



Block Algebraic Multigrid Method for saddle-point problems of various physics

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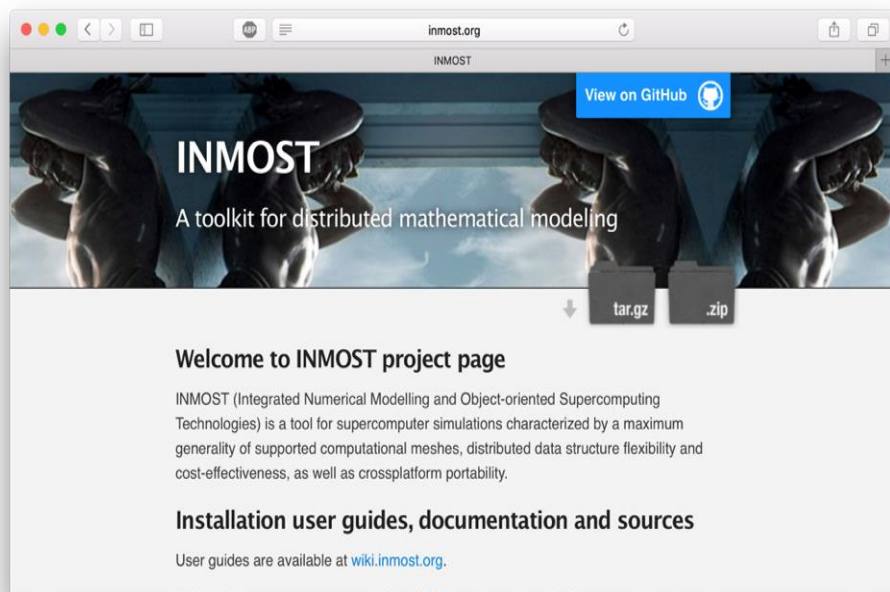
⁵Sirius University





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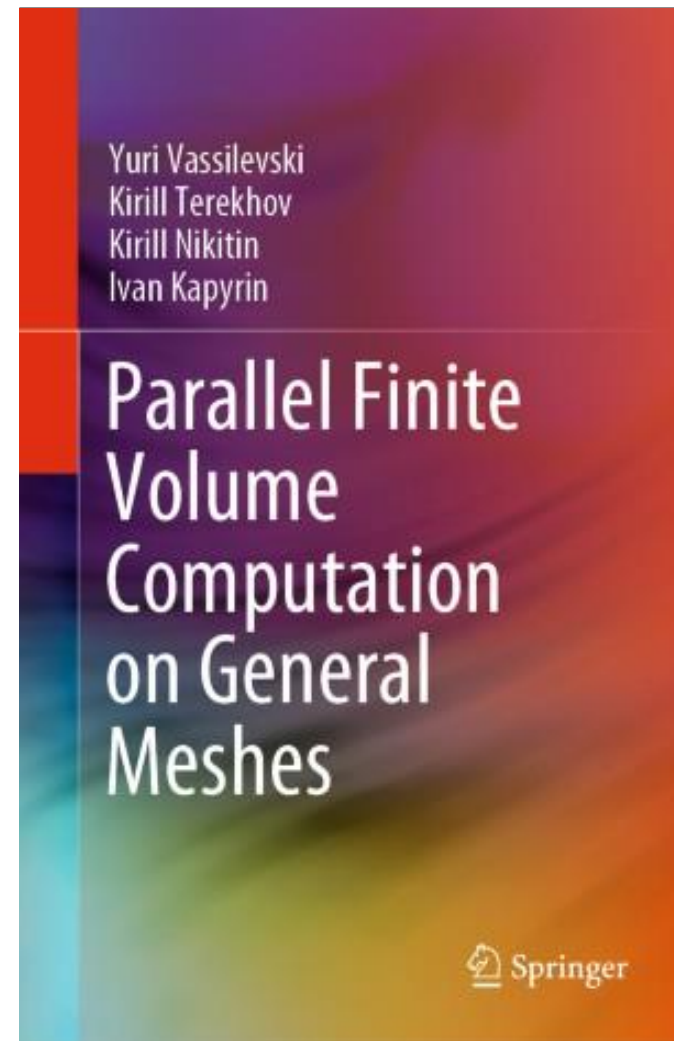
Framework for mathematical modelling



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INMOST

INMOST (www.inmost.org, www.inmost.ru) is a short for:

Integrated

Numerical

Modeling and

Object-oriented

Supercomputing

Technologies

- Distributed meshes (**moving, adaptive**)
- Distributed linear system assembly
- Parallel linear solvers
- Automatic differentiation
- Nonlinear system assembly
- Coupling of unknowns and models

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INMOST Linear Solvers

- Preconditioned **BiCGStab(I)** method¹
- Preconditioner **MPI-parallelization** using **Additive Schwarz Method**
- Preconditioner **OpenMP-parallelization** using **Bordered Block-Diagonal Form**^{9,10}
- **Multi-level preconditioner** based on the second-order **Crout-ILU**^{2,3}
- **Condition estimation** of the inverse factors determines the **coarse system** and tunes dropping tolerances^{4,5}
- **Scaling** and **reordering** of the local system on each successive level^{6,7,8}



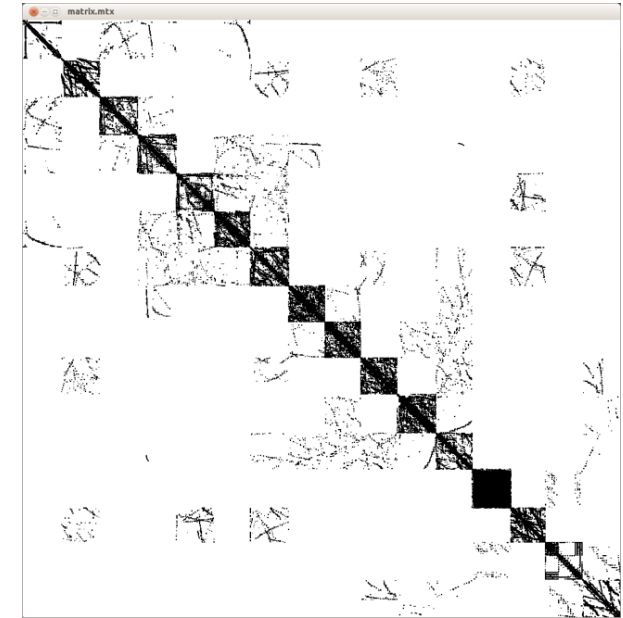
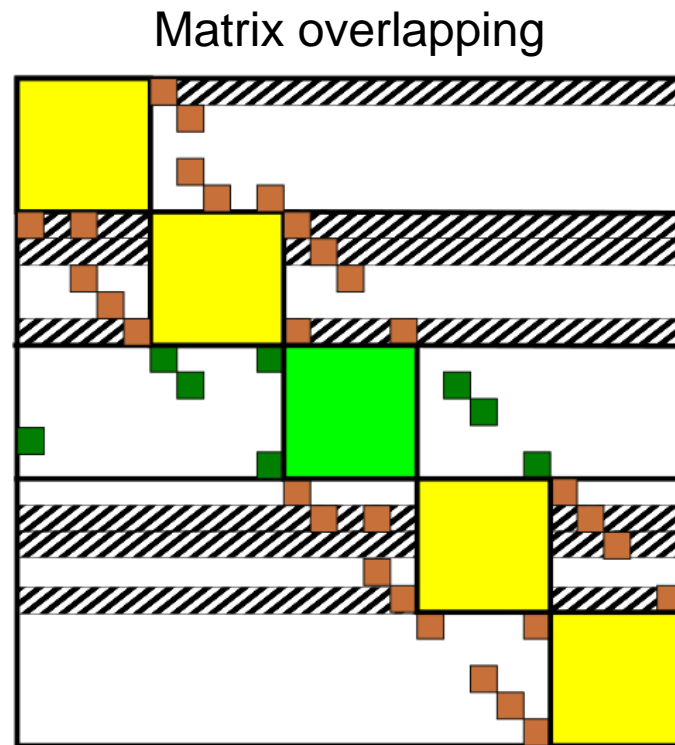
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- 4) Bollhöfer, M.: *A robust ILU with pivoting based on monitoring the growth of the inverse factors*. *Linear Algebra and its Applications* 338.1-3 (2001): 201-218. **(Tuning dropping tolerances)**
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- 7) Olschowka, M., Arnold N.: *A new pivoting strategy for Gaussian elimination*. *Linear Algebra and its Applications* 240 (1996): 131-151. **(Maximizing diagonal product)**
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Additive Schwarz Method

- Global matrix is composed of local blocks.
- Extend blocks to localize the connection.
- **Restricted** version.
- **More iterations with more blocks**



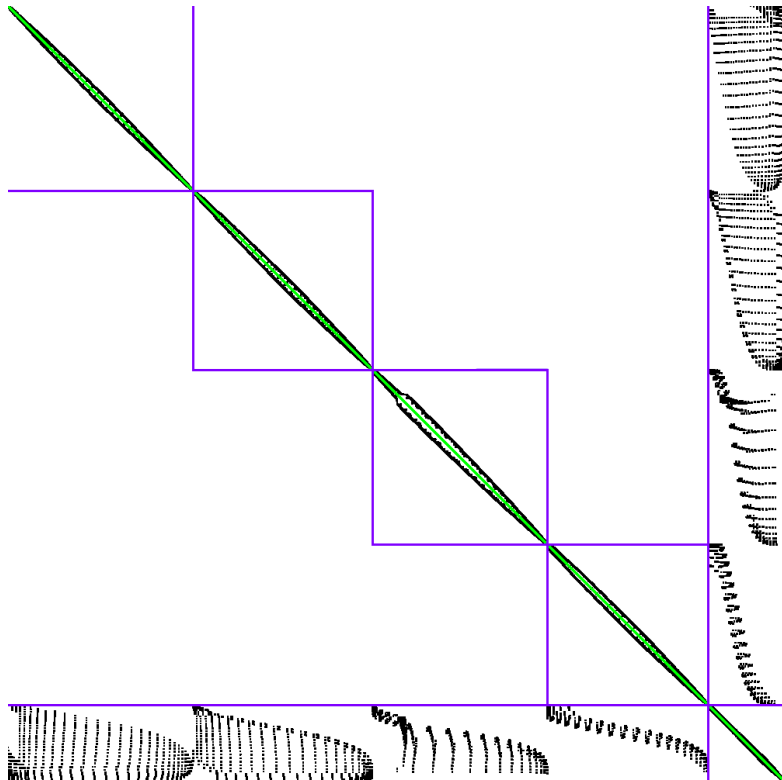
Distributed system

- - Local partition outlier
- - Remote partition outlier
- - Local partition
- - Remote partitions
- ▨ - Extended rows

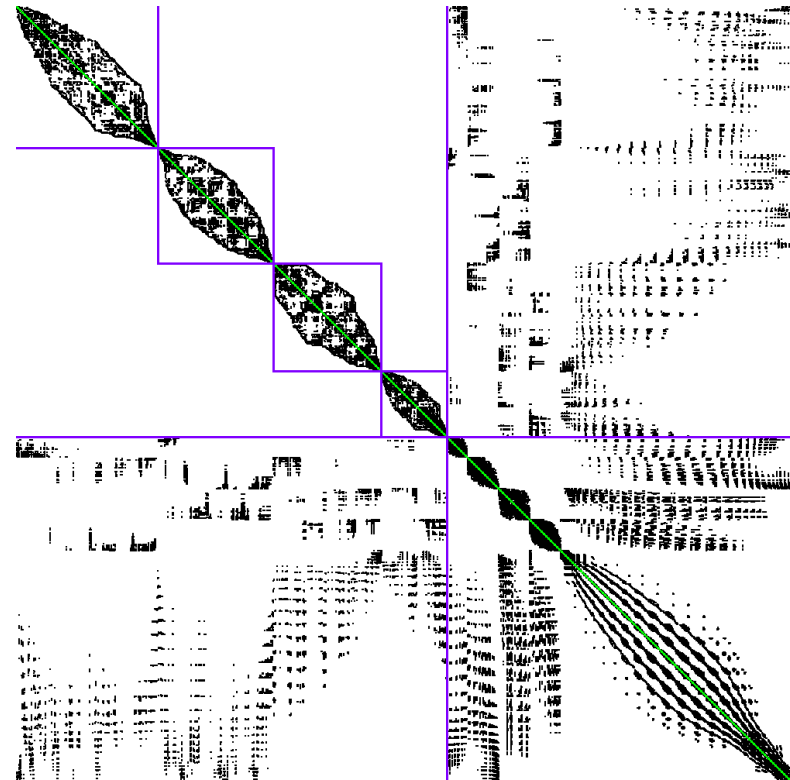


Doubly-Bordered Block-Diagonal Form

First level



Schur complement

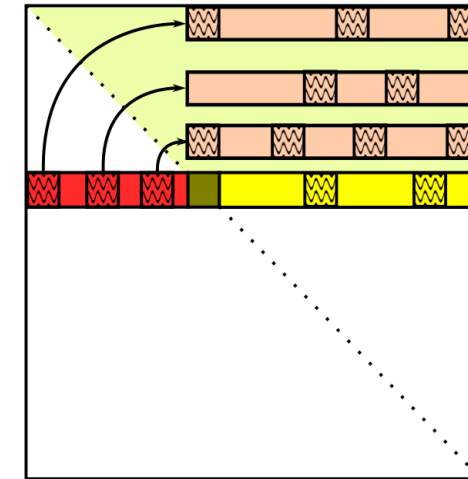
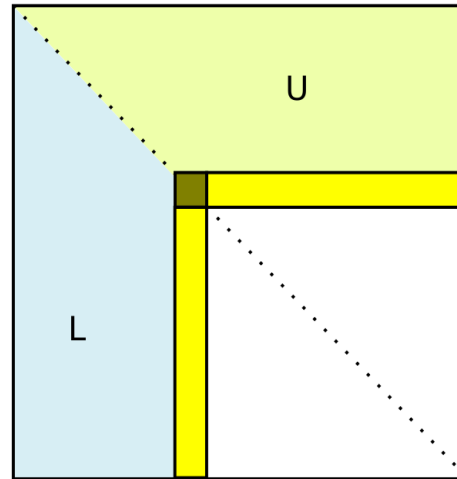


Larger Schur complement with more blocks

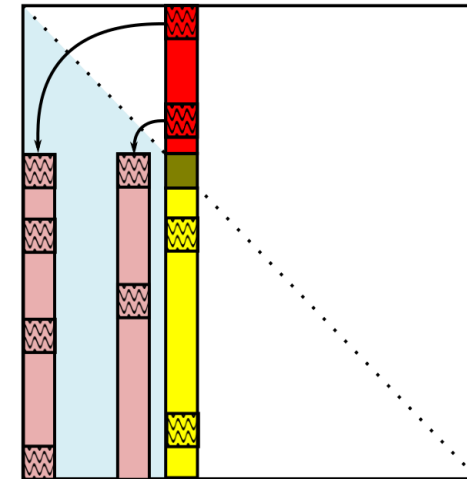


Second-order Crout Incomplete LU

- Dual-threshold dropping:
 - τ^2 for factorization.
 - τ for iterations.
- Running condition estimation:



