Application of a modified multigrid waveform relaxation method as a time-simultaneous approach to convection-diffusion equations

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Motivation

Convection-diffusion equation

$$\begin{aligned} \partial_t u - \nu \Delta u(x,t) + v(x,t) \cdot \nabla u(x,t) &= f(x,t) & (x,t) &\in \Omega \times (0,T) \\ u(x,t) &= g_D(x,t) & (x,t) &\in \Gamma_D \times (0,T) \\ \partial_n u(x,t) &= g_N(x,t) & (x,t) &\in \Gamma_N \times (0,T) \\ u(x,0) &= u_0(x) & x &\in \Omega \end{aligned} \tag{1}$$

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

- Solve the convection-diffusion equation arising as linear sub-problems of the Navier-Stokes equation
- enable a high amount of parallelism
    - even when only a moderate number of spatial unknowns are used
- use in a global-in-time context
- robust convergence bahovior w.r.t. to spatial and temporal mesh sizes h, Δt and number of parallel time-steps K

Outline

1. Motivation
2. Multigrid waveform relaxtion for the heat equation
   - Multigrid wavefrom relaxation
   - An algebraic approach
   - Convergence results
   - Heat equation tests
3. Application of WRMG to convection-diffusion equation
   - Numerical examples
   - Problems in transport dominant cases
   - Stabilization techniques
4. Conclusion

Multigrid Waveform relaxation

- introduced by Lubich, Ostermann (1987)
- semidiscrete linear evolution equation: $\boldsymbol{M}, \boldsymbol{A} \in \mathbb{R}^{n\times n}$, $\boldsymbol{u}, \boldsymbol{f} \in \mathbb{R}^{n\times 1}$

$$\begin{aligned} \partial_t \boldsymbol{M}\boldsymbol{u}(t) + \boldsymbol{A}\boldsymbol{u}(t) &= \boldsymbol{f}(t) \qquad t \in (0,T) \\ \boldsymbol{u}(0) &= \boldsymbol{u}_0 \end{aligned}$$

- introduce splittings $\boldsymbol{M} = \boldsymbol{M}_a + \boldsymbol{M}_b$ and $\boldsymbol{A} = \boldsymbol{A}_a + \boldsymbol{A}_b$
- calculate u^{n+1} by the iteration

$$\begin{aligned} \partial_t \boldsymbol{M}_a\boldsymbol{u}^{n+1}(t) + \boldsymbol{A}_a\boldsymbol{u}^{n+1}(t) &= \boldsymbol{f}(t) - \partial_t \boldsymbol{M}_b\boldsymbol{u}^{n}(t) - \boldsymbol{A}_b\boldsymbol{u}^{n}(t) \quad t \in (0,T) \\ \boldsymbol{u}^{n+1}(0) &= \boldsymbol{u}_0 \end{aligned} \tag{2}$$

- ideally: n decoupled ODEs
- multigrid waveform relaxtion: use multilevel splittings
  - use (2) as smoother
  - restrict the residual *in space* and calculate a correction on a coarser space discretization

An algebraic approach

A linear parabolic evolution equation

$$\begin{aligned} \partial_t u(x,t) - \mathcal{L}u(x,t) &= f(x,t) & (x,t) &\in \Omega_T := \Omega \times (0,T) \\ u(x,t) &= g(x,t) & (x,t) &\in \partial\Omega \times (0,T) \\ u(x,0) &= u_0(x) & x &\in \Omega \end{aligned}$$

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

- FE (/FD) space discretization
- (linear) one- or multistep method, e.g. IE, CN, BDF(k), Runge-Kutta methods,...
- solve the 'all-at-once' system consisting of multiple time steps

An algebraic approach

A linear parabolic evolution equation

$$\begin{aligned} \partial_t u(x,t) - \mathcal{L}u(x,t) &= f(x,t) && (x,t) \in \Omega_T := \Omega \times (0,T) \\ u(x,t) &= g(x,t) && (x,t) \in \partial\Omega \times (0,T) \\ u(x,0) &= u_0(x) && x \in \Omega \end{aligned}$$

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

E.g. a linear one-step method:

