On a Time-Simultaneous Multigrid Method in Combination with Stabilization Techniques for the Convection–Diffusion Equation

Oberseminar WS 22/23

Wiebke Drews, Stefan Turek, Christoph Lohmann

Institute of Applied Mathematics (LS III)
Department of Mathematics
TU Dortmund University

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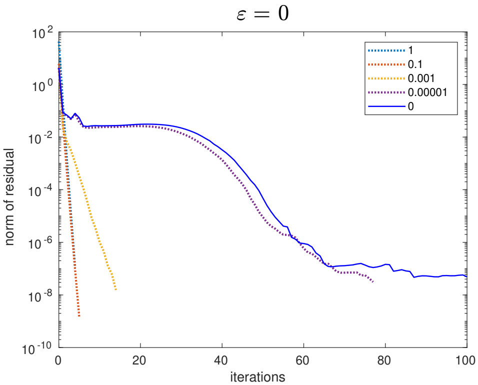
technische universität dortmund
fakultät für mathematik

Motivation



Exemplary convergence behavior for convection-dominated problems.

- solve convection-diffusion equation efficiently $\rightarrow$ parallelization
- use a **time-simultaneous** multigrid method[1]
- stabilization for convection-dominated problems

The perfect algorithm is **not** presented here!

[1] Multigrid Waveform Relaxation (by Lubich, Ostermann (1987)).

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Preliminaries

Convection-diffusion equation in 1D

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\partial_t u(x,t) - \varepsilon u_{xx}(x,t) + v(x,t)u_x(x,t) &= f(x,t) & (x,t) &\in \Omega \times (0,T] \\
u(0,t) = u(1,t) &= 0 & t &\in [0,T] \\
u(x,0) &= u_0(x) & x &\in \Omega
\end{aligned}
$$

with $\Omega = (0,1), T > 0$.

- finite difference (FD) discretization in space

$$\partial_t \boldsymbol{M}_h \boldsymbol{u}_h(t) + \varepsilon \boldsymbol{L}_h \boldsymbol{u}_h(t) = \boldsymbol{f}_h(t)$$

- Crank-Nicolson scheme for discretization in time

$$\boldsymbol{A}\boldsymbol{u}^m + \boldsymbol{B}\boldsymbol{u}^{m-1} = \boldsymbol{f}^m, \quad m = 1, \ldots, K$$

using time step size δt and

$$\boldsymbol{A} := \boldsymbol{M}_h + \tfrac{1}{2}\delta t \varepsilon \boldsymbol{L}_h, \quad \boldsymbol{B} := -\boldsymbol{M}_h + \tfrac{1}{2}\delta t \varepsilon \boldsymbol{L}_h, \quad \boldsymbol{f}^m := \tfrac{1}{2}\delta t \left(\boldsymbol{f}_h^m + \boldsymbol{f}_h^{m-1}\right).$$

Preliminaries

Convection-diffusion equation in 1D

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$$

Algebraic transformations

Blocking all time steps into a global linear system of equations...

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

Note: K time steps $t^1, t^2, ..., t^K$ and N spatial nodes $x_1, ..., x_N$

...and rearranging the degrees of freedom...

$$(u_1^1, u_2^1, \ldots u_N^1, u_1^2, u_2^2, \ldots, u_N^2, \ldots, u_1^K, u_2^K, \ldots, u_N^K)^\top$$

$$\downarrow$$

$$\boldsymbol{u} := (u_1^1, u_1^2 \ldots, u_1^K, u_2^1, u_2^2, \ldots, u_2^K, \ldots, u_N^1, u_N^2, \ldots, u_N^K)^\top$$

Algebraic transformations

...results in a **space-only problem** with vector-valued unknowns for each spatial node:

$$\underbrace{\begin{pmatrix} \# & \# & & \\ \# & \# & \ddots & \\ & \ddots & \ddots & \# \\ & & \# & \# \end{pmatrix}}_{=:\boldsymbol{S}\in\mathbb{R}^{NK\times NK}} \boldsymbol{u} = \boldsymbol{f}, \quad \text{with } \# := \begin{pmatrix} * & & & \\ * & * & & \\ & \ddots & \ddots & \\ & & * & * \end{pmatrix} \in \mathbb{R}^{K\times K}$$

$\rightarrow$ apply geometric multigrid method on $\boldsymbol{S}$ in space!