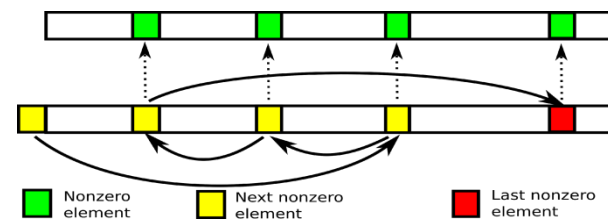
U-factor elimination



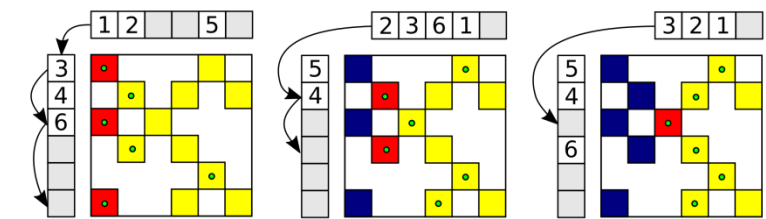
L-factor elimination

- $\kappa = \max(\|L^{-1}\|, \|U^{-1}\|)$

Dense row accumulator:



Transposed matrix traversal:

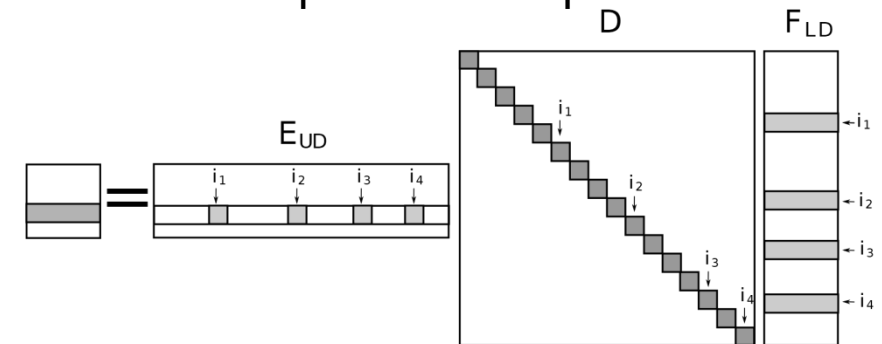
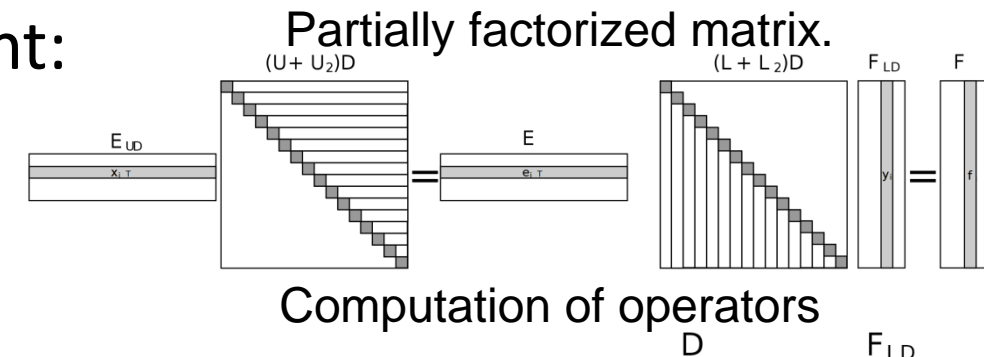
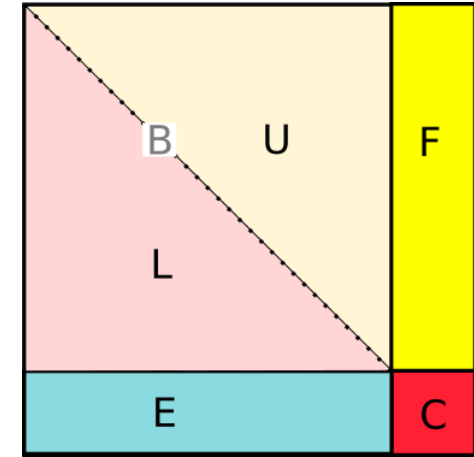


- $\tau/\kappa = \text{const}$ tuning.
- Limit growth of κ .



Schur Complement

- Part that leads to growth of κ is accumulated in **C**:
 - system **reordering** after factorization.
- Next level system is the **Schur** complement:
 - $S = C - E (DU)^{-1} D(LD)^{-1}F$.
 - Requires forward and backward substitution with **sparse** right hand side.
 - **Fill-in control** is critical.
 - **Second-order** ILU is critical.





Analogy to the Algebraic Multigrid

- **Coarse** system should contain the **largest error** of the **smoother**.
- **Condition estimation** reveals the **error** in the **smoother** and provides the *coarse-fine splitting* of the system.
- Ideal prolongation $P=(-EB^{-1}, I)$ and restriction $R=(-FB^{-1}, I)^T$.
 - (not satisfied by the present method).
- Schur complement corresponds to the **coarse** system.
- **Universal but much more computationally complex.**
 - (definitely not linear computational complexity)

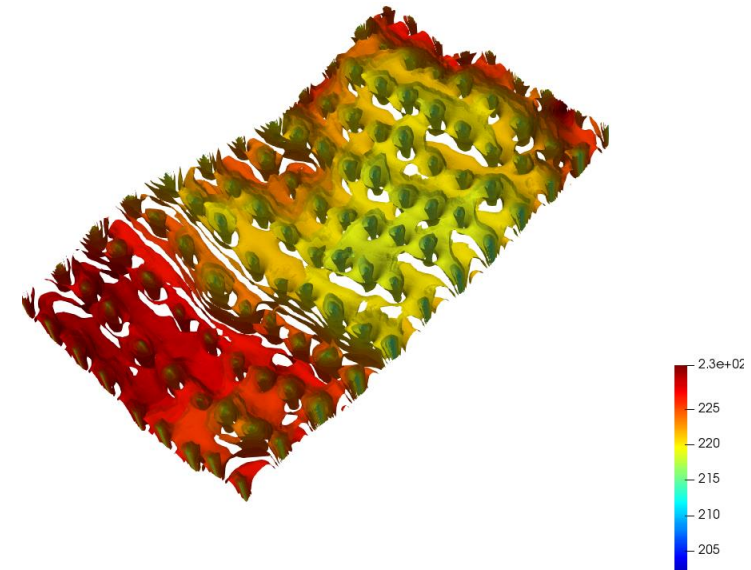
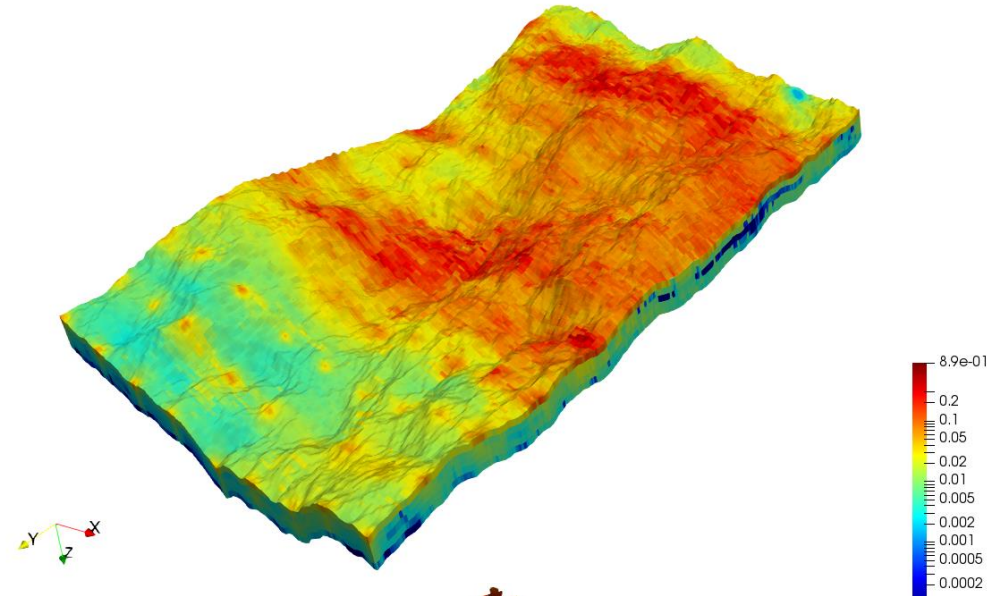


Oil & Gas: Black Oil

- Suitable for large problem solutions:
 - Black oil problem
 - $\times 3$ unknowns per cell
 - **100M** and **200M** cells (320 cores, INM RAS cluster):

Case	T_{mat}	T_{prec}	T_{iter}	T_{sol}	T_{upd}	N_n	N_l
SPE10_100M	14	18.5	55.4	78.6	0.2	402	3.5
SPE10_200M	29.6	34.7	64.1	107.5	0.38	428	3.96

- Scaled up to **1B of cells** on 9600 Cray cores by Ahmad Abushaika at HBKU, Qatar.
- Optimal preconditioner is **Constrained pressure residual method with AMG**.





Oil & Gas: Geomechanics

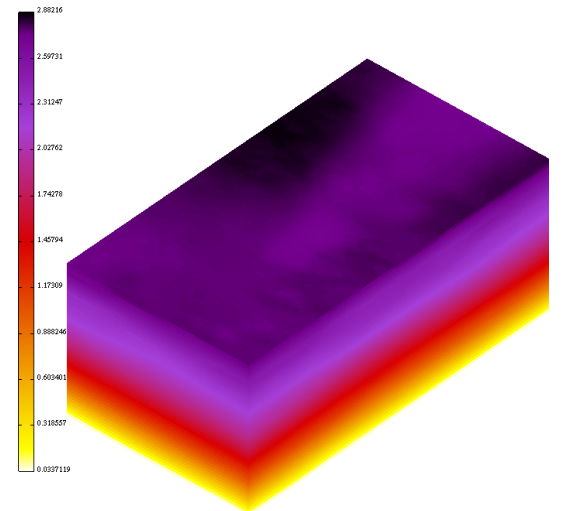
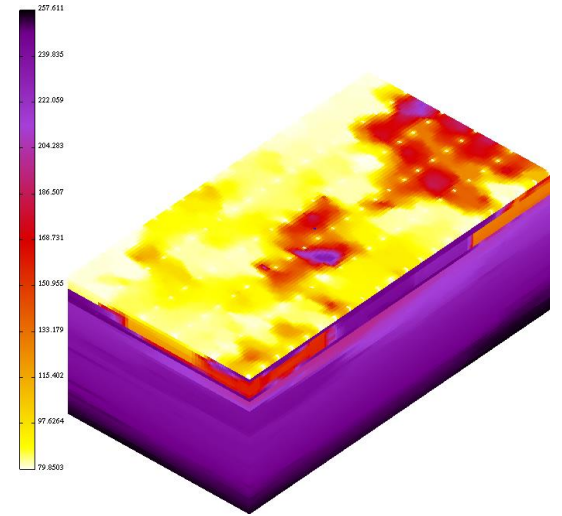
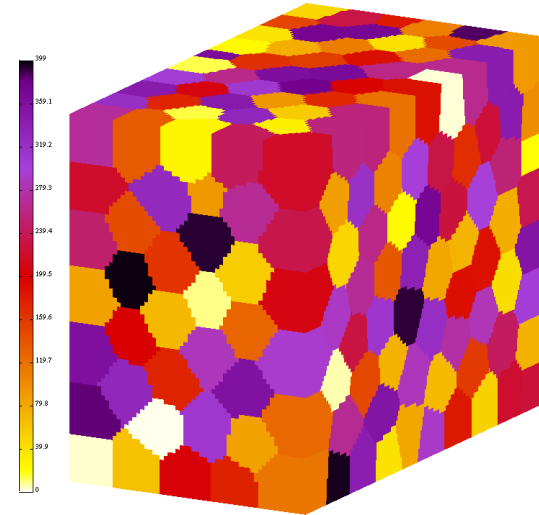
- Poroelasticity:

$$\frac{1}{M} \frac{\partial p}{\partial t} - \operatorname{div} \left(\mathbb{K}(\nabla p - \rho g \nabla z) - \mathbb{B} \frac{\partial \mathbf{u}}{\partial t} \right) = q$$

$$- \operatorname{div} \left(\varepsilon : \frac{\nabla \mathbf{u} + \nabla \mathbf{u}^T}{2} + \mathbb{B} p \right) = \rho g \nabla z$$

- ×4 unknowns per cell
- **1.2M** cells (INM RAS cluster, Lomonosov):

Machine	N_{proc}	T_{tot}	T_{asm}	T_{prec}	T_{iter}	T_{upd}
INM RAS cluster	100	15079.4	1119.8	7245.2	4463	479.7
	200	8791.2	582.9	3926.2	2800.9	252.4
	400	4637	300.3	1965.6	1374.2	127
Lomonosov supercomputer	700	3536	234.1	1071.1	1112.42	70.5

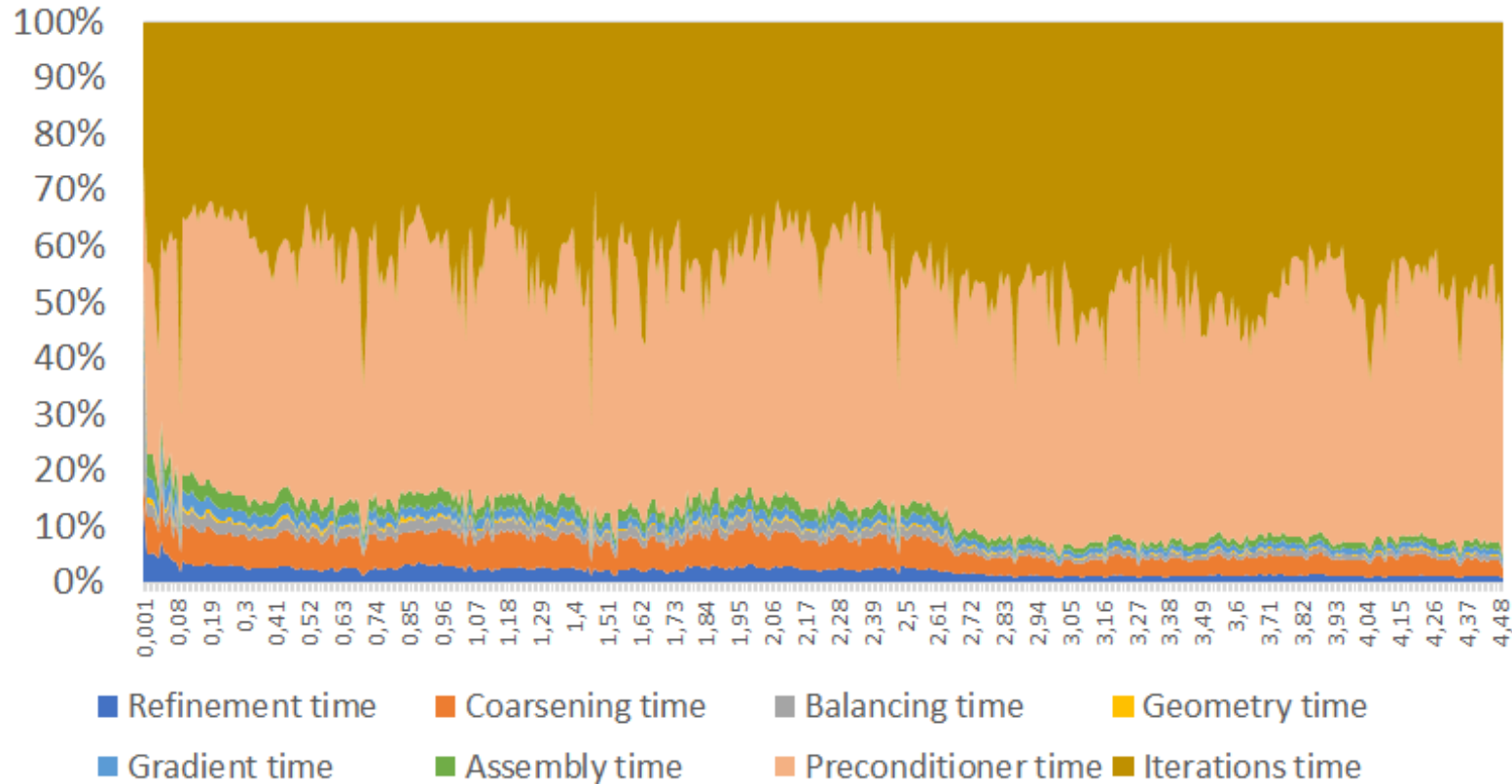


Solution of **saddle-point** problem.

