

A time-parallel Navier-Stokes solver using Augmented Lagrangian acceleration and space-time multigrid methods

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Motivation

Incompressible Navier-Stokes equation

$$\begin{aligned}\partial_t \mathbf{u} - \nu \Delta \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \nabla p &= \mathbf{f} & (x, t) \in \Omega \times (0, T) \\ \nabla \cdot \mathbf{u} &= 0 & (x, t) \in \Omega \times (0, T)\end{aligned}\tag{1}$$

with $\mathbf{u}(x, t) \in \mathbb{R}^d$, $p(x, t) \in \mathbb{R}$.

- FEAT3:
 - FE software package with geometric multigrid solvers (monolithic and splitting approaches)
 - Spatial parallelization by domain decomposition (data parallel)
 - DNS for low and moderate Reynolds numbers
 - Non-Newtonian fluids
 - Only sequential time stepping
- This presentation:
 - Additional parallelism (in space or time) by solving multiple time steps at once
 - LSC preconditioner, Augmented Lagrangian
 - Space-time multigrid for velocity problems
 - Decoupled pressure problems

Test case: DFG-Benchmark 3

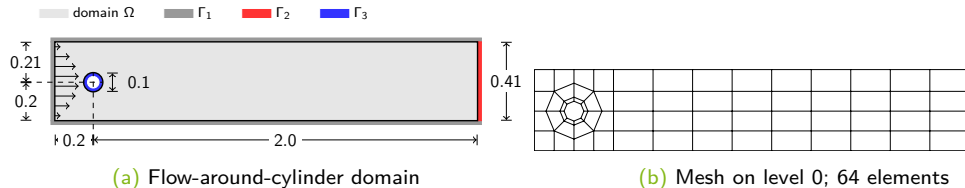


Figure: Test domain

- Instationary parabolic inflow, final time $T = 8$
- Parabolic inflow $\mathbf{v}(x, t) = v_{max} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \sin\left(\frac{1}{8}\pi t\right) \frac{4x_2(0.41-x_2)}{0.41^2}$ on Γ_1
- Standard test case: $Re = 100$, $\nu = 10^{-3}$, $v_{max} = 1.5$
- Modified test case: $Re = 10$, $\nu = 10^{-2}$, $v_{max} = 1.5$
- Modified test case: $Re = 2$, $\nu = 10^{-2}$, $v_{max} = 0.3$

Benchmark 3 - Velocity fields

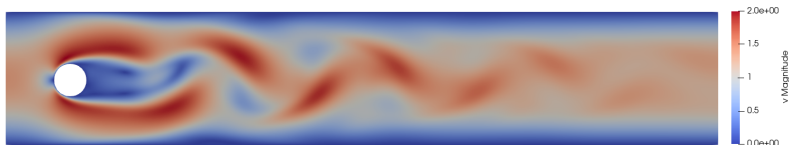


Figure: Bench 3, $\nu = 10^{-3}$, $v_{max} = 1.5$: velocity v at $t = 5$

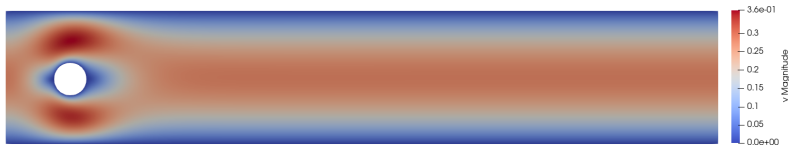


Figure: Bench 3, $\nu = 10^{-2}$, $v_{max} = 0.3$: velocity v at $t = 5$

Outline

1 Motivation

2 Time simultaneous Multigrid methods for linear parabolic problems

- Multigrid waveform relaxation
- Space-time multigrid for linear problems

3 Navier-Stokes solver

- All-at-once LSC preconditioner
- Augmented Lagrangian acceleration

4 Conclusion

Linear Multigrid methods

Linear parabolic evolution equation

$$\partial_t u(x, t) - \mathcal{L}u(x, t) = f(x, t) \quad (x, t) \in \Omega_T := \Omega \times (0, T)$$

$$u(x, t) = g(x, t) \quad (x, t) \in \partial\Omega \times (0, T)$$

$$u(x, 0) = u_0(x) \quad x \in \Omega$$

with $T > 0$, $\Omega \subset \mathbb{R}^d$ and an elliptic differential operator $\mathcal{L}(t)$.