Aim: design of a highly parallelizable solution strategy!

Time-simultaneous multigrid algorithm

- smoothing
  - number of pre-smoothing and post-smoothing steps: ν_1 and ν_2
  - (damped) block Jacobi method: $\boldsymbol{x}^{(\nu)} = \boldsymbol{x}^{(\nu-1)} + \omega \boldsymbol{D}^{-1}(\boldsymbol{f} - \boldsymbol{S}\boldsymbol{x}^{(\nu-1)})$
  - block Jacobi preconditioning embedded into GMRES method:

$$\boldsymbol{D} := \begin{pmatrix} \# & & \\ & \ddots & \\ & & \# \end{pmatrix}, \quad \# = \underbrace{\begin{pmatrix} * & & & \\ * & * & & \\ & \ddots & \ddots & \\ & & * & * \end{pmatrix}}_{K \times K}$$

- intergrid transfer operators
  - standard coarsening in space for each time step
  - prolongation:

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

  - restriction:

$$\boldsymbol{R}_{\delta t,h}^{\delta t,2h} = \boldsymbol{R}_{h}^{2h} \otimes \boldsymbol{I}_K = \frac{1}{2}\left(\boldsymbol{P}_{\delta t,2h}^{\delta t,h}\right)^{\top}$$

Theoretical convergence results

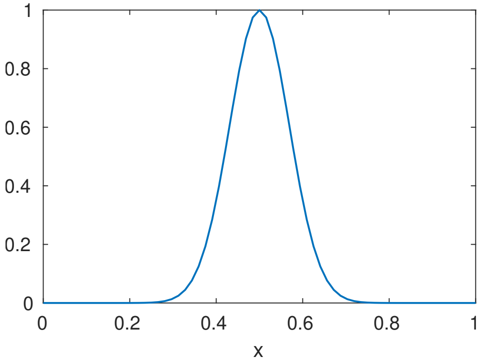
- linear multi-step methods: asymptotic convergence rate is the same as in time-stepping approach [Janssen, Vandewalle (1996)]

- Fourier analysis of time-simultaneous two-grid algorithm [Lohmann et al. (2022)]
  - 1D heat equation on uniform mesh
  - damped Jacobi (waveform relaxation) smoothing
  - spectral norm of two-grid iteration matrix $\boldsymbol{J}$ is uniformly bounded:

$$||\boldsymbol{J}||_2 < C < 1, \quad C \neq C(\delta t, h, K)$$

  for $\theta \geq \frac{1}{2}, \omega = \frac{2}{3}, \nu_1 \geq 1$.

Numerical studies on heat equation



$u(x,t)$ for different time steps.

- manufactured solution

$$u(x,t) = \exp\left(-\eta(\tfrac{1}{2} - x + \tfrac{1}{4}\sin(\tfrac{\pi}{2}t))^2\right)\sin(\pi x)$$

  where $\eta = 100$.

- homogenous Dirichlet boundary conditions

$$u(0,t) = u(1,t) = 0.$$

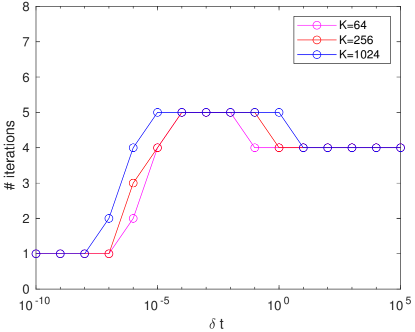
Discretization: FD in space, Crank-Nicolson scheme in time