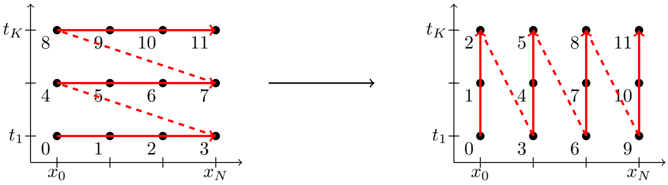
$$\underbrace{\begin{bmatrix} \boldsymbol{A}^1 & & & & \\ \boldsymbol{B}^1 & \boldsymbol{A}^2 & & & \\ & \boldsymbol{B}^2 & \boldsymbol{A}^3 & & \\ & & \ddots & \ddots & \\ & & & \boldsymbol{B}^{K-1} & \boldsymbol{A}^K \end{bmatrix}}_{=:\bar{\boldsymbol{A}} \in \mathbb{R}^{NK \times NK}} \underbrace{\begin{bmatrix} \boldsymbol{u}^1 \\ \boldsymbol{u}^2 \\ \boldsymbol{u}^3 \\ \vdots \\ \boldsymbol{u}^K \end{bmatrix}}_{=:\bar{\boldsymbol{u}} \in \mathbb{R}^{NK}} = \underbrace{\begin{bmatrix} \boldsymbol{f}^1 - \boldsymbol{B}^0 \boldsymbol{u}^0 \\ \boldsymbol{f}^2 \\ \boldsymbol{f}^3 \\ \vdots \\ \boldsymbol{f}^K \end{bmatrix}}_{=:\bar{\boldsymbol{f}} \in \mathbb{R}^{NK}} \tag{3}$$

Reordering

- *space-time grid is a cartesian product of a space and a time grid*
- switch to a 'time-major' ordering

$$\bar{\boldsymbol{u}} = [u_1^1, u_2^1, \ldots, u_N^1, u_1^2, u_2^2, \ldots, u_N^2, \ldots, u_1^K, u_2^K, \ldots, u_N^K]^T$$
$$\downarrow$$
$$\boldsymbol{u} = [u_1^1, u_1^2, \ldots, u_1^K, u_2^1, u_2^2, \ldots, u_2^K, \ldots, u_N^1, u_N^2, \ldots, u_N^K]^T$$

- reorder $\bar{\boldsymbol{A}}$ and $\bar{\boldsymbol{f}}$ accordingly



Multigrid applied to the reordered global matrix (1D)

- transfer operators (semi coarsening in space):
  - standard coarsening for each time step
  - Prolongation:

$$\boldsymbol{P}_{\tau,2h}^{\tau,h} = \boldsymbol{P}_{2h}^{h} \otimes \boldsymbol{I}_K$$

  - Restriction:

$$\boldsymbol{R}_{\tau,h}^{\tau,2h} = \boldsymbol{R}_{h}^{2h} \otimes \boldsymbol{I}_K = \left(\boldsymbol{P}_{\tau,2h}^{\tau,h}\right)^T$$

- damped block-Jacobi smoother:

$$\boldsymbol{x}^{m+1} = \boldsymbol{x}^m + \omega\, \boldsymbol{D}^{-1}(\boldsymbol{f} - \boldsymbol{A}\boldsymbol{x}^m)$$

$$\boldsymbol{D} = \begin{pmatrix} \# & & & \\ & \# & & \\ & & \ddots & \\ & & & \# \end{pmatrix} \in \mathbb{R}^{NK \times NK}$$

$$\underbrace{\begin{pmatrix} \# & \# & & & \\ \# & \# & \# & & \\ & \ddots & \ddots & \ddots & \\ & & \# & \# & \# \\ & & & \# & \# \end{pmatrix}}_{=\boldsymbol{A}} \boldsymbol{u} = \boldsymbol{f}$$

$$\# = \begin{bmatrix} * & & & & \\ * & * & & & \\ & * & * & & \\ & & \ddots & \ddots & \\ & & & * & * \end{bmatrix} \in \mathbb{R}^{K \times K}$$