Optimal preconditioner: **Fixed-stress splitting with AMG**

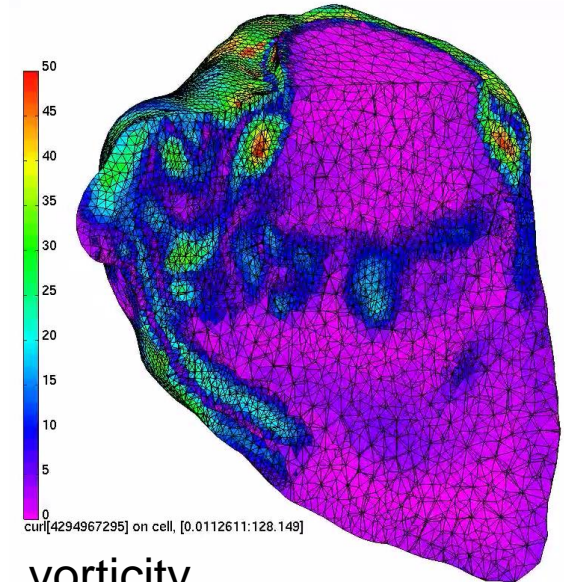


Blood flow: Right Ventricle

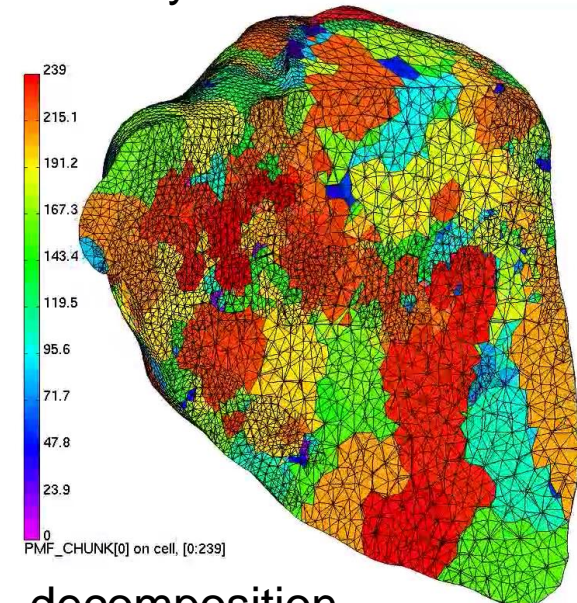


Every step we adapt and balance the mesh, calculate geometry and recompute discretization coefficients, but the biggest challenge is the linear solution of the coupled **saddle-point** system.

Optimal preconditioner: **GMG with Vanka smoother**



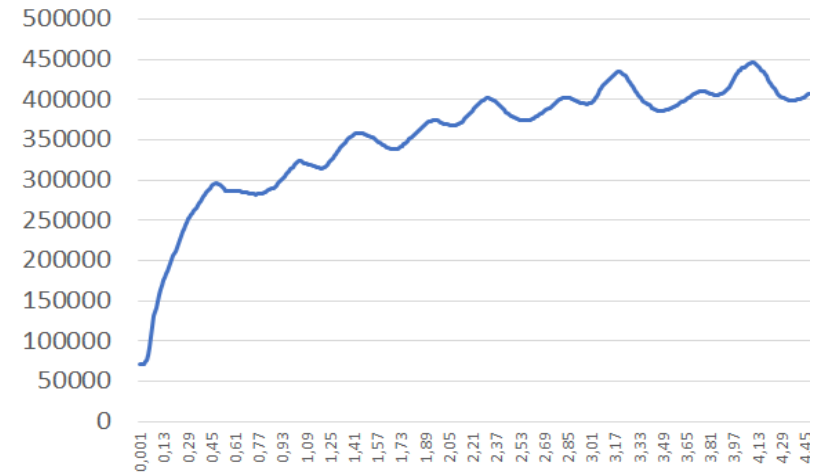
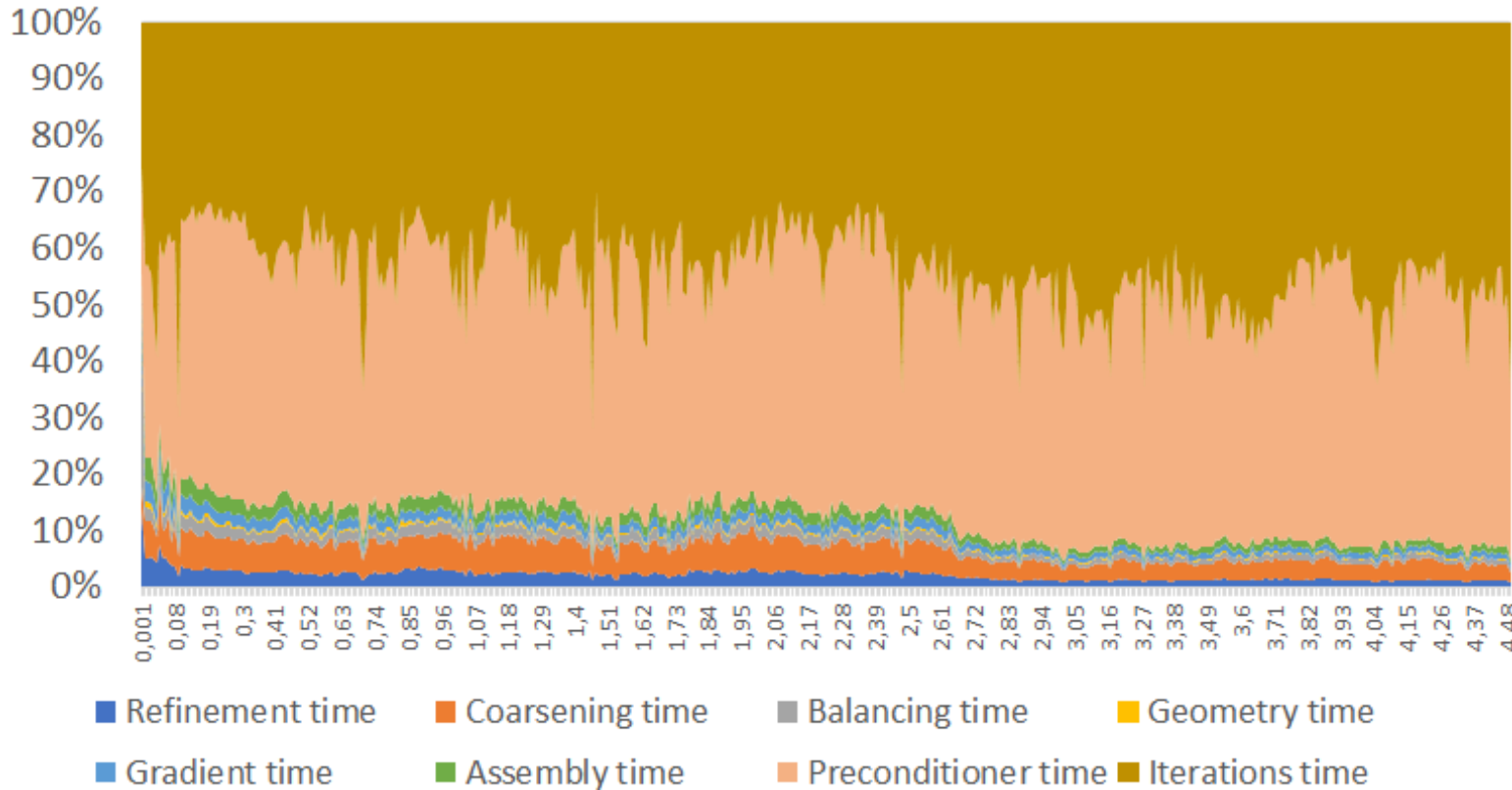
vorticity



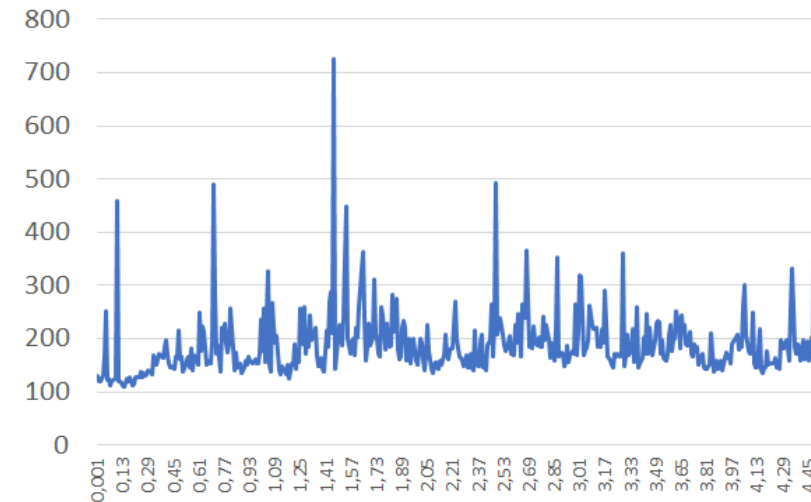
decomposition



Blood flow: Right Ventricle



Number of cells



Linear iterations

Every step we adapt and balance the mesh, calculate geometry and recompute discretization coefficients, but the biggest challenge is the linear solution of the coupled **saddle-point** system.

Optimal preconditioner: **GMG with Vanka smoother**



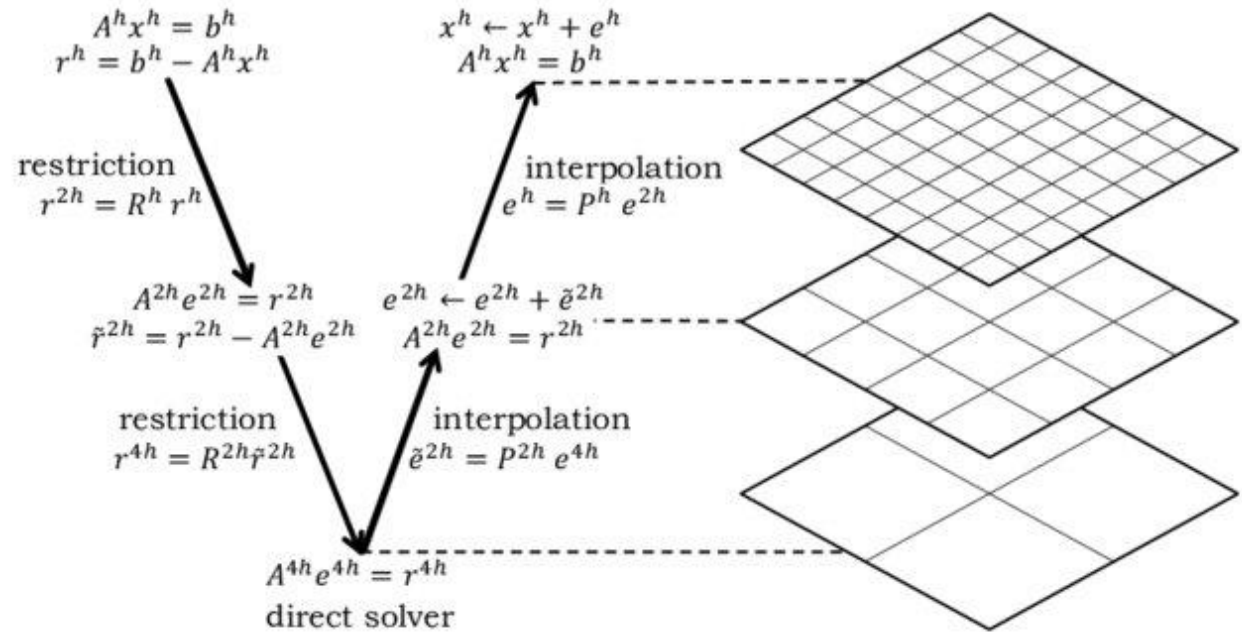
AMG

Classical approaches to coupled problems: bootstrap adaptive AMG, AMG on Schur complement for mimetic finite difference method, constrained pressure residual and AMG for black oil problem, Bramble-Pasciak method with AMG for Stokes and Navier-Stokes



Bootstrap Adaptive Algebraic Multigrid

- **Setup** phase:
 - Smoother or preconditioner setup.
 - **Near null-space approximation.**
 - Coarse-fine space splitting.
 - Interpolation and restriction operators.
 - Coarse space computation: matrix-matrix multiplication.
- **Solve** phase:
 - Smoother application.
 - Matrix-vector multiplication.



(illustration from internet)



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Near Null-Space Vector

- Linear system: $A\mathbf{x} = \mathbf{b}$, where A is $N \times N$ matrix.
- Let $A\mathbf{e} \approx \mathbf{0}$, where vector \mathbf{e} is **near null space** of the system:

$$a_{ii}\mathbf{e}_i \approx - \sum_{i \neq j} a_{ij}\mathbf{e}_j$$

- For elliptic system the best guess is: $\mathbf{e} = \mathbf{1}$ – **classical** AMG.
- **Adaptive multigrid**: exploit information on \mathbf{e} for general systems.
- **Bootstrap process**: try to estimate \mathbf{e} with several iterations of the available smoother

(Ideal \mathbf{e} is an **eigenvector** corresponding to smallest eigenvalue – extremely expensive to find! Instead we search for error outside of smoother range)



Space and Connections Splitting

- **Coarse-fine** splitting of the grid elements: $\Omega = \{1, \dots, N\} = C \cup F$.
- **Connections** of the element: $N_i = \{j \mid i \neq j, a_{ij} \neq 0\}$.
- **Strong-weak** splitting of connections: $N_i = S_i \cup W_i = I_i \cup T_i \cup E_i \cup W_i$.
 - $I_i = S_i \cap C$ – **interpolatory connections**.
 - W_i - **weak connections**, absorbed by the diagonal coefficient.
 - $T_i \cup E_i = S_i \cap F$ – **strong non-interpolatory** connections.
 - T_i – **twice-removed interpolation**, requires $\forall j \in T_i : S_i \cap S_j \cap C \neq \emptyset$.
 - E_i – **absorbed by the coefficient**, do not satisfy the condition.
- **Ruge-Stuben** rules for the **coarse-fine** splitting:
 - $\forall i \in F: \forall j \in S_i \cap F: S_i \cap S_j \cup C \neq \emptyset$ (E_i is always **empty**)
 - C is a maximal independent set in the graph of strong connections.