- Level: fine level with spatial resolution $h = 2^{\text{-Level}}$
- δt: time step size
- K: number of blocked time steps

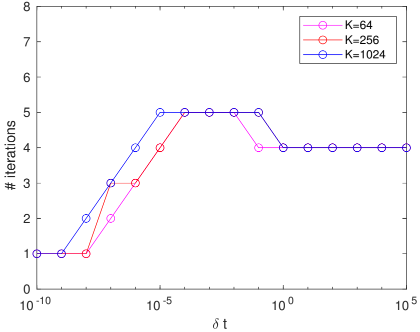
MG algorithm:

- coarse level 1
- GMRES smoother
- $\nu_1 = \nu_2 = 4$

Numerical studies on heat equation: V-cycle, $\varepsilon = 1$



Level 7.



Level 9.

Results:

- independent of K and fine mesh level
- number of iterations $\leq$ 5

Numerical studies on convection-diffusion equation

Convection-diffusion equation in 1D

$$\begin{aligned} \partial_t u(x,t) - \varepsilon u_{xx}(x,t) + \cancel{v(x,t) u_x(x,t)} &= f(x,t) && (x,t) \in \Omega \times (0,T] \\ u(0,t) = u(1,t) &= 0 && t \in [0,T] \\ u(x,0) &= u_0(x) && x \in \Omega \end{aligned}$$

with $\Omega = (0,1), T > 0$.

$$\partial_t \boldsymbol{M}_h \boldsymbol{u}_h(t) + \varepsilon \boldsymbol{L}_h \boldsymbol{u}_h(t) + \boldsymbol{K}_h \boldsymbol{u}_h(t) = \boldsymbol{f}_h(t)$$

- Convection term: discretized with first order upwind scheme
- Numerical studies with
  - $v = 1$ for convenience
  - manufactured solution as above and corresponding right hand side

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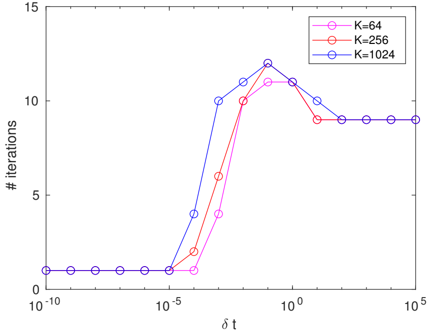
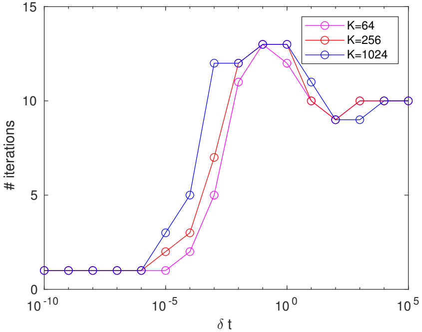
Upwind discretization, V-cycle, $\varepsilon = 10^{-3}$



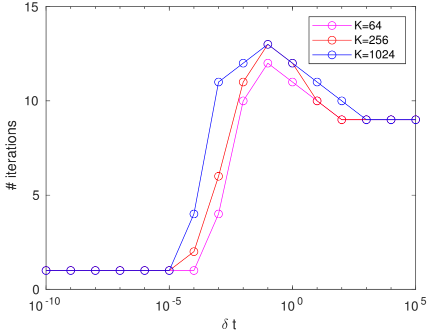
Level 7.



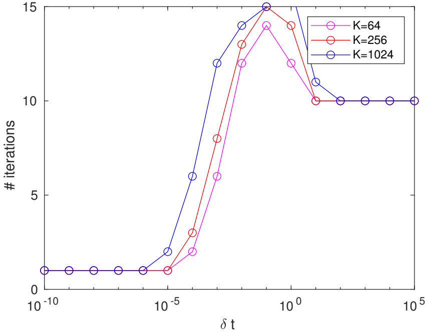
Level 9.