'All-at-once' system with a linear one-step method:

$$\underbrace{\begin{bmatrix} \mathbf{A}_{i,1} & & & & \\ \mathbf{A}_{e,1} & \mathbf{A}_{i,2} & & & \\ & \mathbf{A}_{e,2} & \mathbf{A}_{i,3} & & \\ & & \ddots & \ddots & \\ & & & \mathbf{A}_{e,K-1} & \mathbf{A}_{i,K} \end{bmatrix}}_{=:\mathbf{A}_K \in \mathbb{R}^{NK \times NK}} \underbrace{\begin{bmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \mathbf{u}_3 \\ \vdots \\ \mathbf{u}_K \end{bmatrix}}_{=:\mathbf{u} \in \mathbb{R}^{NK}} = \underbrace{\begin{bmatrix} \mathbf{f}_1 - \mathbf{A}_{e,0}\mathbf{u}_0 \\ \mathbf{f}_2 \\ \mathbf{f}_3 \\ \vdots \\ \mathbf{f}_K \end{bmatrix}}_{=:\mathbf{f} \in \mathbb{R}^{NK}} \quad (2)$$

Multigrid waveform relaxation

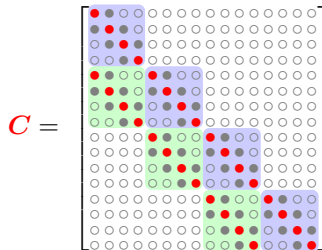
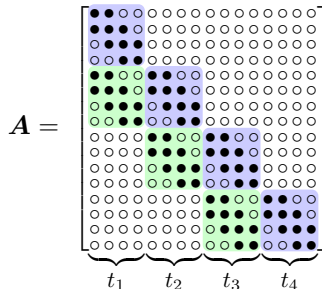
- Multigrid waveform relaxation, Multigrid dynamic iteration [Lubich, Ostermann (1987)]
- Transfer operators (*semi coarsening in space*):
 - Standard coarsening for each time step
 - Prolongation:

$$P_{\tau,2h}^{\tau,h} = I_K \otimes P_{2h}^h$$

- Restriction:

$$R_{\tau,h}^{\tau,2h} = I_K \otimes R_h^{2h} = (P_{\tau,2h}^{\tau,h})^T$$

- Line smoothing in time direction (block preconditioned GMRES smoother)
 - Preconditioner C^{-1}



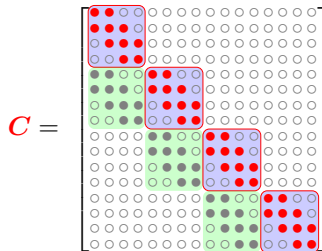
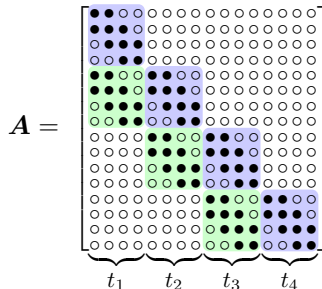
STMG: Multigrid applied to the all-at-once system

- Space-time multigrid [Gander, Neumüller (2016)]
- Transfer operators (*semi coarsening in time*):
 - Coarsening in time direction (restriction forward in time)

$$P_{2\tau,h}^{\tau,h} = P_{2\tau}^{\tau} \otimes I_N$$

$$R_{\tau,h}^{2\tau,h} = R_{\tau}^{2\tau} \otimes I_N = (P_{2\tau,h}^{\tau,h})^T$$

- Block-Jacobi smoother, $\omega = 0.5$ (/block preconditioned GMRES)
 - Preconditionier C^{-1}
 - Approximation of $\bar{C}^{-1}$ by a single V-cycle multigrid step in space
- particularly suited for DG(p) time discretization schemes