Interpolation Method

- Using introduced spaces:

$$a_{ii} \mathbf{e}_i \approx - \sum_{i \neq j} a_{ij} \mathbf{e}_j = - \sum_{j \in I_i} a_{ij} \mathbf{e}_j - \sum_{j \in W_i} a_{ij} \mathbf{e}_j - \sum_{j \in T_i} a_{ik} \mathbf{e}_k - \sum_{j \in E_i} a_{ij} \mathbf{e}_j$$

- Twice-removed interpolation for T_i :

$$a_{ik} \mathbf{e}_k \approx - \sum_{j \in S_i \cap S_k \cap C} \frac{a_{ik} a_{kj} \mathbf{e}_k \mathbf{e}_j}{\sum_{l \in S_i \cap S_k \cap C} a_{kl} \mathbf{e}_l}$$

- Now $A\mathbf{e} \approx \mathbf{0}$ turns into expression:

$$\left(a_{ii} + \sum_{j \in W_i} a_{ij} \frac{\mathbf{e}_j}{\mathbf{e}_i} \right) \mathbf{e}_i \approx - \eta_i \sum_{j \in I_i} \left(a_{ij} + \sum_{k \in T_i} \frac{a_{ik} a_{kj} \mathbf{e}_k}{\sum_{l \in S_i \cap S_k \cap C} a_{kl} \mathbf{e}_l} \right) \mathbf{e}_j$$

- Multiplying coefficient for E_i :

$$\eta_i = \frac{\sum_{k \in S_i} a_{ik} \mathbf{e}_k}{\sum_{k \in S_i \setminus E_i} a_{ik} \mathbf{e}_k}$$



Interpolation Method

- Interpolation:

$$\mathbf{e}_i = \sum_{j \in I_i} \omega_{ij} \mathbf{e}_j$$

- Weights:

$$\omega_{ij} = \frac{-\eta_i \mathbf{e}_i}{a_{ii} + \sum_{j \in W_i} a_{ij} \mathbf{e}_j} \left(a_{ij} + \sum_{k \in T_i} \frac{a_{ik} a_{kj} \mathbf{e}_k}{\sum_{l \in S_i \cap S_k \cap C} a_{kl} \mathbf{e}_l} \right)$$

- Prolongator:

$$P_i = \begin{cases} \sum_{j \in I_i} \omega_{ij} \delta_j & i \in F \\ \delta_i & i \in C \end{cases}$$

- Coarse-space system:

$$B = P^T A P$$



Choosing Spaces

- **Modification** to the Ruge-Stuben **coarse-fine splitting** rules:

- $\forall i \in F: |\eta_i - 1| \leq \kappa$, where κ is a tunable parameter.
- C is a maximal independent set in the graph of strong connections.

- **Classical** selection of strong connections by Ruge-Stuben:

- $S_i = \left\{ j \mid -a_{ij} \geq \theta \max_{k \in N_i} (-a_{ik}) \right\}, \quad \theta = \frac{1}{4}.$

- **Modified** selection of strong connections:

- $S_i = \left\{ j \mid -\text{sgn}(a_{ii} \mathbf{e}_i) a_{ij} \mathbf{e}_j \geq \theta \max_{k \in N_i} (-\text{sgn}(a_{ii} \mathbf{e}_i) a_{ik} \mathbf{e}_k) \right\}, \quad \theta = \frac{1}{4}$

- Additional requirement: $a_{ii} \mathbf{e}_i (a_{ii} \mathbf{e}_i + \sum_{j \in W_i} a_{ij} \mathbf{e}_j) > 0.$



Application to MFD System

Mimetic finite difference scheme for anisotropic diffusion produces a system:

$$A \begin{bmatrix} p_c \\ p_f \end{bmatrix} = \begin{bmatrix} B & E \\ E^T & C \end{bmatrix} \begin{bmatrix} p_c \\ p_f \end{bmatrix} = \begin{bmatrix} q \\ 0 \end{bmatrix},$$

- Schur complement (B is diagonal):

$$S = C - E^T B^{-1} E.$$

- Requires multiplying and subtracting two matrices.
- S- suffix in the methods is the preconditioner applied to the Schur complement.

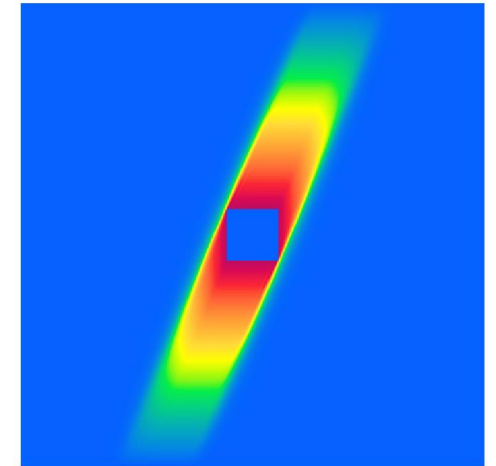


Application to MFD System

κ	T, aAMG	Lit, aAMG	Mem, aAMG
0	36,377	20	800,859
0,1	37,416	21	795,189
0,25	32,369	18	759,875
0,5	34,592	21	727,332
1	39,38	38	469,223
2	40,792	44	420,403
5	43,952	50	398,419
10	42,909	49	394,489

(time in sec) (memory in MB)

Convergence rate depends on κ
(optimal $\kappa = 0.25$)



Single well problem with anisotropic diffusion
2,241,216 unknowns
746,496 cells

Classical and adaptive multigrid for scaled systems:

$$A_* = D_L A D_R$$

- A_s – symmetric scaling
- A_w – Sinkhorn scaling
- A_m – maximum transversal
- A_r – random scaling

	AMG					α AMG				
	A	A_s	A_w	A_m	A_r	A	A_s	A_w	A_m	A_r
T	363	54448.5	26040.4	—	1754.9	352	383.9	328	596.2	492
Ts	20.6	25.5	25.2	20.5	20.5	31	33.4	33.4	34.6	31.5
Tit	342.4	54423	26065.7	—	1734.4	321.1	350.4	290.6	561.5	460.5
Nit	89	11581	5563	>15000[‡]	447	82	89	76	143	115
Lvl	9	17	17	11	11	10	11	10	10	10
Mem	1.8 GB	2.3 GB	2.3 GB	1.8 GB	1.8 GB	1.8 GB	1.8 GB	1.8 GB	1.8 GB	1.8 GB

(system with 3 904 281 unknowns)



Multistage Methods

Multistage strategies:

- Two stage – a way to combine multiple preconditioners and solve $(AM^{-1})(Mx)=b$ with

$$M^{-1} = M_1^{-1} + \sum_{i=2}^{n_{st}} M_i^{-1} \prod_{j=1}^{i-1} (I - AM_j^{-1}),$$

- Two stage Gauss-Seidel – use Gauss-Seidel on 2×2 block matrix with individual preconditioner M_1 and M_2 :

$$\begin{bmatrix} B & E \\ F & C \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} \Longrightarrow \begin{bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{bmatrix} = \begin{bmatrix} B & E \\ F & C \end{bmatrix}^{-1} \left(\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} - \begin{bmatrix} 0 & E \\ 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \right),$$
$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} B & E \\ C & F \end{bmatrix}^{-1} \left(\begin{bmatrix} b_1 \\ b_2 \end{bmatrix} - \begin{bmatrix} 0 & 0 \\ F & 0 \end{bmatrix} \cdot \begin{bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \end{bmatrix} \right).$$

$$\tilde{x}_1 = M_1^{-1}(b_1 - Ex_2), \quad x_2 = M_2^{-1}(b_2 - F\tilde{x}_1), \quad x_1 = M_1^{-1}(b_1 - Ex_2).$$



Multistage Methods

Multistage strategies:

- CPR – constrained pressure residual:
 - Using black-oil problem structure, multiply from the left by a matrix to approximately decouple the pressure system:

$$\begin{bmatrix} A_{pp} & A_{ps} \\ A_{sp} & A_{ss} \end{bmatrix} \cdot \begin{bmatrix} p \\ s \end{bmatrix} = \begin{bmatrix} b_p \\ b_s \end{bmatrix} \implies \begin{bmatrix} B_{pp} & Z_{ps} \\ A_{sp} & A_{ss} \end{bmatrix} \cdot \begin{bmatrix} p \\ s \end{bmatrix} = \begin{bmatrix} b_p - D_{ps} D_{ss}^{-1} b_s \\ b_s \end{bmatrix} \quad \begin{aligned} B_{pp} &\equiv A_{pp} - D_{ps} D_{ss}^{-1} A_{ps} \\ Z_{ps} &\equiv A_{ps} - D_{ps} D_{ss}^{-1} A_{ss} \approx 0 \end{aligned}$$

- Use a two-stage method to solve the system.
- M_1 - for pressure system, M_2 - for either complete system or saturations system (**two-stage GS**).

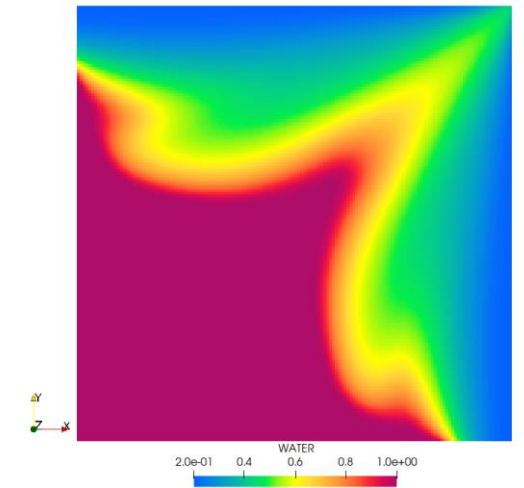
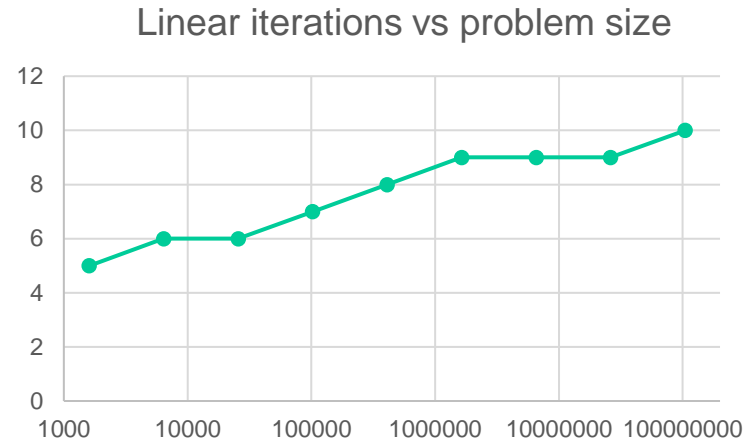


Application to Two-Phase Problem

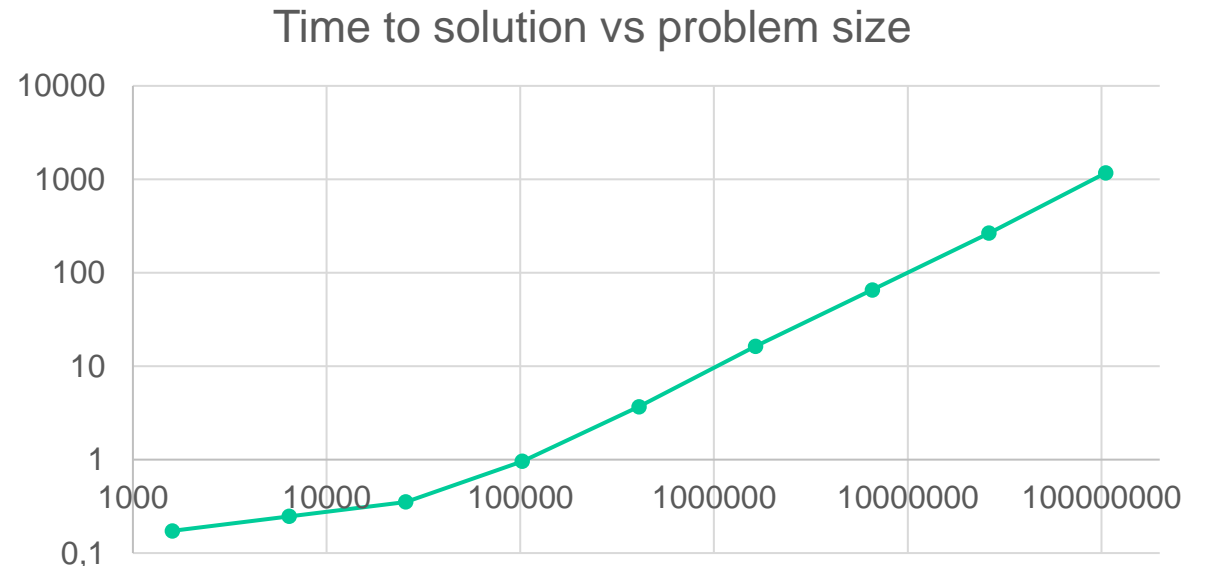
Using CPR rescaling,
AMG at pressure block, and
block Gauss-Seidel at first stage

Cells	T (sec)	Lit
1600	0,173	5
6400	0,248	6
25600	0,354	6
102400	0,961	7
409600	3,691	8
1638400	16,376	9
6553600	65,404	9
26214400	265,432	9
104857600	1163,921	10

Almost linear scaling! **Sequential** code.



