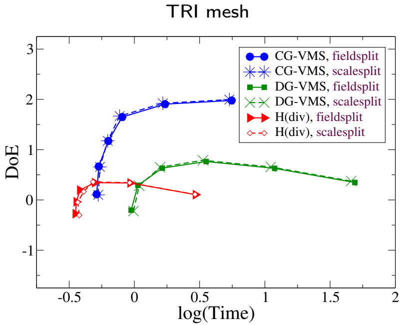
2D ←

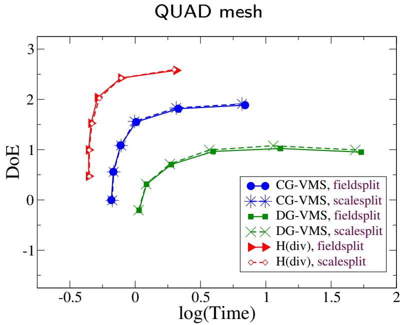
3D ←

- H(div) formulation processes its DoF count faster than either of the VMS formulations.
- Assembly algorithm in 2D vs 3D

FEs comparisons (Digits of Efficacy)

Macro velocity





- DoE: CG-VMS $\gg$ DG-VMS > H(div).
- DoE: H(div) > CG-VMS > DG-VMS.

Solver strategies comparisons (Strong-scaling @ 200K DoF)

Field-splitting | Scale-splitting

H(div)

No. of MPI proc.	Field-splitting: Time Assembly	Solver	Total	KSP	Parallel eff. (%)	Scale-splitting: Time Assembly	Solver	Total	KSP	Parallel eff. (%)
1	9.11E-01	6.62E-01	1.57E+00	15	100	9.14E-01	6.19E-01	1.53E+00	15	100
2	6.25E-01	5.20E-01	1.15E+00	16	68.7336	6.07E-01	4.92E-01	1.10E+00	16	69.8543
4	4.10E-01	3.51E-01	7.60E-01	16	51.7627	4.25E-01	3.36E-01	7.61E-01	16	50.4008
8	3.63E-01	2.70E-01	6.33E-01	16	31.092	3.81E-01	2.83E-01	6.63E-01	16	28.9085
12	3.87E-01	3.04E-01	6.90E-01	16	18.9986	3.36E-01	2.68E-01	6.04E-01	16	21.168
16	3.63E-01	3.00E-01	6.62E-01	16	14.8513	3.82E-01	2.73E-01	6.55E-01	16	14.6352

CG-VMS

No. of MPI proc.	Field-splitting: Time Assembly	Solver	Total	KSP	Parallel eff. (%)	Scale-splitting: Time Assembly	Solver	Total	KSP	Parallel eff. (%)
1	1.23E+01	5.01E+00	1.73E+01	13	100	1.25E+01	4.14E+00	1.66E+01	13	100
2	7.95E+00	3.39E+00	1.13E+01	15	76.455	7.84E+00	2.80E+00	1.06E+01	15	77.9605
4	4.81E+00	1.99E+00	6.80E+00	15	63.7406	4.84E+00	1.64E+00	6.48E+00	15	64.0244
8	3.16E+00	1.26E+00	4.42E+00	16	49.0052	3.32E+00	1.11E+00	4.43E+00	16	46.8009
12	2.99E+00	1.06E+00	4.05E+00	16	35.6702	2.90E+00	9.59E-01	3.86E+00	16	35.8439
16	2.42E+00	9.54E-01	3.38E+00	16	32.1111	2.44E+00	8.38E-01	3.28E+00	16	31.6313

DG-VMS

No. of MPI proc.	Field-splitting: Time Assembly	Solver	Total	KSP	Parallel eff. (%)	Scale-splitting: Time Assembly	Solver	Total	KSP	Parallel eff. (%)
1	8.08E+00	5.40E+00	1.35E+01	19	100	7.81E+00	4.11E+00	1.19E+01	19	100
2	4.76E+00	8.27E+00	1.30E+01	79	51.7268	4.57E+00	6.62E+00	1.12E+01	79	53.2618
4	2.55E+00	5.45E+00	7.99E+00	102	42.1566	2.54E+00	4.43E+00	6.97E+00	102	42.7301
8	1.91E+00	3.37E+00	5.27E+00	109	31.9492	1.85E+00	2.88E+00	4.73E+00	109	31.5077
12	1.98E+00	2.69E+00	4.67E+00	111	24.0646	1.88E+00	2.36E+00	4.24E+00	111	23.4498
16	1.61E+00	2.52E+00	4.13E+00	119	20.4045	1.61E+00	2.26E+00	3.87E+00	119	19.2556

All tables: TET mesh.

- Scale-splitting methodology slightly more efficient in terms of time-to-solution.
- Both methods have same KSP counts.

Concluding remarks:

- Proposed a framework for performance analysis of various “enriched FEs” for the DPP model.
- The VMS formulations yield much higher overall numerical accuracy for all velocity and pressure fields.
- Type of mesh (simplicial or non-simplicial) affects the digits of efficacy.
- Regardless of mesh type, DoFs are processed the fastest under the H(div) formulation compared to other formulations.
- Both composable solvers are scalable in both parallel and algorithmic senses.
- Both solvers exert similar overall effects on performance metrics.

Dissemination of this work

- M. S. Joshaghani, J. Chang, K. B. Nakshatrala, and M. G. Knepley, "*On composable block solvers and performance spectrum analysis for double porosity/permeability model*," Journal of Computational Physics, 2019.
- M. S. Joshaghani, S. H. Joodat, and K. B. Nakshatrala, "*A stabilized mixed discontinuous Galerkin formulation for double porosity/permeability model*," Tentatively accepted in Computer Methods in Applied Mechanics and Engineering, 2019.

Thank you

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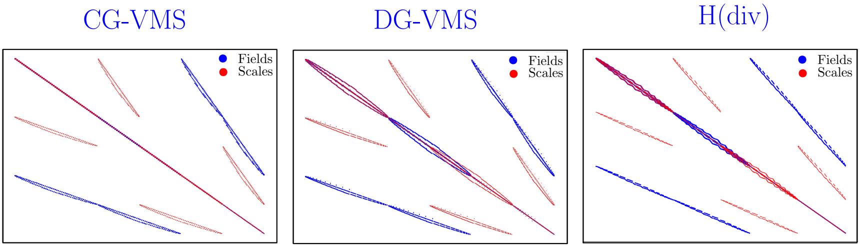
Field-splitting vs Scale-splitting

Global matrix with DoF=1k



- Smaller bandwidth in scale-split method → better performance wrt time.
- The sparsity pattern of the subblocks → the performance differences of solvers.