Linearized test problem

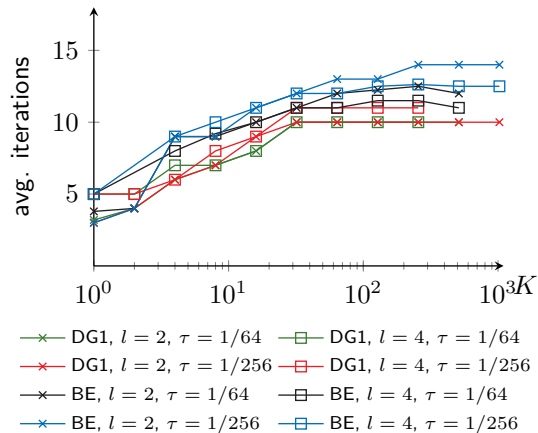
Convection-diffusion-reaction equation

$$\begin{aligned}\partial_t \mathbf{u} - \nu \Delta \mathbf{u} + (\mathbf{v} \cdot \nabla) \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{v} &= f & (x, t) \in \Omega \times (0, T) \\ \mathbf{u}(x, t) &= \mathbf{g}_D & (x, t) \in \Gamma_D \times (0, T) \\ \partial_n \mathbf{u} &= \mathbf{g}_N & (x, t) \in \Gamma_N \times (0, T) \\ \mathbf{u}(x, 0) &= \mathbf{u}_0(x) & x \in \Omega\end{aligned}\tag{3}$$

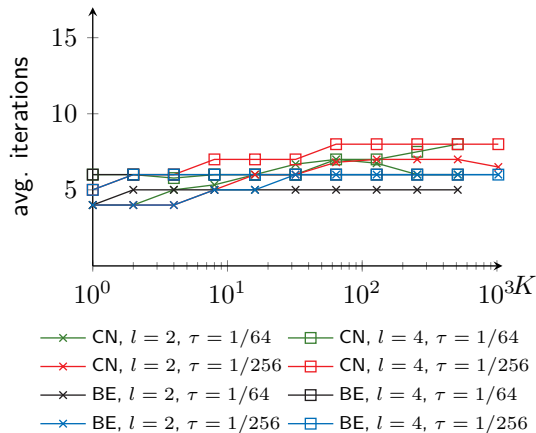
with $T > 0$, $\Omega \subset \mathbb{R}^d$ and $\Gamma_D \dot{\cup} \Gamma_N = \partial\Omega$.

- Convection-diffusion(-reaction) equation
- Reactive term from linearization by Newton's method
- Velocity field $\mathbf{v}$ is the solution of the non-linear Benchmark

Bench3 - Newton linearization - $\nu = 0.01$, $u_{max} = 0.3$



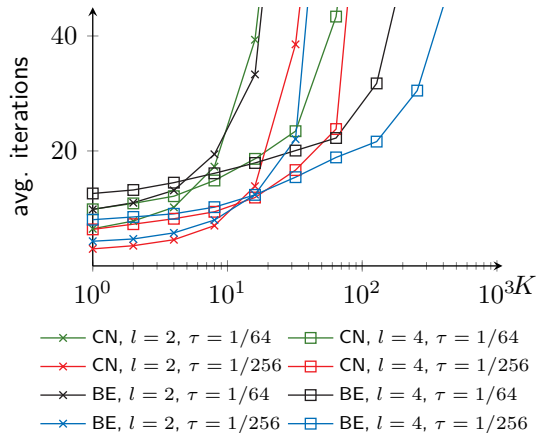
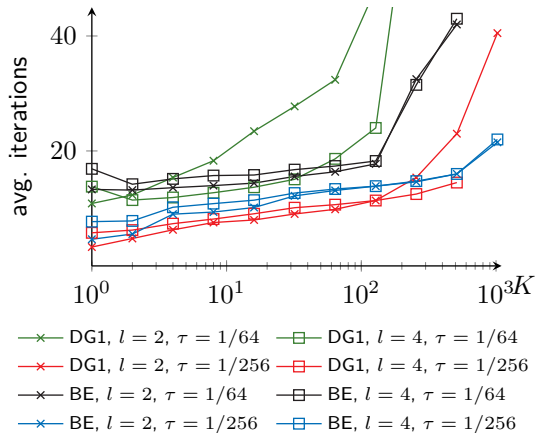
(a) STMG: 2+2 FGMRES smoothing steps, V-cycle



(b) WRMG: V-cycle, 4+4 FGMRES smoothing steps

Figure: Linearized test problem: number of iterations

Bench3 - Newton linearization - $\nu = 0.001$, $u_{max} = 1.5$



(a) STMG: F-cycle, 2+2 FGMRES smoothing steps

(b) WRMG: F-cycle, 4+4 FGMRES smoothing steps

Figure: Linearized test problem: number of iterations

WRMG: Strong scaling test

- Fritz@FAU (2x Intel Xeon Platinum 8360Y “Ice Lake” and 256GB DDR4 RAM per node, Blocking HDR 100 Infiniband interconnect)
- 2 FGMRES pre- and post-smoothing steps, F-cycle
- Level 5, 2048 total time steps
- Mesh with 48 coarse grid elements