- use a block-wise geometric multigrid method on $\boldsymbol{A}$ in space

Theoretical convergence results

- linear multi-step methods: the asymptotic convergence rates are the same as in a time-stepping approach [Janssen, Vandewalle (1996)]
- Notay (2022):
  - symmetric elliptic operators, backward Euler
  - Fourier analysis applicable to the stationary problem
  - aware Jacobi smoothing: only damp stiffness matrix

$$D = \omega \Delta t \, \mathrm{diag}(\boldsymbol{A}) + \mathrm{diag}(\boldsymbol{M})$$

  $\Rightarrow$ 2-norm of iteration matrix is uniform bounded w.r.t h, Δt and K
- Lohmann et al. (accepted)
  - 1D heat equation on uniform meshes
  - naive Jacobi smoothing

  $\Rightarrow$ 2-norm of iteration matrix is uniform bounded w.r.t h, Δt and K

Influence of the damping parameter and mass lumping

- with mass lumping and $\lambda = \frac{\Delta t}{h^2} \to 0$ an undamped Jacobi-smoother becomes exact
- in general damping is necessary

=> use Krylov subspace smoothers with block-Jacobi preconditioning

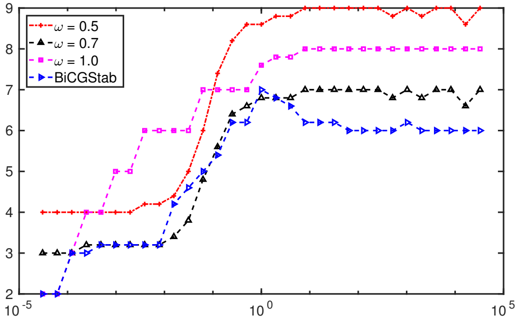
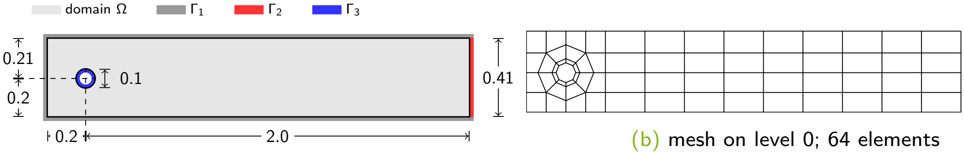


Figure: F-cycle, 2 pre- and postsmoothing steps (1 BiCGStab step), Q1 elements, CN, $h = \frac{1}{128}$, 500 time steps, 100 blocked steps

Numerical example: heat equation



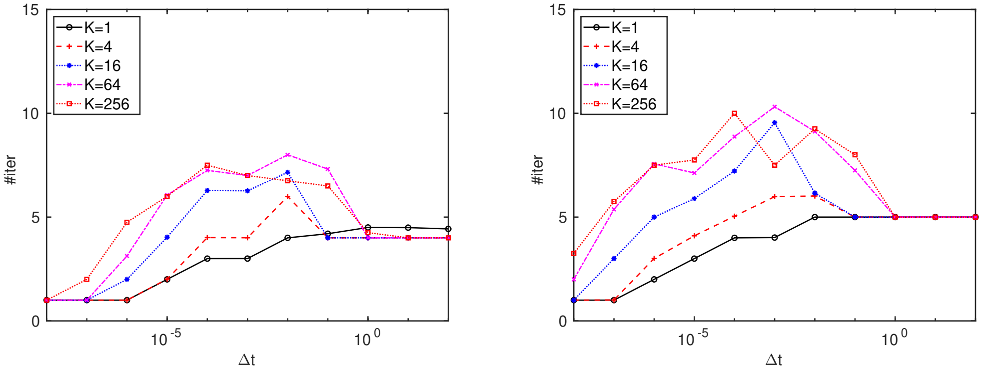
(a) Flow-around-cylinder domain

(b) mesh on level 0; 64 elements

Figure: Test domain

- homogenous Dirichlet b.c. and i.c
- $f(x,t) = 1 + 0.1\sin(t)$, $\nu = 1$
- Q1-FEM in space, Crank Nicolson in time
- 4 BiCGSTAB pre- and post-smoothing steps, V-cycle
- uniform refinement