Quarter-five spot problem

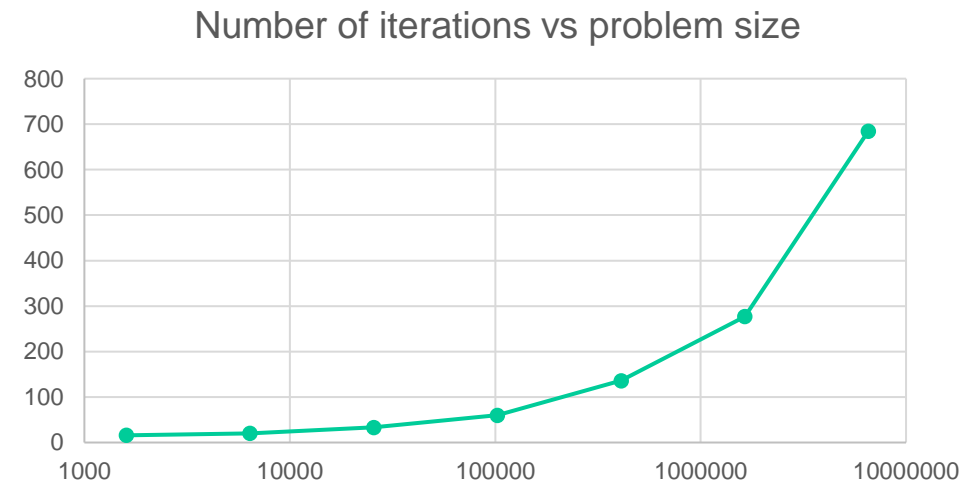
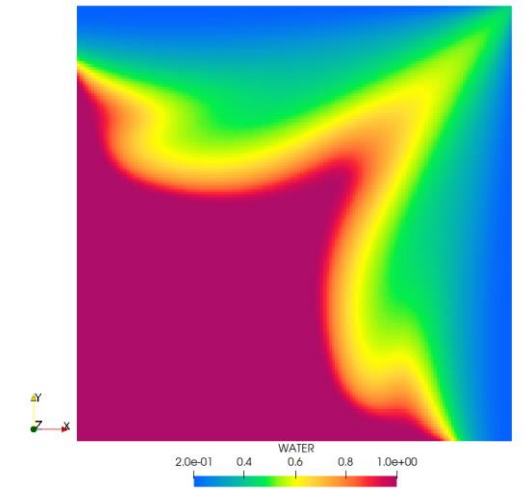
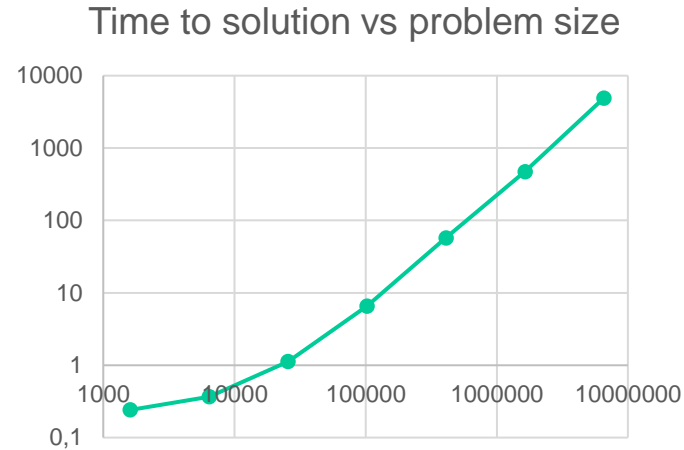




Application to Two-Phase Problem

Using **bootstrap adaptive AMG**
on **original** system
Classic AMG **not applicable**

Cells	T (sec)	Lit
1600	0,242	16
6400	0,368	20
25600	1,124	33
102400	6,591	60
409600	57,441	136
1638400	472,973	277
6553600	4922,85	685



Adaptive multigrid is **directly** applied to the **entire** system!
(maybe we need more test vectors or block version)



Bramble-Pasciak method

- Initial System:

$$\begin{bmatrix} B & F \\ E & -C \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \end{bmatrix},$$

- Assumptions: $B > 0, C \geq 0, E = F^T$

- Modified** System:

$$\begin{bmatrix} B - P^{-1} & \\ & \mathbb{I} \end{bmatrix} \begin{bmatrix} \mathbb{I} & \\ E & -\mathbb{I} \end{bmatrix} \begin{bmatrix} P & \\ & \mathbb{I} \end{bmatrix} \begin{bmatrix} B & F \\ E & -C \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} BPf_1 - f_1 \\ EPf_1 - f_2 \end{bmatrix}$$

- Collapses into:

$$\begin{bmatrix} BPB - B & BPF - F \\ EPB - E & C + EPF \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} BPf_1 - f_1 \\ EPf_1 - f_2 \end{bmatrix}$$

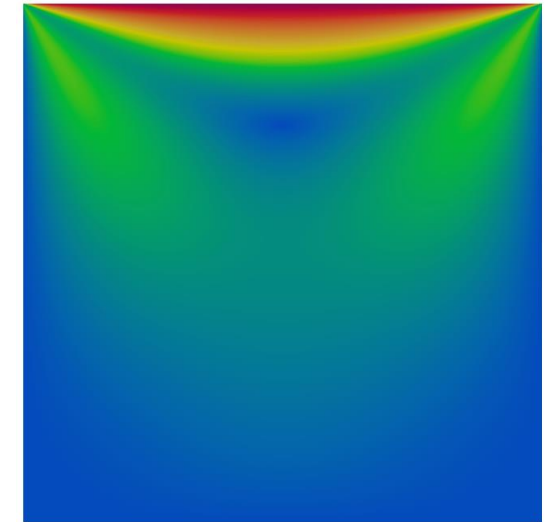
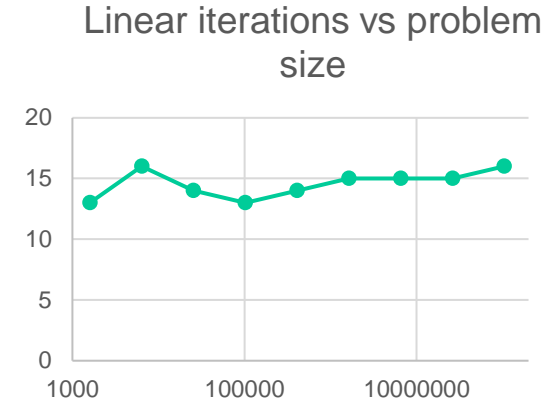
- Do not require P^{-1} , Krylov solver with multiplication by modified matrix, **spd** for CG if P is properly scaled.
- Applicable with BiCGStab without P scaling and to moderately **non-symmetric systems**.



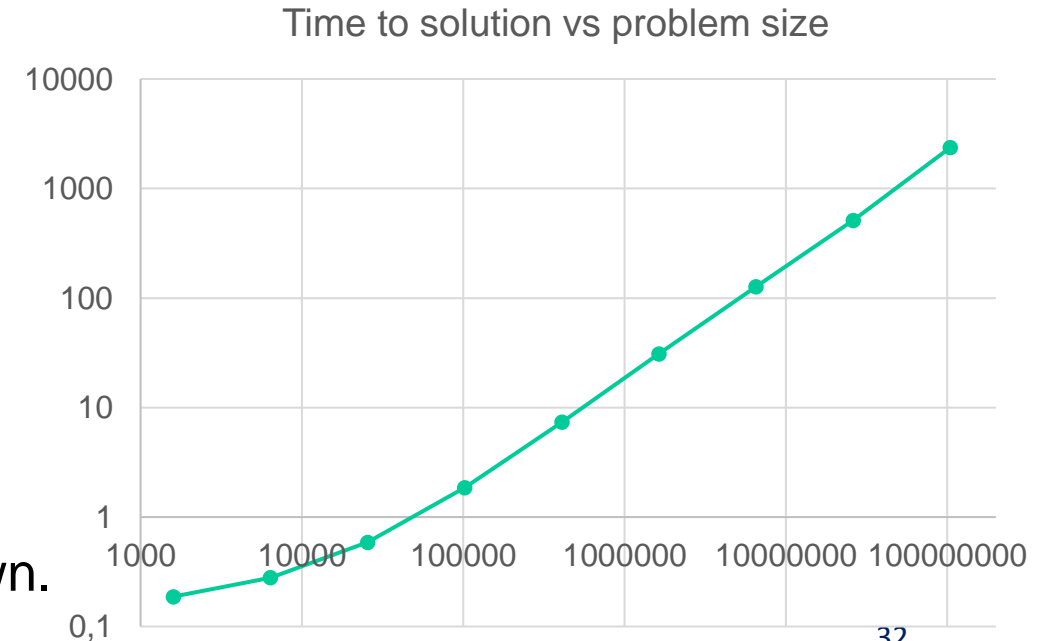
Application to Stokes Problem

Cells	Time (sec)	Nit	Lit
1600	0,188	1	13
6400	0,28	1	16
25600	0,59	1	14
102400	1,862	1	13
409600	7,365	1	14
1638400	31,012	1	15
6553600	127,189	1	15
26214400	511,757	1	15
104857600	2373,665	1	16

Staggered discretization: around 3 equations per cell.
Symmetric with $C = 0$. **ILU** methods typically breakdown.
Linear scaling! **Sequential** code.

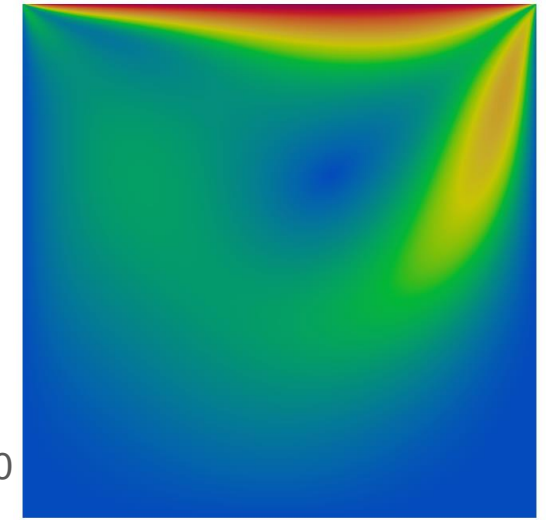
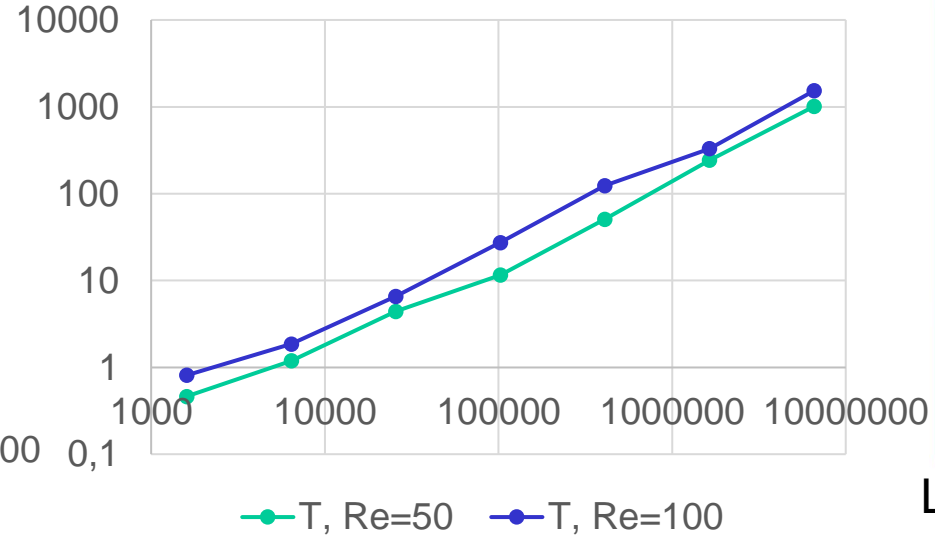
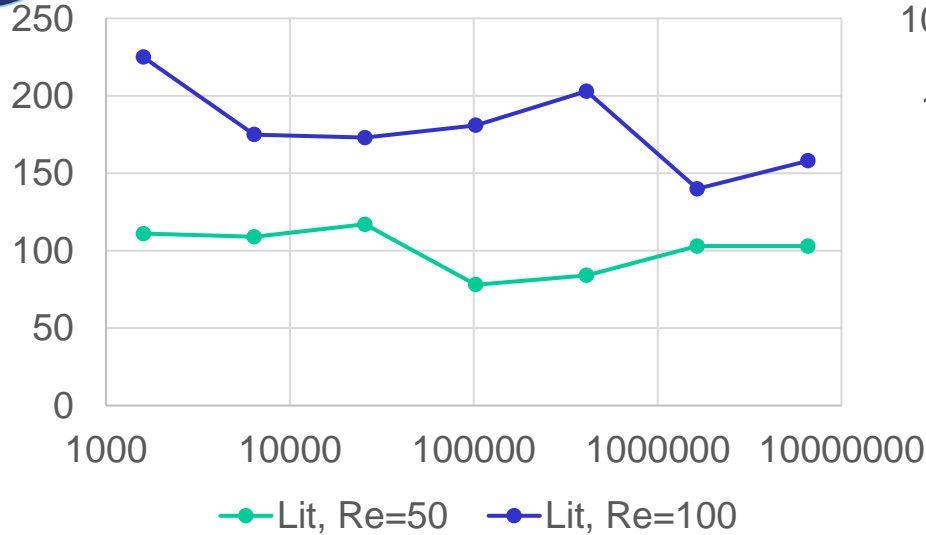


Lid-driven cavity problem





Application to Navier-Stokes Problem



Lid-driven cavity problem

Newton iterations to **steady-state**. **Non-symmetric** with $C = 0$.

Cells	Lit, Re=50	Lit, Re=100	Nit, Re=50	Nit, Re=100	T, Re=50	T, Re=100
1600	111	225	3	4	0,462	0,814
6400	109	175	3	3	1,192	1,858
25600	117	173	3	3	4,418	6,578
102400	78	181	2	3	11,596	27,4
409600	84	203	2	3	50,956	123,725
1638400	103	140	2	2	243,345	329,94
6553600	103	158	2	2	1011,053	1534,724

(time in sec)



Block AMG

For general **collocated** finite-volume discretization: exactly follows Ruge-Stuben scheme with blocks and uses block Gauss-Seidel smoother



Interpolation Method (Block version)

- Selection of strong connections:

$$S_i = \left\{ j \mid \|a_{ij}\| \geq \theta \max_{k \in N_i} (\|a_{ik}\|) \right\}, \quad \theta = \frac{1}{4}.$$

- Interpolation ($\kappa = 0 \Rightarrow E_i = \emptyset$):

$$\mathbf{e}_i = \sum_{j \in I_i} \omega_{ij} \mathbf{e}_j, \quad \omega_{ij} = - \left(\mathbf{a}_{ii} + \sum_{j \in W_i} \mathbf{a}_{ij} \right)^{-1} \left(\mathbf{a}_{ij} + \sum_{k \in T_i} \frac{\mathbf{a}_{ik} \|\mathbf{a}_{kj}\|}{\sum_{l \in S_i \cap S_k \cap C} \|\mathbf{a}_{kl}\|} \right)$$

- Prolongator:

$$P_i = \begin{cases} \sum_{j \in I_i} \omega_{ij} \delta_j & i \in F \\ \mathbb{I} \delta_i & i \in C \end{cases}$$

- Coarse-space system:

$$B = P^T A P$$



General Concept for Differential Equations

System of PDE equations:

$$\frac{\partial \tau(q)}{\partial t} + \mathbf{div}(\mathcal{A}(q)) = \mathcal{R}(q),$$

Where

- q is $N \times 1$ vector of unknowns of the system,
- $\tau(q)$ corresponds to the accumulation,
- $\mathcal{R}(q)$ represents **body forces** and **reactions** – discretized with matrix-weighted Euler method:
 - I. Butakov, K. Terekhov. **Two Methods for the Implicit Integration of Stiff Reaction Systems**. CMAM, submitted.
- $\mathcal{A}(q)$ represents **conservative forces** – addressed by the general finite volume framework:
 - K.Terekhov. **General finite-volume framework for saddle-point problems of various physics**. RJNAMM, 2021

Ultimate goal: automatic **collocated** finite-volume discretization for a given system.

Complications: inf-sup condition, convective instability and other problems...

We get a system with $N \times N$ **blocks**. At the core we get a **symmetric quasi-definite** system.