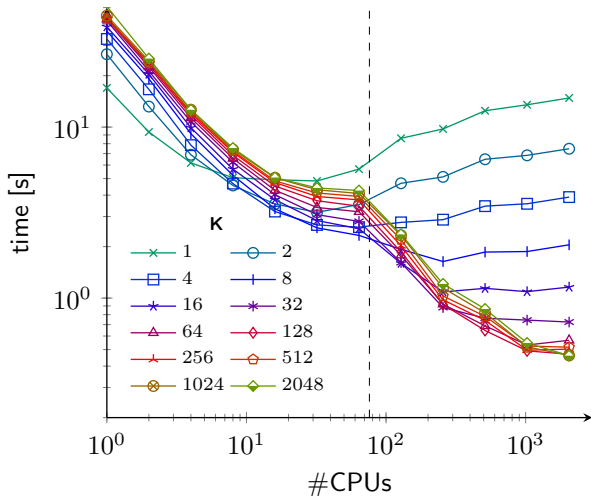


Figure: Solver time per iteration

Navier-stokes solver - Discretization

Incompressible Navier-Stokes equation

$$\begin{aligned}\partial_t \mathbf{u} - \nu \Delta \mathbf{u} + (\mathbf{u} \cdot \nabla) \mathbf{u} - \nabla p &= \mathbf{f} & (x, t) \in \Omega \times (0, T) \\ \nabla \cdot \mathbf{u} &= 0 & (x, t) \in \Omega \times (0, T)\end{aligned}$$

with $\mathbf{u}(x, t) \in \mathbb{R}^d$, $p(x, t) \in \mathbb{R}$.

- Linearization by Newton's method
- Space discretization: LBB-stable FE-pair Q2-P1(disc)
- Quadrature-based mass lumping
- For illustration: Backward Euler discretization in time

Linear system in each time step

$$\begin{aligned}(\mathbf{M} + \tau \mathbf{K} + \tau \mathbf{C}(v_k) + \tau \mathbf{R}(v_k)) \mathbf{u}_k + \tau \mathbf{B} p_k &= \mathbf{f}_k + \mathbf{M} \mathbf{u}_{k-1} \\ \mathbf{B}^T \mathbf{u}_k &= \mathbf{g}_k\end{aligned} \quad k = 1, \dots, K$$

All at once system

$$\mathbf{A}_{i,m} = \mathbf{M} + \tau \mathbf{K} + \tau \mathbf{C}(v_m) + \tau \mathbf{R}(v_m) \quad \mathbf{A}_{e,m} = -\mathbf{M}$$

$$\left(\begin{array}{cccc|cccc} \mathbf{A}_{i,1} & & & & \tau \mathbf{B} & & & \\ \mathbf{A}_{e,1} & \mathbf{A}_{i,2} & & & & \tau \mathbf{B} & & \\ & \mathbf{A}_{e,2} & \mathbf{A}_{i,3} & & & & \tau \mathbf{B} & \\ & & \ddots & \ddots & & & & \ddots \\ & & & \mathbf{A}_{e,K-1} & \mathbf{A}_{i,K} & & \tau \mathbf{B} & \\ \hline \tau \mathbf{B}^T & & & & & & & \\ & \tau \mathbf{B}^T & & & & & & \\ & & \tau \mathbf{B}^T & & & & & \\ & & & \tau \mathbf{B}^T & & & & \\ & & & & \tau \mathbf{B}^T & & & \end{array} \right) \begin{pmatrix} \mathbf{u}_1 \\ \mathbf{u}_2 \\ \mathbf{u}_3 \\ \vdots \\ \mathbf{u}_K \\ \mathbf{p}_1 \\ \mathbf{p}_2 \\ \mathbf{p}_3 \\ \vdots \\ \mathbf{p}_K \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 - \mathbf{A}_{e,0} \mathbf{u}_0 \\ \mathbf{f}_2 \\ \mathbf{f}_3 \\ \vdots \\ \mathbf{f}_K \\ \hline \tau \mathbf{g}_1 \\ \tau \mathbf{g}_2 \\ \tau \mathbf{g}_3 \\ \vdots \\ \tau \mathbf{g}_K \end{pmatrix}$$

$$\Leftrightarrow \begin{bmatrix} \mathbf{A}_K & \tilde{\mathbf{B}}_K \\ \tilde{\mathbf{B}}_K^T & \mathbf{0} \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{f} \\ \tilde{\mathbf{g}} \end{bmatrix}, \quad \tilde{\mathbf{B}}_K := \mathbf{I}_K \otimes \tilde{\mathbf{B}} := \mathbf{I}_K \otimes \tau \mathbf{B}$$