Convergence behavior



(a) Level 3 (b) Level 5

Figure: Number of iterations

Computational characteristics

- slightly higher computational costs
  - increased bandwidth of all-at-once systems
- same amount of communicated data per iterations between nodes
- lower number of communication operations
  - more data is transmitted at once
  - latency induced run-time can be reduced
- parallelization still limited by the number of spatial DoFs
- has to be combined with a telescopic / hierarchical multigrid approach
- additional parallelization in time is possible

Strong scaling test

- executed on LiDO3 (2x Intel Xeon E5-2640v4 and 64GB memory per node, Infiniband QDR interconnect (40Gbps))
- 4 BiCGSTAB pre- and post-smoothing steps, V-cycle

- time spent on coarse levels can not be lowered when more CPUs are used
- moderate numbers of simultaneous time steps K yield better scaling, higher K will not improve the run time

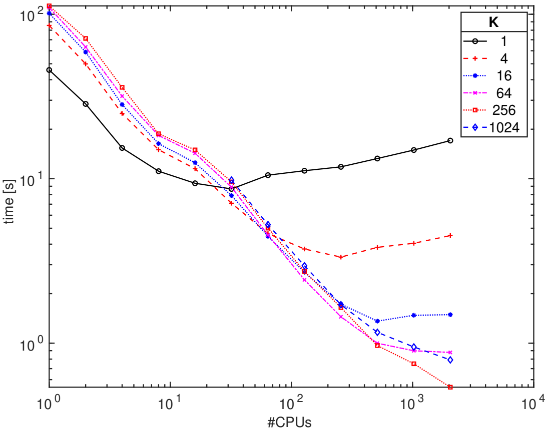


Figure: Solver time per iteration

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Convection diffusion equation - first order upwind (1D)

uniform grid, $L = 6, h = \frac{1}{512}$

$$v(x,t) = \sin(\pi x)\sin(2t)$$
$$u_0(x) = \exp(4(x - x^2)) - 1$$
$$g_D(x,t) = 0$$
$$f(x,t) = x\sin(t)$$

robust convergence behavior due to numerical diffusion

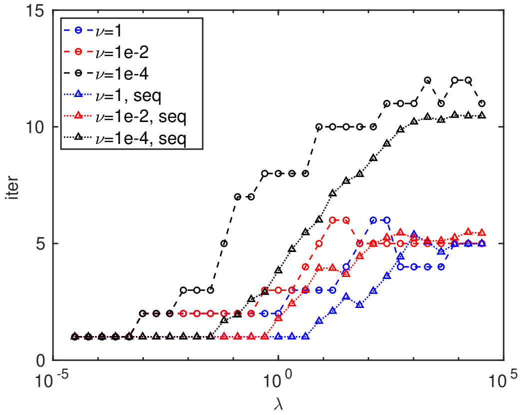
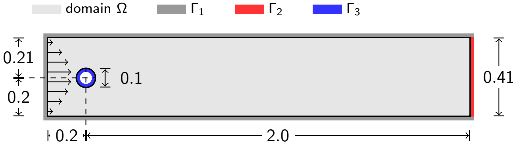
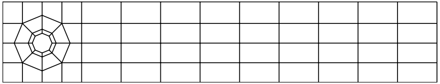


Figure: number of iterations, W-cycle, 1 pre- and postsmoothing step, FD with upwind, backward Euler, 1000 blocked time steps, $h = \frac{1}{1024}$