Collocated Finite Volume Method

- Gauss-Green theorem :

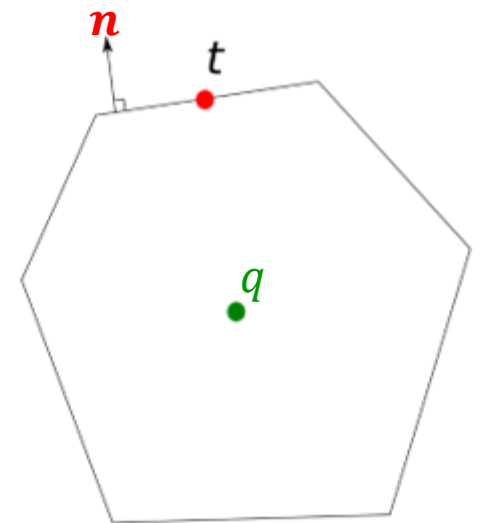
$$\operatorname{div}(\mathcal{A}(q)) = g \Rightarrow \oint_{\partial V} \mathcal{A}(q) d\mathbf{S} = \int_V \mathbf{g} dV \Rightarrow \frac{1}{|V|} \sum_{f \in \mathcal{F}(V)} \mathcal{A}_f \mathbf{n} |f| = \mathbf{g}_V$$

- Requires flux approximation on a face:

$$\mathbf{t} = \mathcal{A}_f \mathbf{n}$$

- Which flux?

- $\mathcal{A} = -\mu^{-1}(\nabla p - \rho g \nabla z)^T \mathbb{K}$, (Darcy)
- $\mathcal{A} = -\mathcal{C} : (\mathbf{u} \nabla^T + \nabla \mathbf{u}^T) / 2$, (elasticity)
- $\mathcal{A} = \begin{cases} -\mathcal{C} : \frac{\mathbf{u} \nabla^T + \nabla \mathbf{u}^T}{2} + \mathbb{B} p \\ -\mu^{-1} \mathbb{K} (\nabla p - \rho g \nabla z) + \mathbb{B} \frac{\partial \mathbf{u}}{\partial t} \end{cases}$, (Biot)
- $\mathcal{A} = \begin{cases} \rho \mathbf{u} \mathbf{u}^T - \mu \nabla \mathbf{u} + \mathbb{I} p \\ \rho \mathbf{u} \end{cases}$, (Navier-Stokes)
- $\mathcal{A} = \begin{cases} -R(\mathbf{H} \otimes \mathbb{I}) \\ R(\mathbf{E} \otimes \mathbb{I}) \end{cases}, R = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & -1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \end{bmatrix}$, (Maxwell)
- $\mathcal{C}, \mathbb{K}, \mathbb{B}$ — piecewise-constant tensors with discontinuity at mesh faces.





General Framework

- Gauss-Green theorem:

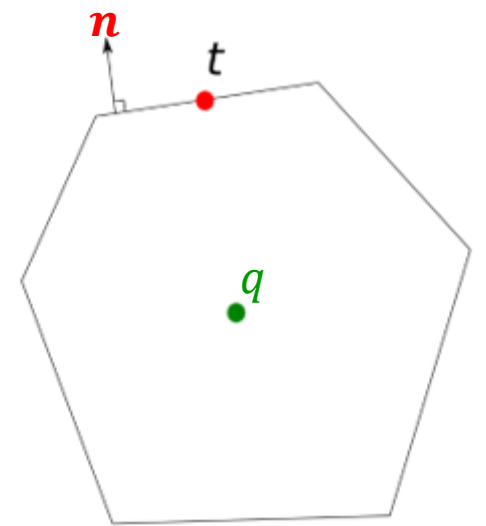
$$\operatorname{div}(\mathcal{A}(q)) = g \Rightarrow \oint_{\partial V} \mathcal{A}(q) d\mathbf{S} = \int_V g dV \Rightarrow \frac{1}{|V|} \sum_{f \in \mathcal{F}(V)} \mathcal{A}_f \mathbf{n} |f| = \mathbf{g}_V$$

- General flux formula:

$$\mathbf{t} = \mathcal{A}_f \mathbf{n} = \mathcal{A}(q_f) \mathbf{n} = M(\mathbf{n}) q_f + W(\mathbf{n})(q \otimes \nabla) + R,$$

- Here

- q_f - $m \times 1$ unknown vector at interface,
- $(q \otimes \nabla)$ - $md \times 1$ gradient of unknown at cell center,
- $M(\mathbf{n})$ - $m \times m$ matrix of **hyperbolic** component,
- $W(\mathbf{n})$ - $m \times md$ matrix of **elliptic** component,
- R - $m \times 1$ additional terms (gravity, previous time step, etc).





General Framework

- General flux expression:

$$\mathbf{t}_i = M_i \mathbf{q}_{f_i} + W_i(q_i \otimes \nabla) + R_i.$$

- Condition with constraints C (i.e. sliding) and condition F (i.e. friction):

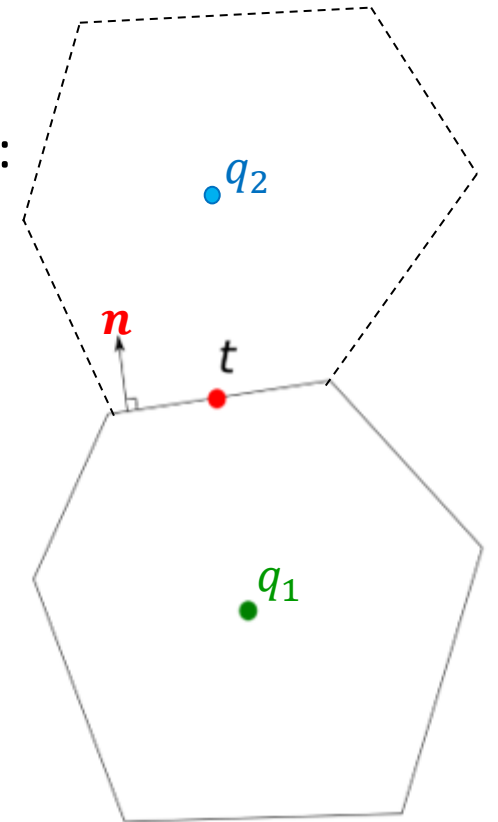
$$(\mathbb{I} - C)\mathbf{t}_i = \mathbf{F}, \quad C \mathbf{q}_{f_1} = C \mathbf{q}_{f_2}.$$

- Decompositions:

- $M_i = M_i^+ + M_i^-$ - eigen-decomposition of the matrix,
- $W_i = \Lambda_i(\mathbb{I} \otimes \mathbf{n}^T) + \Gamma_i$ - normal projection,
- $(q_i \otimes \nabla) \approx \frac{1}{r_i}(q_{f_i} - q_i)\mathbf{n} + \left(\mathbb{I} - \frac{1}{r_i}\mathbf{n}(x_f - x_i)^T\right)(q_i \otimes \nabla).$

- Assumption (unknown is piecewise-continuous):

- $(\mathbb{I} - \mathbf{nn}^T)(q_1 \otimes \nabla) = (\mathbb{I} - \mathbf{nn}^T)(q_2 \otimes \nabla) = G_\tau.$





General Framework

- General flux expression:

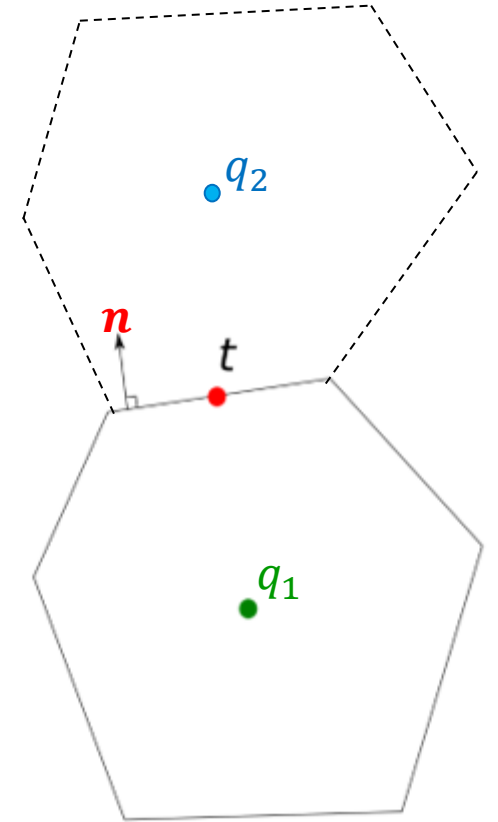
$$\mathbf{t}_i = M_i \mathbf{q}_{f_i} + W_i (q_i \otimes \nabla) + R_i.$$

- System of conditions:

$$\begin{bmatrix} r_1^{-1} \Lambda_1 + M_1^+ & & -C \\ & r_2^{-1} \Lambda_2 - M_2^- & C \\ -C & & C \end{bmatrix} \begin{bmatrix} \mathbf{q}_{f_1} \\ \mathbf{q}_{f_2} \\ \mathbf{t} \end{bmatrix} = \begin{bmatrix} (r_1^{-1} \Lambda_1 - M_1^-) \mathbf{q}_1 \\ (r_2^{-1} \Lambda_2 + M_2^+) \mathbf{q}_2 \end{bmatrix}$$

$$- \begin{bmatrix} (r_1^{-1} \Lambda_1 - M_1^-) \otimes \mathbf{y}_1^T + M_1 \otimes \mathbf{x}_f^T - (r_1^{-1} \Lambda_1 + M_1^+) X_h^T + \Gamma_1 \\ (r_2^{-1} \Lambda_2 + M_2^+) \otimes \mathbf{y}_2^T + M_2 \otimes \mathbf{x}_f^T - (r_2^{-1} \Lambda_2 - M_2^-) X_h^T - \Gamma_2 \end{bmatrix} G_\tau$$

$$- \begin{bmatrix} r_1 M_1^- \otimes n^T (q_1 \otimes \nabla) + R_1 \\ r_2 M_2^+ \otimes n^T (q_2 \otimes \nabla) - R_2 \end{bmatrix}$$

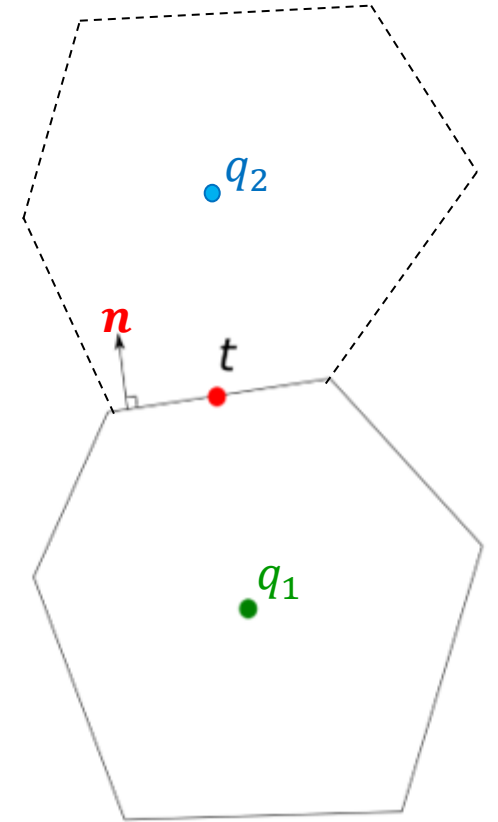




General Framework

- Solve the system:
 - for Ct to get the flux expression $t = Ct + F$.
 - Two-point part and transversal correction.
 - for q_{f_1}, q_{f_2} and tune X_h to eliminate G_τ to get the interpolation.
- Similar concept to obtain q_f and the flux from the boundary conditions:

$$\alpha q_f + \beta q \otimes \nabla = \gamma$$





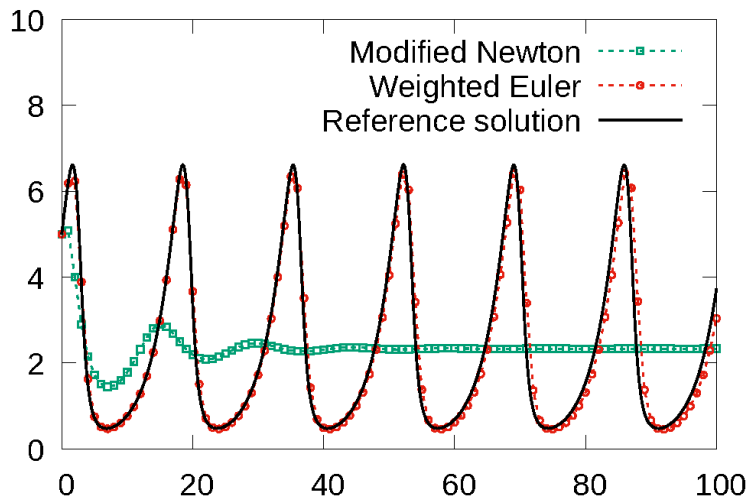
Reactions

- System of reactions:

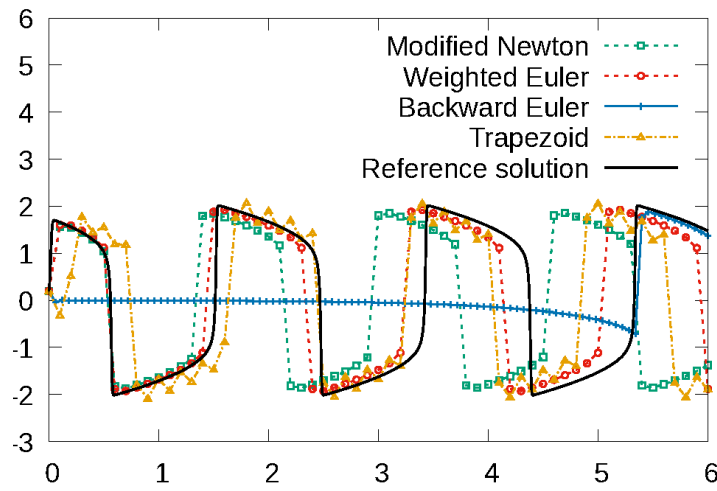
$$\frac{\partial \mathbf{x}}{\partial t} = \mathbf{r}, \rightarrow |V^{n+1}| \mathbf{x}^{n+1} - |V^n| \mathbf{x}^n = |V(t)| (\mathbf{W} \mathbf{r}^{n+1} + (\mathbb{I} - \mathbf{W}) \mathbf{r}^n),$$

- where \mathbf{W} is a matrix, filtering eigenvalues in $\mathbf{J} = \frac{\partial \mathbf{r}^{n+1}}{\partial \mathbf{x}^T}$, and reproducing exponential integrator:

$$\mathbf{W} = \phi \left(\frac{|V(t)|}{|V^{n+1}|} \mathbf{J} \right), \quad \phi(z) = z^{-1} - (e^z - 1)^{-1}.$$



Lotka-Volterra system



Van der Pol system

I. Butakov and K. Terekhov **Two Methods for the Implicit Integration of Stiff Reaction Systems**. Computational Methods in Applied Mathematics, 2022