■ Similar structure for different time discretizations

Preconditioning

- Based on decomposition

$$\begin{bmatrix} \mathbf{A}_K & \tilde{\mathbf{B}}_K \\ \tilde{\mathbf{B}}_K^T & \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_K & \mathbf{0} \\ \tilde{\mathbf{B}}_K^T & -\mathbf{S}_K \end{bmatrix} \begin{bmatrix} \mathbf{I}_K & \mathbf{A}_K^{-1} \tilde{\mathbf{B}}_K \\ \mathbf{0} & \mathbf{I}_K \end{bmatrix} \quad \text{with} \quad \mathbf{S}_K = \tilde{\mathbf{B}}_K^T \mathbf{A}_K^{-1} \tilde{\mathbf{B}}_K$$

- Use FGMRES solver with block preconditioner $\mathbf{P}^{-1}$

$$\mathbf{P}^{-1} = \begin{bmatrix} \mathbf{A}_K & \mathbf{0} \\ \tilde{\mathbf{B}}_K^T & -\mathbf{C}_K \end{bmatrix}^{-1}$$

Preconditioning

- Based on decomposition

$$\begin{bmatrix} \mathbf{A}_K & \tilde{\mathbf{B}}_K \\ \tilde{\mathbf{B}}_K^T & \mathbf{0} \end{bmatrix} = \begin{bmatrix} \mathbf{A}_K & \mathbf{0} \\ \tilde{\mathbf{B}}_K^T & -\mathbf{S}_K \end{bmatrix} \begin{bmatrix} \mathbf{I}_K & \mathbf{A}_K^{-1} \tilde{\mathbf{B}}_K \\ \mathbf{0} & \mathbf{I}_K \end{bmatrix} \quad \text{with} \quad \mathbf{S}_K = \tilde{\mathbf{B}}_K^T \mathbf{A}_K^{-1} \tilde{\mathbf{B}}_K$$

- Use FGMRES solver with block preconditioner $\mathbf{P}^{-1}$

$$\mathbf{P}^{-1} = \begin{bmatrix} \mathbf{A}_K & \mathbf{0} \\ \tilde{\mathbf{B}}_K^T & -\mathbf{C}_K \end{bmatrix}^{-1}$$

- approximate Schur complement by least squares commutator (LSC) preconditioner

$$\mathbf{C}_K^{-1} := \tilde{\mathbf{D}}_{p,K}^{-1} \tilde{\mathbf{B}}_K^T \mathbf{M}_{u,K}^{-1} \tilde{\mathbf{A}}_K \mathbf{M}_{u,K}^{-1} \tilde{\mathbf{B}}_K^T \tilde{\mathbf{D}}_{p,K}^{-1} \approx \mathbf{S}_K^{-1}$$

- With Pressure Laplace matrix $\tilde{\mathbf{D}}_{p,K} = \tilde{\mathbf{B}}_K^T \mathbf{M}_{u,K} \tilde{\mathbf{B}}_K$ and $\mathbf{M}_{u,K} = \mathbf{I}_K \otimes \mathbf{M}_u$

$$\mathbf{C}_K^{-1} := (\mathbf{I}_K \otimes (\tilde{\mathbf{D}}_p^{-1} \tilde{\mathbf{B}}^T \mathbf{M}_u^{-1})) \tilde{\mathbf{A}}_K (\mathbf{I}_K \otimes (\mathbf{M}_u^{-1} \tilde{\mathbf{B}}^T \tilde{\mathbf{D}}_p^{-1})) \approx \mathbf{S}_K^{-1}$$

⇒ 2x K independent pressure Laplace solves in space, 1 space-time velocity problem

- $\mathbf{D}_p^{-1}$, $\mathbf{A}_K^{-1}$ are approximated by a few (1-4) multigrid steps

Results

- Modified DFG95-Benchmark 3: $Re = 10$
- Linear solver stagnates:

K	2	5	10	20	50	100	200	400	800
nonlinear iters.	1.97	1.99	2	2.23	2.69	4.88	7.75	-	-
linear iters.	25.2	34.5	54.9	78.3	132	396	699	-	-
linear per nonlin.	12.8	17.3	27.5	35.2	49.1	81.2	90.2	-	.