- Result: similar behavior as for heat equation, but only 1st order accuracy
- Goal: higher order of convergence $\rightarrow$ central difference scheme?

Upwind discretization, V-cycle, $\varepsilon = 0$



Level 7.



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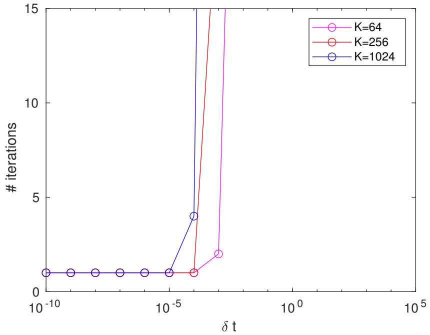
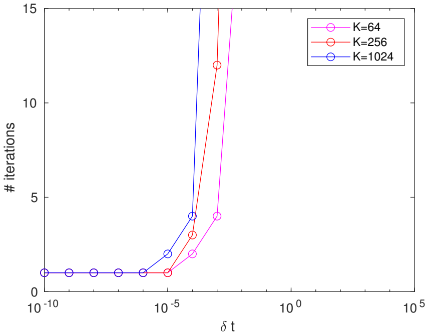
- Result: similar behavior as for heat equation, but only 1st order accuracy
- Goal: higher order of convergence $\rightarrow$ central difference scheme?

Central discretization, V-cycle, $\varepsilon = 10^{-3}$



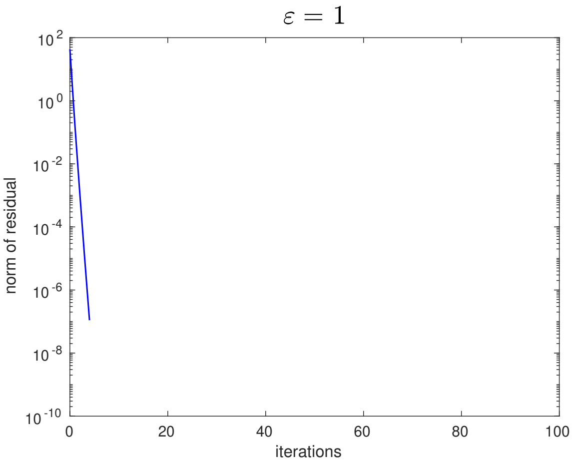
Level 7.



Level 9.

- Convection term discretized using second order central discretization
- Result: extremely increasing number of iterations!

Central discretization



Convergence behavior for different values of ε.

TG algorithm:
level $= 7$, $\delta t = \frac{1}{128}, K = 64.$

- fixed $v = 1$, varying ε

  $\rightarrow$ stability issues arise for convection-dominated problems

Higher order stabilization

- add diffusive term with stabilization parameter $\alpha_{add} \geq 0$ and compensation term[2]

$$(\partial_t u_h, \varphi_h) + \varepsilon(\nabla u_h, \nabla \varphi_h) + (v \cdot \nabla u_h, \varphi_h) + \alpha_{add}(\nabla u_h, \nabla \varphi_h) - \alpha_{add}(\mathbf{g}_h, \nabla \varphi_h) = (f, \varphi_h) \quad \forall \varphi_h \in V_h$$
$$(\mathbf{g}_h - \nabla u_h, \boldsymbol{\psi}_h) = 0 \qquad \forall \boldsymbol{\psi}_h \in (V_h)^d$$

- semi-discrete formulation in matrix form: $\boldsymbol{M}_h \sim \mathrm{id}, \boldsymbol{B}_h \sim \mathrm{grad}, \boldsymbol{B}_h^\top \sim \mathrm{div}$

$$\partial_t \boldsymbol{M}_h \boldsymbol{u}_h(t) + \varepsilon \boldsymbol{L}_h \boldsymbol{u}_h(t) + \boldsymbol{K}_h \boldsymbol{u}_h(t) + \alpha_{add} \underbrace{(\boldsymbol{L}_h - \boldsymbol{B}_h^\top \boldsymbol{M}_h^{-1} \boldsymbol{B}_h)}_{(*)} \boldsymbol{u}_h(t) = \boldsymbol{f}_h(t)$$