Publications on FV

- K. Terekhov, B. Mallison, and H. Tchelepi. **Cell-centered nonlinear finite-volume methods for the heterogeneous anisotropic diffusion problem.** Journal of Computational Physics, 2017.
- K. Terekhov, and Yu. Vassilevski. **Finite volume method for coupled subsurface flow problems, I: Darcy problem.** Journal of Computational Physics, 2019
- K. Terekhov, and H. Tchelepi. **Cell-centered finite-volume method for elastic deformation of heterogeneous media with full-tensor properties.** Journal of Computational and Applied Mathematics, 2020
- K. Terekhov. **Cell-centered finite-volume method for heterogeneous anisotropic poromechanics problem.** Journal of Computational and Applied Mathematics, 2020
- K. Terekhov. **Collocated Finite-Volume Method for the Incompressible Navier-Stokes Problem,** Journal of Numerical Mathematics, 2020
- Yu. Vassilevski, K. Terekhov, K. Nikitin, I. Kapyrin. **Parallel finite volume computation on general meshes,** Springer Book, 2020
- K. Terekhov. **Multi-physics flux coupling for hydraulic fracturing modelling within INMOST platform.** Russian Journal of Numerical Analysis and Mathematical Modelling, 2020
- K. Terekhov. **Fully-Implicit Collocated Finite-Volume Method for the Unsteady Incompressible Navier-Stokes Problem,** Lecture Notes in Computational Science and Engineering, 2021
- K. Terekhov, and Yu. Vassilevski. **Finite volume method for coupled subsurface flow problems, II: Poroelasticity.** Journal of Computational Physics, 2022
- K. Terekhov **Pressure boundary conditions in the collocated finite-volume method for the steady Navier–Stokes equations.** Computational Mathematics and Mathematical Physics, 2022
- I. Butakov and K. Terekhov **Two Methods for the Implicit Integration of Stiff Reaction Systems.** Computational Methods in Applied Mathematics, 2022
- K. Terekhov, I. Butakov., A. Danilov, Yu. Vassilevski, **Dynamic adaptive moving mesh finite-volume method for the blood flow and coagulation modeling.** *International Journal for Numerical Methods in Biomedical Engineering*, e3731, 2023
- **K. Terekhov. General finite-volume framework for saddle-point problems of various physics. Russian Journal of Numerical Analysis and Mathematical Modelling, 2021**
 - **We consider problems from this work**



Numerical experiments



Problem 1

Problem 1 (Ph2-z) *Two-phase oil recovery problem* ($\mathbf{b} = 2$)

O-type multi-point flux approximation for water-oil flow.

Fully-implicit cell-centered finite-volume discretization method.

2D grids $16 \times 16 \times 1$, $32 \times 32 \times 1$, $64 \times 64 \times 1$ with time steps 2.0, 1.0, 0.5 days.

At 13-th time step: Ph2-z1, Ph2-z2, Ph2-z3.

$$\partial_t(\phi(p)\rho_\alpha(p)S_\alpha) - \operatorname{div}(\rho_\alpha(p)k_{r\alpha}(S_\alpha)\mu_\alpha(p)^{-1}\mathbb{K}\nabla p) = q_\alpha, \quad \alpha = w, o.$$

where p is the water pressure and S_o is the oil saturation with constraint $S_w + S_o = 1$.



Problems 2-3

Problem 2 (Ph3-injg) *Three-phase black-oil recovery with **gas** injection ($\mathbf{b} = 3$)*

Water-oil-gas flow with two wells.

2D grids $16 \times 16 \times 1$, $32 \times 32 \times 1$, $64 \times 64 \times 1$ with time steps 0.0008, 0.0004, 0.0002 days.

$$\partial_t(\phi(p)\rho_\alpha(p)S_\alpha) - \operatorname{div}(\rho_\alpha(p)k_{r\alpha}(S_\alpha)\mu_\alpha(p)^{-1}\mathbb{K}\nabla p) = q_\alpha, \quad \alpha = w, o.$$

$$\partial_t(\phi\rho_g S_g + \phi R_s \rho_{og} S_o) - \operatorname{div}((\rho_g k_{rg} \mu_g^{-1} + R_s \rho_{og} k_{ro} \mu_o^{-1}) \mathbb{K} \nabla p) = q_g$$

Problem 3 (Ph3-injw) *Three-phase black-oil recovery with **water** injection ($\mathbf{b} = 3$)*

Water-oil-gas flow with two wells.

2D grids $16 \times 16 \times 1$, $32 \times 32 \times 1$, $64 \times 64 \times 1$ with time steps 0.002, 0.001, 0.0005 days.



Problems 4-5

Problem 4 (Ccfv-sh, Ccfv-st, Ccfv-sd) *Linear elasticity: beam under **shear** ($\mathbf{b} = 3$)*

Cell-centered finite-volume (Ccfv) method for the stationary heterogeneous anisotropic linear elasticity problem for compressible materials.

hex-grid: $4 \times 4 \times 20$, $8 \times 8 \times 40$, $16 \times 16 \times 80$; **tet-grid:** $4 \times 4 \times 20 \times 6$, $8 \times 8 \times 40 \times 6$, $16 \times 16 \times 80 \times 64$;
dual-grid: 525, 3321, 23409

$$-\mathbf{div}(\mathbf{C} : \boldsymbol{\epsilon}) = \mathbf{b}, \quad \boldsymbol{\epsilon} = \frac{\mathbf{u}\nabla^T + \nabla\mathbf{u}^T}{2}$$

Problem 5 (Ccfv-th, Ccfv-tt, Ccfv-td) *Linear elasticity: beam under **torsion** ($\mathbf{b} = 3$)*

Cell-centered finite-volume (Ccfv) method for the stationary heterogeneous anisotropic linear elasticity problem for compressible materials.

The same grids and equations.



Problems 6

Problem 6 (NS-t) *Navier–Stokes flow in a tube* ($\mathbf{b} = 4$)

The Poiseuille flow through a cylindrical pipe with the prismatic mesh for a cylinder with radius $1/2$ and length 5.

3D grids: 820, 5600, 40720 and time steps 1.0, 0.5, 0.25 sec.

$$\partial_t \rho \mathbf{u} + \mathbf{div} (\rho \mathbf{u} \mathbf{u}^T - \mu \nabla \mathbf{u} + \mathbb{I} p) = \mathbf{0}, \quad \mathbf{div} (\mathbf{u}) = 0$$

for velocity \mathbf{u} and pressure p , subject to appropriate boundary conditions.



Problems 7-8

Problem 7 (Rigid-s) *Stationary incompressible elasticity: beam under **shear** ($\mathbf{b} = 4$)*

As the incompressible linear elasticity problem we consider the equation for the elastic body equilibrium.

3D grid sizes: $8 \times 8 \times 20$, $16 \times 16 \times 40$, $32 \times 32 \times 80$.

$$-\mathbf{div}(\boldsymbol{\sigma} - \mathbb{I}p) = \mathbf{g}, \quad K^{-1}p + \mathbf{div}(\mathbf{u}) = 0, \quad \mathbf{S} : \boldsymbol{\sigma} = \frac{\mathbf{u}\nabla^T + \nabla\mathbf{u}^T}{2}$$

for displacement \mathbf{u} and structural pressure p with the proper boundary conditions.

Problem 8 (Rigid-t) *Stationary incompressible elasticity: beam under **torsion** ($\mathbf{b} = 3$)*

The same grids and equations.



Problems 9-10

Problem 9 (Biot) *Biot poroelasticity problem* ($\mathbf{b} = 4$)

Interaction between a compressible fluid and a compressible porous body in the absence of gravitational forces.

2D grids $22 \times 22 \times 1$, $46 \times 46 \times 1$, $94 \times 94 \times 1$ with time steps 4, 2, 1 sec.

$$-\operatorname{div}(\mathbf{C} : \boldsymbol{\epsilon} - Bp) = \mathbf{g}, \quad M^{-1} \partial_t p + B : \partial_t \boldsymbol{\epsilon} - \operatorname{div}(\mu^{-1} \mathbb{K} \nabla p) = q$$

for displacement \mathbf{u} and fluid pressure p with the proper boundary conditions.

Problem 10 (Poromech) *Barry & Mercer poromechanics problem* ($\mathbf{b} = 4$)

Barry & Mercer test with pulsating source for the above Biot system of equations.

2D grids $22 \times 22 \times 1$, $46 \times 46 \times 1$, $94 \times 94 \times 1$ with time steps 4, 2, 1 sec.

The linear system stored from the first time step.



Problem 11

Problem 11 (Maxwell) *Non-stationary Maxwell problem* ($\mathbf{b} = 6$)

Maxwell equations for the interaction of electric and magnetic fields.

The bounded square cavity problem with the parameter $k = 1/24$ is considered.

3D grids $8 \times 8 \times 8$, $16 \times 16 \times 16$, $32 \times 32 \times 32$ with time steps 0.04, 0.02, 0.01 sec.

$$\partial_t \epsilon \mathbf{E} + \sigma \mathbf{E} = \nabla \times \mathbf{H} - \mathbf{I}, \quad \partial_t \mu \mathbf{H} = -\nabla \times \mathbf{E}$$

for electric field \mathbf{E} and magnetic field \mathbf{H} with the proper boundary conditions.



Structural properties [1/2]...

Problem	b	N	N_{nd}	N_{nz}	N_{zr}	Description
Ph2-z1	2	512	0	3695	7.2	Two-phase oil recovery problem
Ph2-z2	2	2048	0	12576	6.1	
Ph2-z3	2	8192	0	46427	5.6	
Ph3-injg1	3	768	512	10344	13.4	Three-phase black-oil recovery (gas injection)
Ph3-injg2	3	3072	2048	42702	13.9	
Ph3-injg3	3	12288	8192	173454	14.1	
Ph3-injw1	3	768	502	10308	13.4	Three-phase black-oil recovery (water injection)
Ph3-injw2	3	3072	2032	42652	13.8	
Ph3-injw3	3	12288	8162	173330	14.1	
Ccfv-sd1	3	1575	0	55053	34.9	Beam under shear (dual)
Ccfv-sd2	3	9963	0	391473	39.2	
Ccfv-sd3	3	70227	0	2945241	41.9	
Ccfv-sh1	3	960	0	35127	36.5	Beam under shear (hex)
Ccfv-sh2	3	7680	0	291739	37.9	
Ccfv-sh3	3	61440	0	2336498	38.0	
Ccfv-st1	3	5760	0	222144	38.5	Beam under shear (tet)
Ccfv-st2	3	46080	0	1922481	41.7	
Ccfv-st3	3	368640	0	15977699	43.3	
Ccfv-td1	3	1575	0	55053	34.9	Beam under torsion (dual)
Ccfv-td2	3	9963	0	391473	39.2	
Ccfv-td3	3	70227	0	2945241	41.9	



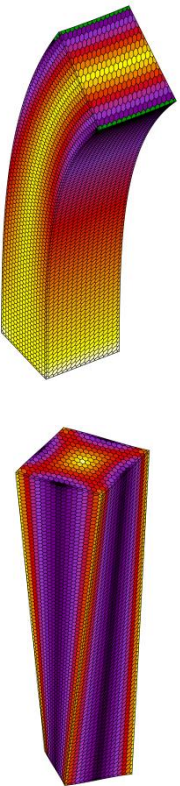
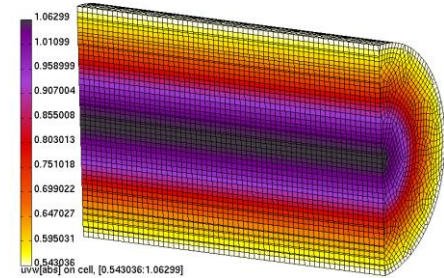
Structural properties ...[2/2]

Problem	b	N	N_{nd}	N_{nz}	N_{zr}	Description
Ccfv-th1	3	960	0	35012	36.4	Beam under torsion (hex)
Ccfv-th2	3	7680	0	291997	38.0	
Ccfv-th3	3	61440	0	2335467	38.0	
Ccfv-tt1	3	5760	0	222145	38.5	Beam under torsion (tet)
Ccfv-tt2	3	46080	0	1922484	41.7	
Ccfv-tt3	3	368640	0	15977695	43.3	
NS-t1	4	11040	0	1709692	154.8	Navier–Stokes flow in a tube
NS-t2	4	80640	0	13248296	164.2	
NS-t3	4	614400	0	97042502	157.9	
Rigid-s1	4	5120	0	190022	37.1	Incompressible elasticity (beam under shear)
Rigid-s2	4	40960	0	1319887	32.2	
Rigid-s3	4	327680	0	9799749	29.9	
Rigid-t1	4	5120	0	190058	37.1	Incompressible elasticity (beam under torsion)
Rigid-t2	4	40960	0	1319758	32.2	
Rigid-t3	4	327680	0	9799179	29.9	
Biot1	4	1936	0	38246	19.7	Biot poroelasticity problem
Biot2	4	8464	0	167070	19.7	
Biot3	4	35344	0	791236	22.3	
Poromech1	4	1936	0	47175	24.3	Barry & Mercer poromechanics
Poromech2	4	8464	0	209244	24.7	
Poromech3	4	35344	0	930623	26.3	
Maxwell1	6	3072	0	59136	19.2	Non-stationary Maxwell problem
Maxwell2	6	24576	0	519168	21.1	
Maxwell3	6	196608	0	4337664	22.0	



Block AMG on Saddle-Point Problems

NS: analytical Pousielle solution in a pipe
rigid-s: analytical solution for rigid beam under shear
rigid-t: analytical solution for rigid beam under torsion



Problem	Size	Block GS, T	Block GS, Nit	Block AMG, T	AMG, Nit	Block Size
NS-1	11040	0,581	64	1,089	5	4
NS-2	80640	3,127	133	3,262	4	4
NS-3	614400	38,044	270	20,6	6	4
rigid-s-1	5120	-	-	1,196	30	4
rigid-s-2	40960	-	-	2,552	42	4
rigid-s-3	327680	-	-	16,614	58	4
rigid-t-1	5120	-	-	0,883	29	4
rigid-t-2	40960	-	-	2,657	44	4
rigid-t-3	327680	-	-	16,314	62	4

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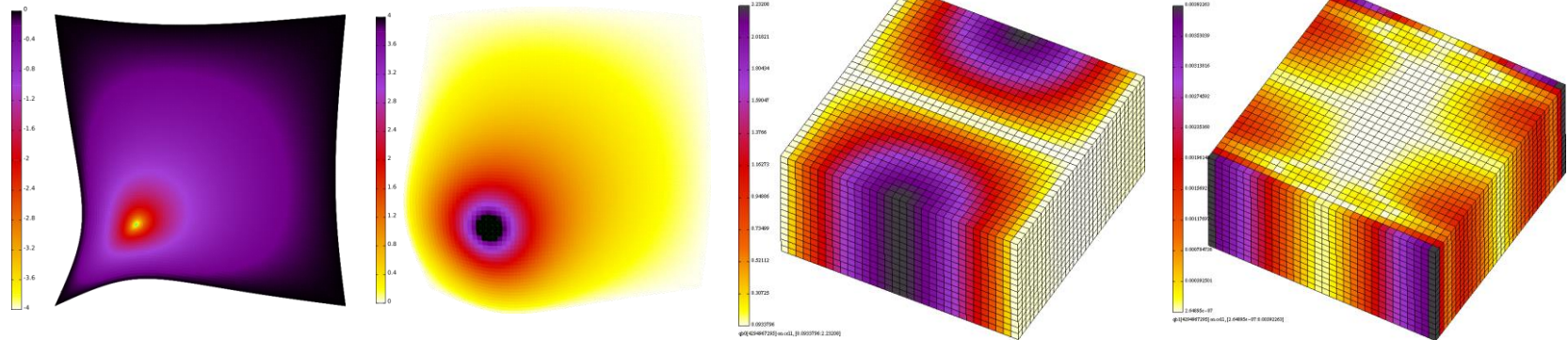
Almost linear scaling!