Table: Number of iterations (averaged over imte domain); level 3

- Stokes test case

K	2	5	10	20	50	100	200	400	800
$\nu = 0.01$	14.58	17.78	26.75	39.5	66.5	94.5	100	158	184
$\nu = 10$	77.96	80.9	76.1	84.2	89.75	105	118	126	132

Table: Number of linear iterations (averaged over imte domain); level 3

Augmented Lagrangian - single time step

$$\begin{bmatrix} A_{i,k} & \tilde{B} \\ \tilde{B}^T & \end{bmatrix} \begin{bmatrix} u_k \\ p_k \end{bmatrix} = \begin{bmatrix} f_k - A_{e,0} u_{k-1} \\ \tilde{g}_k \end{bmatrix}$$

- Augmented Lagrangian (AL) modification [Benzi, Olshanskii (2006)]
- Modify the linear system

$$\begin{bmatrix} A_{i,k} + \gamma \tilde{B} W \tilde{B}^T & \tilde{B} \\ \tilde{B}^T & \end{bmatrix} \begin{bmatrix} u_k \\ p_k \end{bmatrix} = \begin{bmatrix} f_k - A_{e,k-1} u_{k-1} + \gamma \tilde{B} W \tilde{g}_k \\ \tilde{g}_k \end{bmatrix} \quad \text{with} \quad W = \frac{1}{\tau} M_p^{-1}$$

- Notation: $A_{i,\gamma} = A_{i,k} + \gamma \tilde{B} W \tilde{B}^T$
- Does not change the solution

Augmented Lagrangian - single time step

$$\begin{bmatrix} A_{i,k} & \tilde{B} \\ \tilde{B}^T & \end{bmatrix} \begin{bmatrix} u_k \\ p_k \end{bmatrix} = \begin{bmatrix} f_k - A_{e,0} u_{k-1} \\ \tilde{g}_k \end{bmatrix}$$

- Augmented Lagrangian (AL) modification [Benzi, Olshanskii (2006)]
- Modify the linear system

$$\begin{bmatrix} A_{i,k} + \gamma \tilde{B} W \tilde{B}^T & \tilde{B} \\ \tilde{B}^T & \end{bmatrix} \begin{bmatrix} u_k \\ p_k \end{bmatrix} = \begin{bmatrix} f_k - A_{e,k-1} u_{k-1} + \gamma \tilde{B} W \tilde{g}_k \\ \tilde{g}_k \end{bmatrix} \quad \text{with} \quad W = \frac{1}{\tau} M_p^{-1}$$

- Notation: $A_{i,\gamma} = A_{i,k} + \gamma \tilde{B} W \tilde{B}^T$
- Does not change the solution
- Sherman-Morrison-Woodbury identity yields:

$$S_\gamma^{-1} = \tilde{B}^T A_{i,\gamma} \tilde{B}^{-1} = (\tilde{B}^T A_i \tilde{B})^{-1} + \frac{\gamma}{\tau} M_p^{-1}$$

- LSC preconditioner:

$$C_\gamma^{-1} := C^{-1} + \frac{\gamma}{\tau} M_p^{-1} = (\tilde{D}_p^{-1} \tilde{B}^T M_u^{-1}) A_{i,\gamma} (M_u^{-1} \tilde{B} \tilde{D}_p^{-1}) \approx S_\gamma^{-1}$$

Augmented Lagrangian - all-at-once system

- Make the same modification to the time diagonal

$$\begin{bmatrix} \mathbf{A}_K + \gamma \tilde{\mathbf{B}}_K \mathbf{W}_K \tilde{\mathbf{B}}_K^T & \tilde{\mathbf{B}}_K \\ \tilde{\mathbf{B}}_K^T & \end{bmatrix} \begin{bmatrix} \mathbf{u} \\ \mathbf{p} \end{bmatrix} = \begin{bmatrix} \mathbf{f} + \gamma \tilde{\mathbf{B}}_K \mathbf{W}_K \tilde{\mathbf{g}} \\ \tilde{\mathbf{g}} \end{bmatrix} \quad \text{with} \quad \mathbf{W}_K = \frac{1}{\tau} \mathbf{I}_K \otimes \mathbf{M}_p^{-1}$$