- $(*)$ 1D with linear FEM, uniform grid, quadrature based mass-lumping:

$$\tilde{\boldsymbol{L}}_h = \boldsymbol{M}_h^{-1} \boldsymbol{L}_h \sim -\frac{1}{h^2}[1, -2, 1], \qquad \tilde{\boldsymbol{L}}_{2h} = \boldsymbol{M}_h^{-1} \boldsymbol{B}_h^\top \boldsymbol{M}_h^{-1} \boldsymbol{B}_h \sim -\frac{1}{(2h)^2}[1, 0, -2, 0, 1]$$

$$\Longrightarrow \quad \tilde{\boldsymbol{L}}_h - \tilde{\boldsymbol{L}}_{2h} \sim \frac{1}{(2h)^2}[1, -4, 6, -4, 1]$$

[2] Fast, Mierka, Turek (2022), John, Kaya, Layton (2006).

Choice of α_{add} in multigrid algorithm

$$\alpha_{add} := \alpha \left(\frac{h_f}{h}\right)^{\gamma} \quad \Rightarrow \quad \alpha \left(\frac{h_f}{h}\right)^{\gamma} (\tilde{\boldsymbol{L}}_h - \tilde{\boldsymbol{L}}_{2h})\boldsymbol{u}_h$$

where $\alpha > 0, \gamma = 2$, $\quad h_f$: mesh size of fine level, $\quad h$: mesh size of current level.

- stabilization term corresponds to the biharmonic operator with a certain factor

  $\Rightarrow$ second order of accuracy

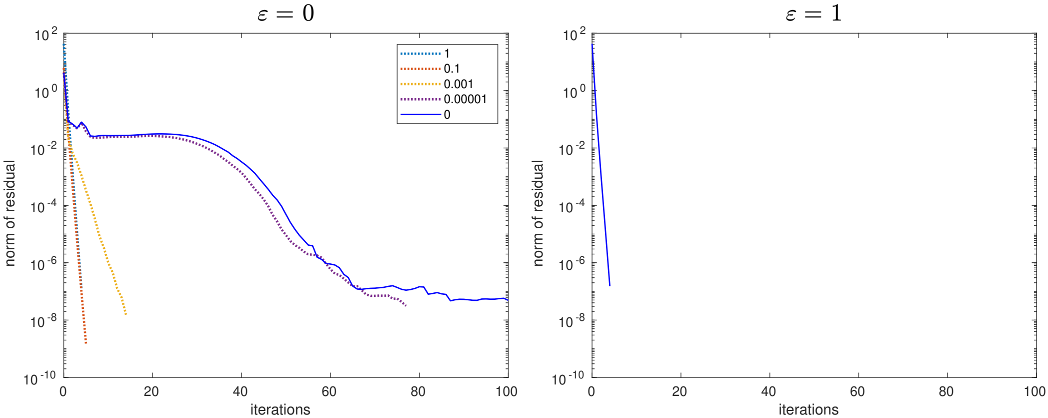
$$\begin{array}{rclllll}
\tilde{\boldsymbol{L}}_h \boldsymbol{u}_h & \sim & \frac{1}{h^2}(& h^2 u_{xx} + & C h^4 u_{xxxx} + & O(h^6)) \\
\tilde{\boldsymbol{L}}_{2h} \boldsymbol{u}_h & \sim & \frac{1}{4h^2}(& 4h^2 u_{xx} + & 2^4 C h^4 u_{xxxx} + & O(h^6)) \\
\hline
(\tilde{\boldsymbol{L}}_h - \tilde{\boldsymbol{L}}_{2h}) \boldsymbol{u}_h & \sim & & & \tilde{C} h^2 u_{xxxx} + & O(h^4)
\end{array}$$

- solve the same continuous problem on each level, **but** less stabilization on coarser levels

$$\alpha \left(\frac{h_f}{h}\right)^{\gamma} (\tilde{\boldsymbol{L}}_h - \tilde{\boldsymbol{L}}_{2h})\boldsymbol{u}_h \sim \alpha \left(\frac{h_f}{h}\right)^{\gamma} \tilde{C} h^2 u_{xxxx} = \alpha h_f^2 \tilde{C} u_{xxxx}, \qquad \text{for } \gamma = 2$$

- The stabilization term is treated fully implicit!