'FAC-like' test case



(a) Flow-around-cylinder domain



(b) mesh on level 0; 64 elements

Figure: Test domain

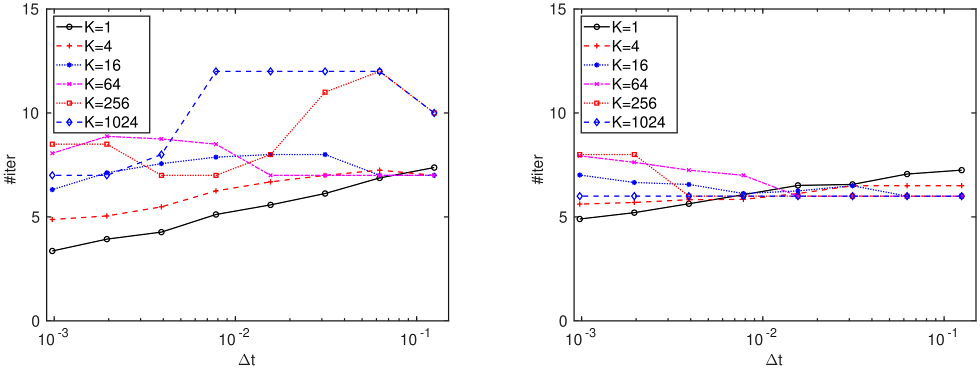
- $\Gamma_D = \Gamma_1 \cup \Gamma_3$, $\Gamma_N = \Gamma_2$: $g_D(x,t) = \mathbb{1}_{\Gamma_3}(x)\,\mathbb{1}_{(0,0.5)}(t)$
- Q2-FEM in space, Crank Nicolson in time
- stationary parabolic velocity field

$$v(x,t) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \frac{6x_2(0.41 - x_2)}{0.41^2}$$

- 'smoothed' stationary parabolic velocity field

$$v_s(x,t) = v(x,t)\tanh\left(20\,\mathrm{dist}(x,\Gamma_3)\right)$$

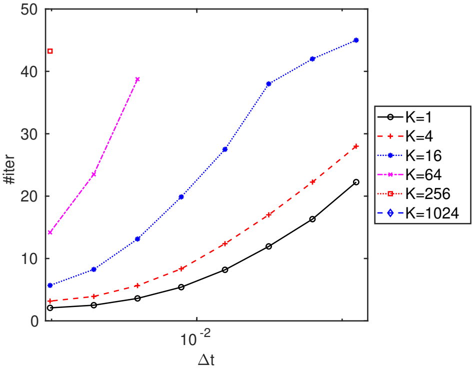
'FAC'-like test case: $\nu = 0.01$



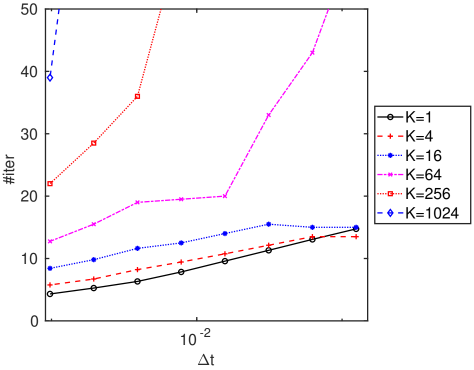
(a) Level 3 (b) Level 5

Figure: Number of iterations: 4 GMRES pre- and postsmooting steps, F-cycle, Q2, Crank-Nicolson, $\nu = 1e-2$

'FAC'-like testcase: $\nu = 0.001$



(a) Level 3



(b) Level 5

Figure: Number of iterations: 4 GMRES pre- and postsmooting steps, F-cycle, Q2, Crank-Nicolson, $\nu = 1e - 3$

Two-level variational multiscale stabilization

- additional diffusive stabilization terms [John, Kaya, Layton (2006)]

$$(\partial_t u_h, \varphi_h) + \nu(\nabla u_h, \nabla\varphi_h) + (v, \nabla u_h) + \alpha(\nabla u_h, \nabla\varphi_h) - \alpha(g_h, \nabla\varphi_h) = (f, \varphi_h) \quad \forall\varphi_h \in V_h$$

$$(\boldsymbol{g}_h - \nabla u_h, \psi_h) = 0 \quad \forall\varphi_h \in (V_h)^d$$

- semi-discrete formulation

$$\partial_t \boldsymbol{M}_h \boldsymbol{u}_h(t) + (\nu + \alpha)\boldsymbol{L}_h \boldsymbol{u}_h(t) + \boldsymbol{K}_h(t)\boldsymbol{u}_h(t) - \alpha \boldsymbol{B}_h^t \bar{\boldsymbol{M}}_h^{-1} \boldsymbol{B}_h \boldsymbol{u}_h(t) = \boldsymbol{f}_h(t)$$