- Sherman-Morrison-Woodbury identity holds:

$$\mathbf{S}_{K,\gamma}^{-1} = \mathbf{S}_K^{-1} + \frac{\gamma}{\tau} \mathbf{I}_K \otimes \mathbf{M}_p^{-1}$$

- LSC preconditioner:

$$\mathbf{C}_{K,\gamma}^{-1} := \mathbf{C}_K^{-1} + \frac{\gamma}{\tau} \mathbf{I}_K \otimes \mathbf{M}_p^{-1} = (\mathbf{I}_K \otimes (\tilde{\mathbf{D}}_p^{-1} \tilde{\mathbf{B}}^T \mathbf{M}_u^{-1})) \mathbf{A}_{K,\gamma} (\mathbf{I}_K \otimes (\mathbf{M}_u^{-1} \tilde{\mathbf{B}}^T \tilde{\mathbf{D}}_p^{-1})) \approx \mathbf{S}_{K,\gamma}^{-1}$$

Velocity solver for Augmented Lagrangian ($Q_2 - P_1$)

- Discrete equation (single time step):

$$\mathbf{A}_{i,k} \mathbf{u}_k + \gamma \tau \mathbf{B} \mathbf{M}_p^{-1} \mathbf{B}^T \mathbf{u}_k = \mathbf{f}_k - \mathbf{A}_{e,k-1} \mathbf{u}_{k-1}$$

- $\mathbf{B} \mathbf{M}_p^{-1} \mathbf{B}^T$ is singular, system ill-conditioned for large γ
- Tailored multigrid methods necessary [Wechsung (2019)]
- Domain decomposition into local patches $\bigcup_i V_{h,i} = V_h$
- kernel of the AL operator:

$$\mathcal{N}_h = \text{kern}(\mathbf{B} \mathbf{M}_p^{-1} \mathbf{B}^T) = \{v \in V_h : \nabla \cdot v = 0\}$$

- kernel capturing property:

$$\mathcal{N}_h = \bigcup_i (V_{h,i} \cap \mathcal{N}_h)$$

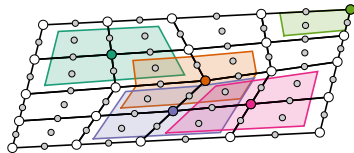


Figure: Decomposition of $V_h = \bigcup_i V_{h,i}$

Stationary AL multigrid solver

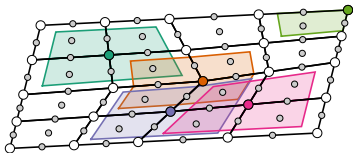


Figure: Smoother

- Smoother

- GMRES with overlapping additive schwarz preconditioner
- Patches around each mesh node

$$C = \sum_j \mathcal{I}_j \tilde{A}_j^{-1} \mathcal{I}_j^T$$

- Transfers

- Correction by solving local problems on each coarse cell

$$P_\gamma = \left(I - \left(\sum_r \mathcal{I}_r \tilde{A}_r^{-1} \mathcal{I}_r^T \right) \gamma^\tau B M_p^{-1} B^T \right) P$$

$$R_\gamma = P_\gamma^T$$

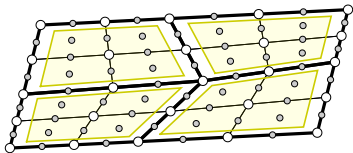


Figure: Prolongation

MG and AL

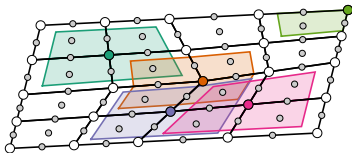


Figure: Smoother

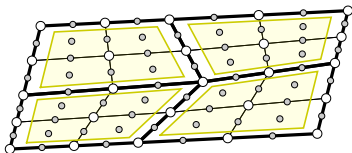
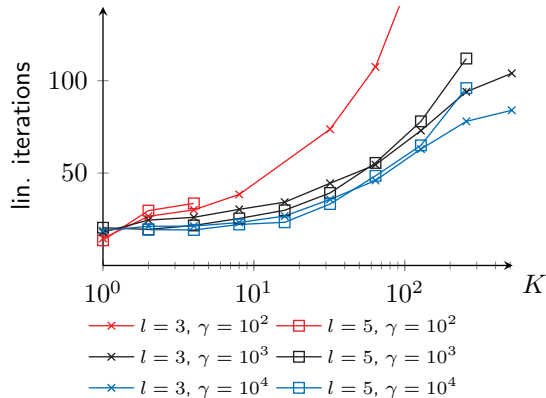