Numerical studies: stabilization



No stabilization. Stabilization with $\alpha = 0.1$.

- number of iterations hardly increases for small values of ε
- the plateau disappears

$\rightarrow$ stabilization can help! How to choose α quantitatively?

Choice of α

$\delta t = h$	$\alpha = 0$	$\alpha = 0.01$	$\alpha = 0.1$	$\alpha = 1$	$\alpha = 10$
1/64	2.0e-03	2.1e-03	6.9e-03	4.8e-02	1.3e-01
1/128	4.8e-04	5.1e-04	1.7e-03	1.6e-02	7.8e-02
1/256	1.2e-04	1.3e-04	4.4e-04	4.2e-03	3.4e-02

Discrete L_2-error at final time $T = 1$, $\varepsilon = 10^{-3}$.

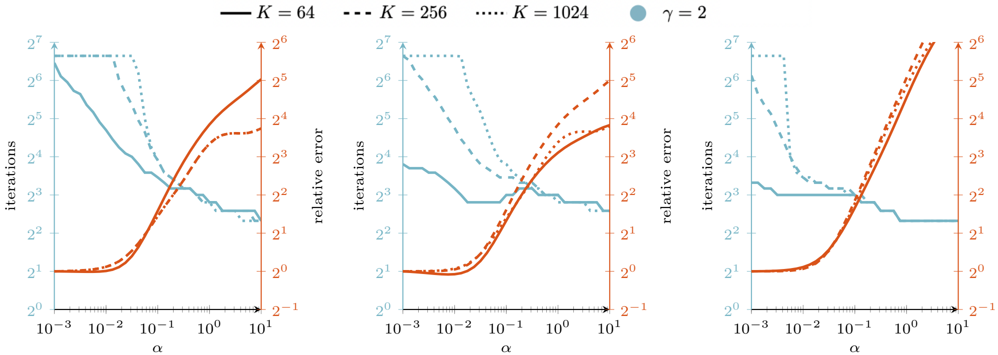
$\delta t = h$	$\alpha = 0$	$\alpha = 0.01$	$\alpha = 0.1$	$\alpha = 1$	$\alpha = 10$
1/64	5.0e-03	2.1e-03	7.0e-03	4.8e-02	1.3e-01
1/128	1.2e-03	5.1e-04	1.8e-03	1.6e-02	7.9e-02
1/256	3.0e-04	1.3e-04	4.4e-04	4.2e-03	3.4e-02

Discrete L_2-error at final time $T = 1$, $\varepsilon = 10^{-9}$.

- the error is reduced by a factor of $\approx$ 4 $\rightarrow$ 2nd order of convergence observed
- loss of accuracy for larger α

$\rightarrow$ do not choose α too large

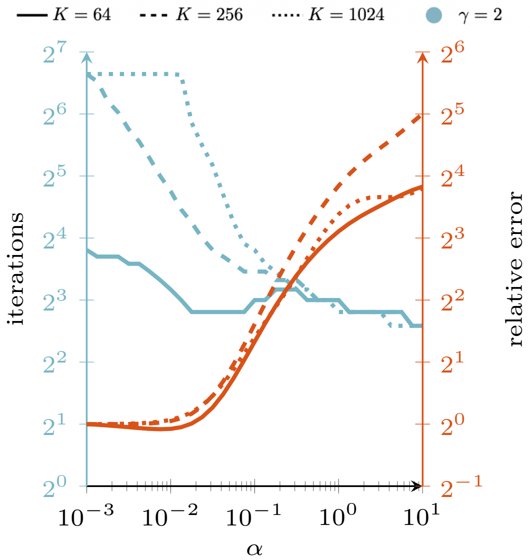
Choice of α, $\varepsilon = 10^{-3}$



Level 5, $\delta t = \frac{1}{32}$. Level 5, $\delta t = \frac{1}{128}$. Level 7, $\delta t = \frac{1}{128}$.