- FE-basis funciton $\psi_l \in V_h$, $\boldsymbol{\psi}_k \in (V_h)^d$

$$(\boldsymbol{M}_h)_{i,j} = (\psi_j, \psi_i) \qquad (\boldsymbol{L}_h)_{i,j} = (\nabla\psi_j, \nabla\psi_i) \qquad (\boldsymbol{K}_h(t))_{i,j} = (v(\cdot, t)\cdot\nabla\psi_j, \nabla\psi_i)$$

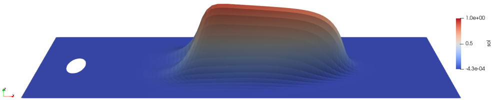
$$(\boldsymbol{B}_h)_{i,j} = (\nabla\psi_j, \boldsymbol{\psi}_i) \qquad (\bar{\boldsymbol{M}}_h)_{i,j} = (\boldsymbol{\psi}_j, \boldsymbol{\psi}_i)$$

Two-level variational multiscale stabilization

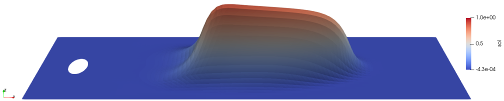
$$\partial_t \boldsymbol{M}_h \boldsymbol{u}_h(t) + (\nu + \alpha)\boldsymbol{L}_h \boldsymbol{u}_h(t) + \boldsymbol{K}_h(t)\boldsymbol{u}_h(t) - \alpha \boldsymbol{B}_h^t \bar{\boldsymbol{M}}_h^{-1} \boldsymbol{B}_h \boldsymbol{u}_h(t) = \boldsymbol{f}_h(t)$$

- stabilization term is treated implicitly
- 1D, uniform grids, linear FEM: behaves like $ch^2 u_{xxxx}(x,t)$
  - α needs to be level-dependent to solve the corresponding coarse grid problem: $\alpha_{l-1} = \alpha_l \left(\frac{h_l}{h_{l-1}}\right)^\gamma$ with $\gamma = 2$
  - less stabilization on coarser levels
- use mass-lumping to solve $\bar{\boldsymbol{M}}_h^{-1}$ easily
  - Lagrange basis functions with consistent mass lumping (cubature): $\boldsymbol{L}_h - \boldsymbol{B}_h^t \bar{\boldsymbol{M}}_h^{-1} \boldsymbol{B}_h$ is singular
  - Bernstein with row-sum mass lumping: $\boldsymbol{L}_h - \boldsymbol{B}_h^t \bar{\boldsymbol{M}}_h^{-1} \boldsymbol{B}_h$ stabilizes the solver

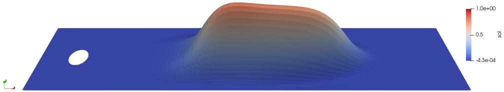
Suitable choices of α: 'FAC-like' test case