Figure: Prolongation

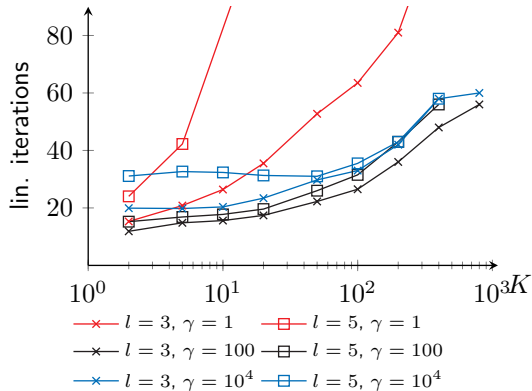
- STMG: apply specialized multigrid to each time step
 - Apply smoother to all stages in each inner spatial block
 - Larger local solves with increasing polynomial degree
 - Apply space transfers to each stage and time step
- WRMG:
 - apply specialized MG in a waveform relaxation manner
 - smoother: preconditioned GMRES
 - PC: for each patch solve the evolution equation
 - apply specialized transfers in each time step

Convergence results w.r.t γ , $Re = 10$

FGMRES(4), 1 velocity mg iteration, 4 pressure mg iterations



(a) STMG, $\tau = 1/64$, DG(0) / BE



(b) WRMG, $\tau = 0.01$, BDF2

Figure: Number of linear iterations: avg. over time domain

(Preliminary) scaling behavior of WRMG solver, $Re = 10$

- LiDO3 (2x Intel Xeon E5-2640v4 and 64GB memory per node, Infiniband QDR interconnect (40Gbps))
- 16 processes per node
- Level 4, CN, $\tau = 0.01$, 800 total time steps
- Unoptimized implementation
- Scaling bottleneck for large K : pressure coarse grid solver due to unsuited implementation

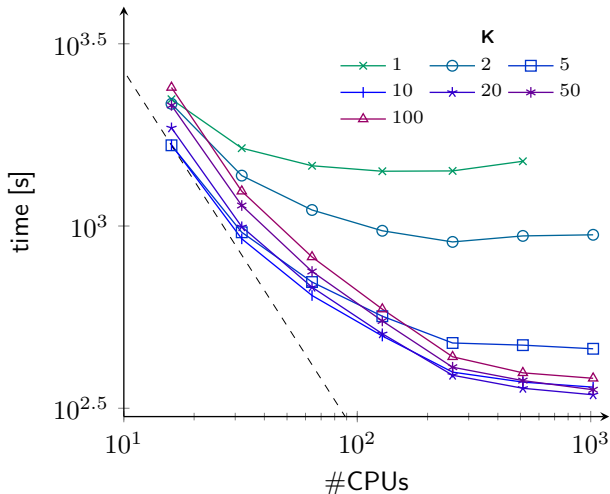


Figure: Total solver time

Convergence results w.r.t γ , $Re = 100$

- FGMRES(4), 1 velocity mg iteration, 4 pressure mg iterations
- Alpine: alternating between Picard and Newton
- Number of nonlinear iterations increases slightly
- Velocity solver convergence deteriorates

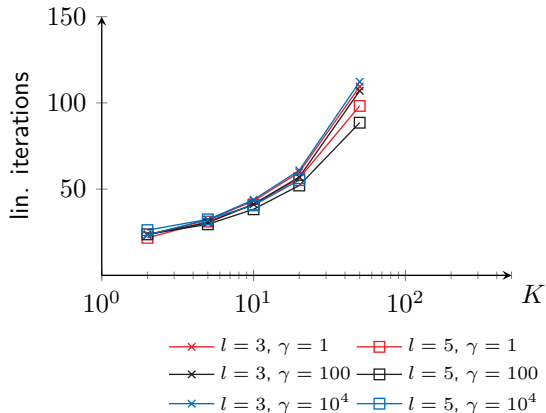


Figure: WRMG, $\tau = 0.01$, BDF2: Number of linear iterations, avg. over time domain

Conclusion

- LSC preconditioner with AL acceleration can lead to robust convergence behavior
- Low diffusion is problematic
- WRMG methods demonstrates speedup in a like-for-like comparison

Future research:

- Improve convergence behavior of STMG approach
- Time parallelization in the STMG method
- Efficient implementation of the pressure solver (multiple r.h.s)
- Block Krylov methods in the pressure solver

References

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