Block AMG on Saddle-Point Problems

biot: Barry & Mercer analytical solution for pulsating source

maxwell: analytic solution for cavity bounded by perfect electric conductor



Problem	Size	Block GS, T	Block GS, Nit	Block AMG, T	AMG, Nit	Block Size
biot-1	1936	0,353	56	0,603	8	4
biot-2	8464	0,737	92	0,787	9	4
biot-3	35344	1,261	206	1,212	10	4
maxwell-1	3072	0,221	7	0,323	3	6
maxwell-2	24576	0,49	7	1,365	3	6
maxwell-3	196608	2,545	7	5,615	3	6

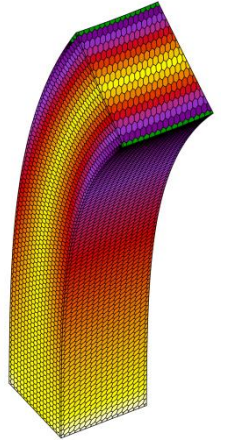
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Almost linear scaling!



Block AMG on Block Elliptic Problems



shear: analytical solution for elastic beam under share
tet, hex, dual: tetrahedral, hexahedral and dual meshes

Problem	Size	Block GS, T	Block GS, Nit	Block AMG, T	AMG, Nit	Block Size
shear-tet-1	5760	0,732	325	0,804	62	3
shear-tet-2	46080	-	-	2,626	69	3
shear-tet-3	363640	-	-	23,392	89	3
shear-hex-1	960	0,4	114	0,475	24	3
shear-hex-2	7680	0,873	276	1,123	31	3
shear-hex-3	61440	3,087	507	3,363	35	3
shear-dual-1	1575	0,523	131	0,51	34	3
shear-dual-2	9963	0,801	285	1,299	45	3
shear-dual-3	70227	3,892	609	3,4	56	3

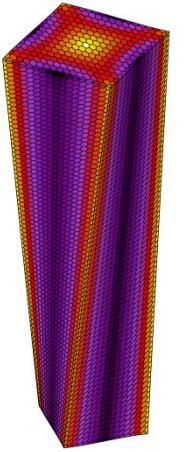
Almost linear scaling!

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Block AMG on Block Elliptic Problems



torsion: analytical solution for elastic beam under torsion

tet, hex, dual: tetrahedral, hexahedral and dual meshes

Problem	Size	Block GS, T	Block GS, Nit	Block AMG, T	AMG, Nit	Block Size
torsion-tet-1	5760	2,113	972	0,83	62	3
torsion-tet-2	46080	11,764	4220	2,7	69	3
torsion-tet-3	368640	-	-	18,775	88	3
torsion-hex-1	960	0,353	106	0,74	23	3
torsion-hex-2	7680	0,677	210	1,017	34	3
torsion-hex-3	61440	3,326	382	3,615	61	3
torsion-dual-1	1575	0,425	126	0,695	32	3
torsion-dual-2	9963	1,318	535	1,018	49	3
torsion-dual-3	70227	10,783	2336	3,974	79	3

Almost linear scaling!

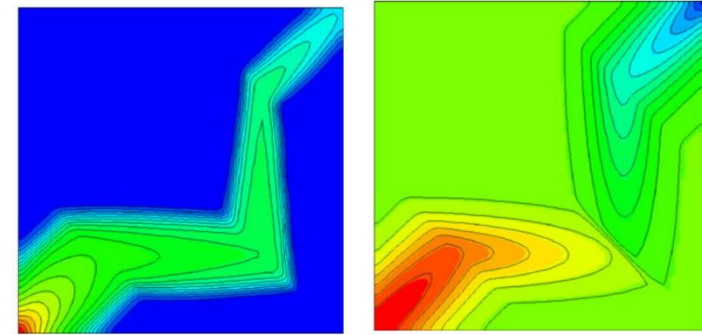
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Block AMG on Oil & Gas Systems

twophase: oil recovery with water
threephase: black oil recovery
gas, water: gas or water are injected



Problem	Size	Block GS, T	Block GS, Nit	Block AMG, T	AMG, Nit	Block Size
twophase-1	512	0,229	64	0,232	11	2
twophase-2	2048	0,329	148	0,249	14	2
twophase-3	8192	0,749	295	1,445	22	2
threephase-gas-1	768	0,179	7	0,184	4	3
threephase-gas-2	3072	0,285	16	0,265	9	3
threephase-gas-3	12288	0,328	22	0,945	25	3
threephase-water-1	768	0,423	7	0,18	4	3
threephase-water-2	3072	0,223	15	0,22	6	3
threephase-water-3	12288	0,372	21	0,889	23	3

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Almost linear scaling! Black oil systems **break down** on **phase switch**: mixing gas saturation and bubble point pressure in interpolation.

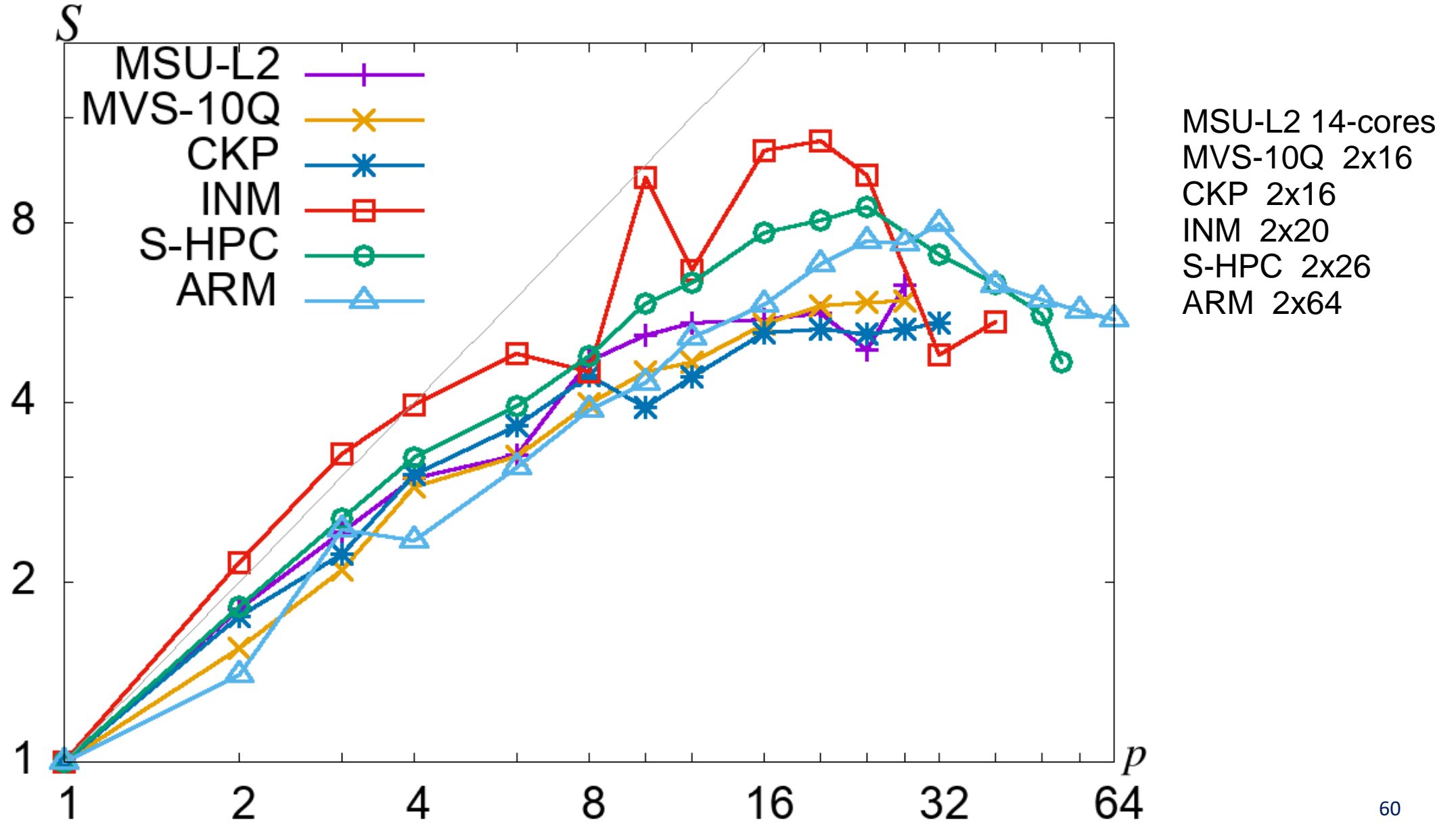


BAMG for 16 cores on INM RAS cluster

Problem	T	T _s	T _{it}	Nit	Lvl	S	S _s	S _{it}
Ph2-z3	0.1224	0.0323	0.0919	27	6	1.06	1.24	0.99
Ph3-injg3	0.1762	0.0535	0.1231	23	7	1.36	1.08	1.48
Ph3-injw3	0.1809	0.0529	0.1284	24	7	1.33	1.10	1.42
Ccfv-sd3	8.7520	0.3974	8.4062	546	5	2.52	1.87	2.54
Ccfv-sh3	1.8455	0.5675	1.2839	56	5	3.51	1.98	4.17
Ccfv-st3	17.9705	1.7372	16.2523	186	6	7.56	2.15	8.13
Ccfv-td3	1.8186	0.4040	1.4218	70	5	3.68	1.88	4.17
Ccfv-th3	2.6281	0.5804	2.0560	95	5	3.46	1.91	3.89
Ccfv-tt3	9.7643	1.5889	8.1925	93	6	6.68	2.37	7.50
NS-t3	16.3802	13.4383	2.9429	6	6	3.18	2.23	7.47
Rigid-s3	35.4617	3.0153	32.4814	312	6	2.97	2.71	2.99
Rigid-t3	12.0035	3.0038	9.0131	87	6	10.58	2.72	13.19
Biot3	0.2299	0.1434	0.0881	11	5	2.65	1.88	3.87
Poromech3	0.2692	0.1747	0.0959	12	5	2.58	1.74	4.07
Maxwell3	2.5852	2.3507	0.2347	3	6	2.59	2.19	6.54

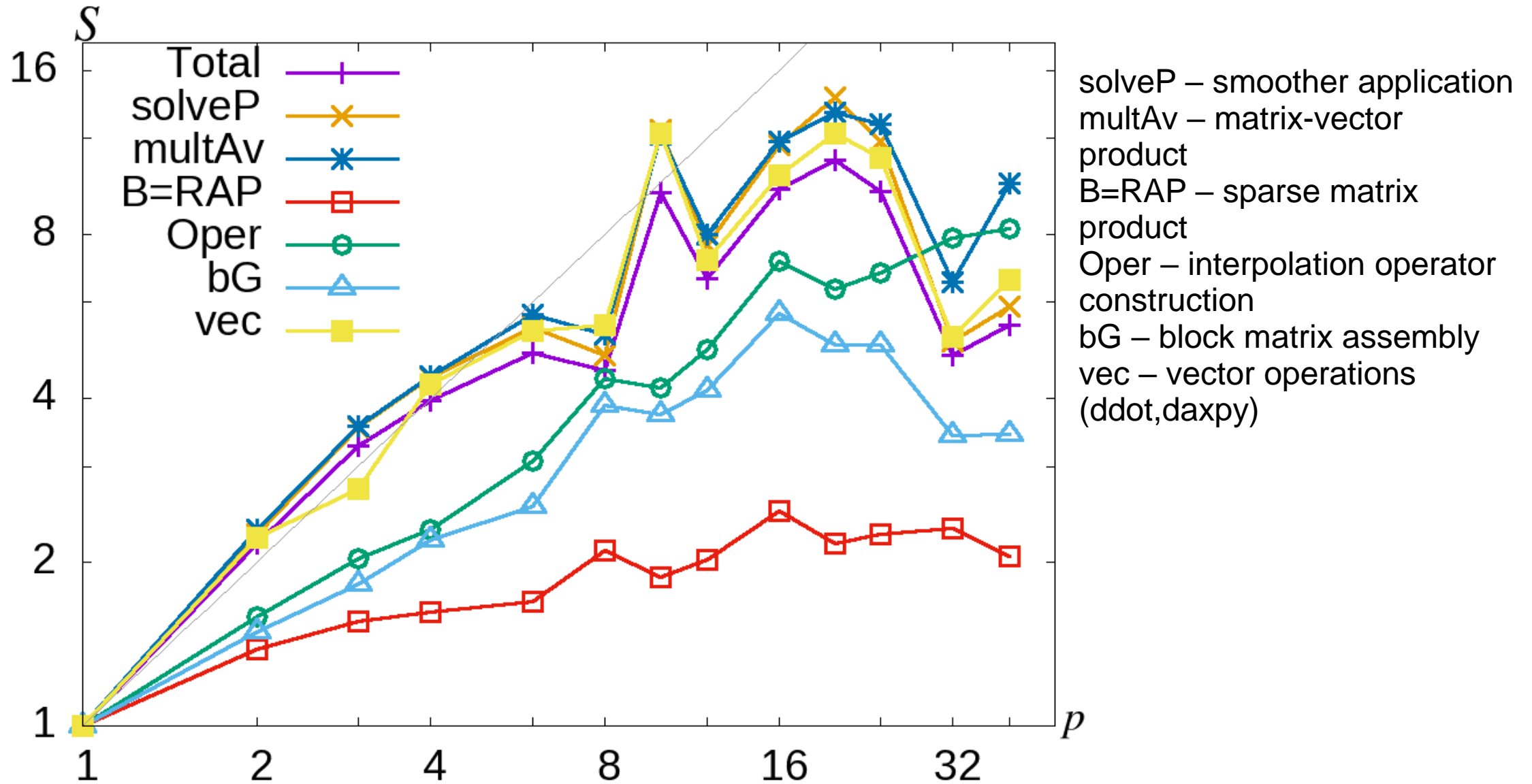


Actual speedup of BAMG for Rigid-t3 problem





Procedure scalability over 40 processors





Future Works

- Tackle problems that block AMG can't solve yet:
 - blood coagulation, mixed Darcy
 - method **breaks down** if block weights become **singular**
- Support **variable block** size:
 - fluid-structure interaction problems
 - mixed physics problems
- Bootstrap adaptive version
- SVD to make positive definite diagonal: $A_{ii} = USV^T \rightarrow \bar{A}_{ii} = VU^T A_{ii}$
- Eigen-splitting to detect strong connections: $A_{ik} = A_{ik}^+ + A_{ik}^-$ with $A_{ik}^+ \geq 0$ contributing to diagonal and $A_{ik}^- < 0$ contributing to weight

Thank you for your attention

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