(a) $\alpha = 0$



(b) $\alpha = 0.01$



(c) $\alpha = 0.1$

Figure: Solution at $t = 1$: $\nu = 1e - 3$, $t = 1$, level 3

Suitable choices of α: DFG Bench2

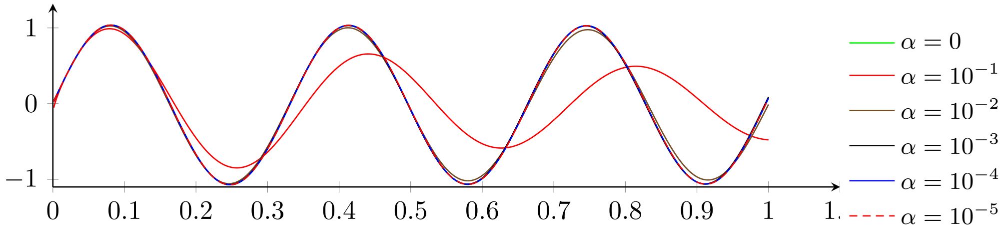
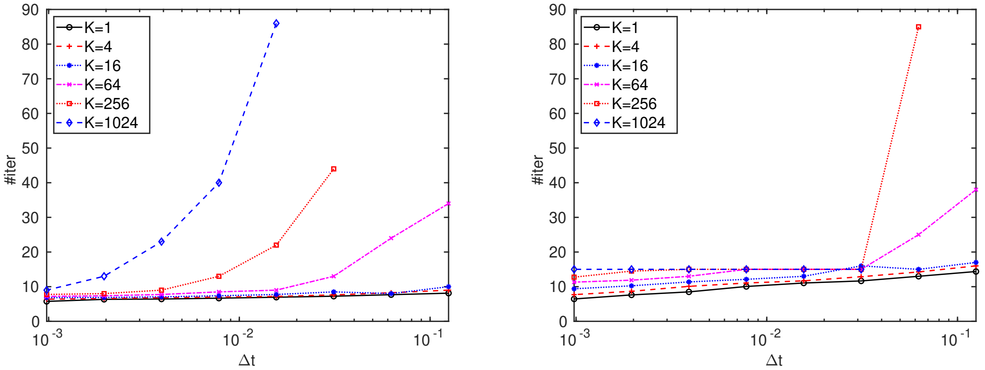


Figure: DFG Bench2: Lift; Bernstein basis, level 3

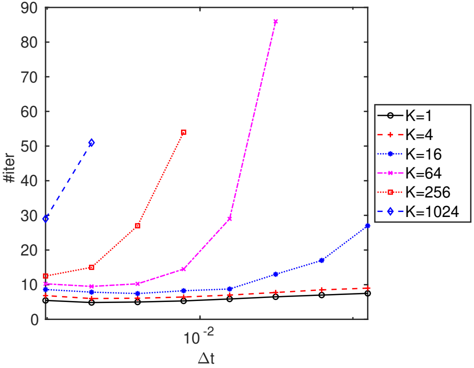
Convergence behavior with stabilization - $\alpha = 0.1$



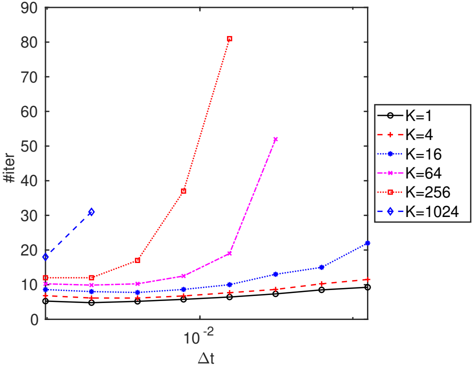
(a) $\gamma = 2$ (b) $\gamma = 1$

Figure: Number of iterations: $\nu = 1e-3$, level 3, 4 GMRES pre- and postsmoothing steps, F-cycle

Convergence behavior with stabilization - $\alpha = 0.01$



(a) $\gamma = 2$



(b) $\gamma = 1$

Figure: Number of iterations: $\nu = 1e-3$, level 3, 4 GMRES pre- and postsmoothing steps, F-cycle

Conclusion

Conclusion:

- Multigrid wavefrom relaxation methods are well-suited to solve parabolic PDEs with enough diffusivity
- significantly lower wall time can be achieved
- convection dominant equations pose problems
- stabilization can help

Outlook:

- choice of α remains diffcult
- α dependent on mesh width and velocity field
- biharmonic stabilization $(\alpha h^3 \boldsymbol{L}\boldsymbol{M}^{-1}\boldsymbol{L})$ seems promising

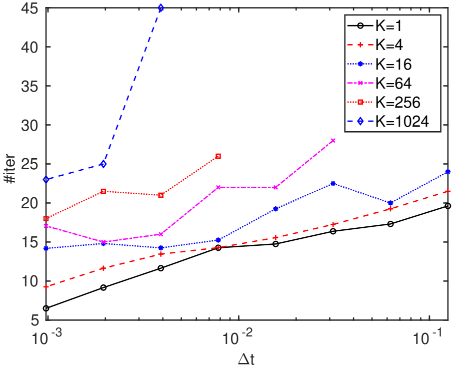


Figure: Number of iterations: Biharmonic stabilization: $\alpha = 0.1$, $\gamma = 2$, level 3, FAC-test case

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