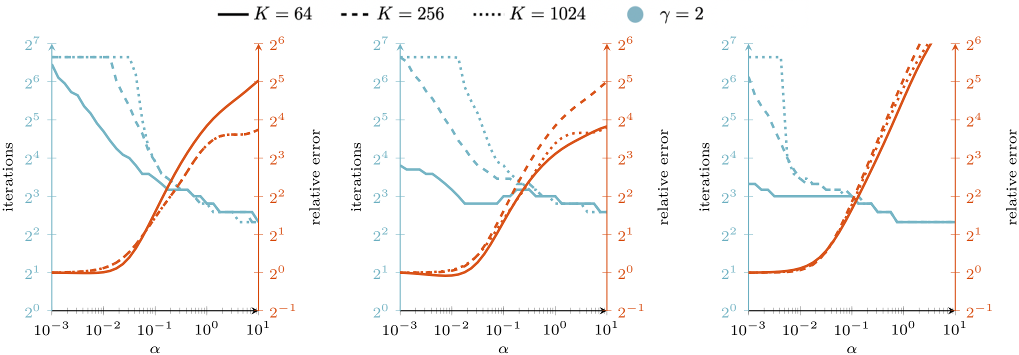
TG algorithm:
maximum number of iterations: 100.

Choice of α, $\varepsilon = 10^{-3}$



Level 5, $\delta t = \frac{1}{128}$.

Choice of α, $\varepsilon = 10^{-3}$



Level 5, $\delta t = \frac{1}{32}$. Level 5, $\delta t = \frac{1}{128}$. Level 7, $\delta t = \frac{1}{128}$.

Results:

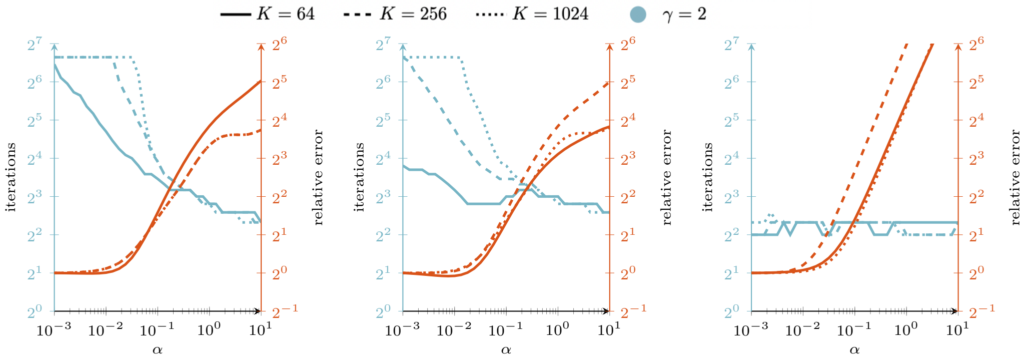
- number of iterations decreases as $\alpha \to \infty$
- independent of number of blocked time steps K and δt for sufficiently large $\alpha \approx 0.1$
- similar convergence behavior for different fine levels

$\rightarrow$ do not choose α too small

Results without stabilization:

- increasing/many iterations for large K
- δt- and level-dependency

Choice of α, $\varepsilon = 10^{-3}$



Level 5, $\delta t = \frac{1}{32}$. Level 5, $\delta t = \frac{1}{128}$. Level 9, $\delta t = \frac{1}{128}$.

Results:

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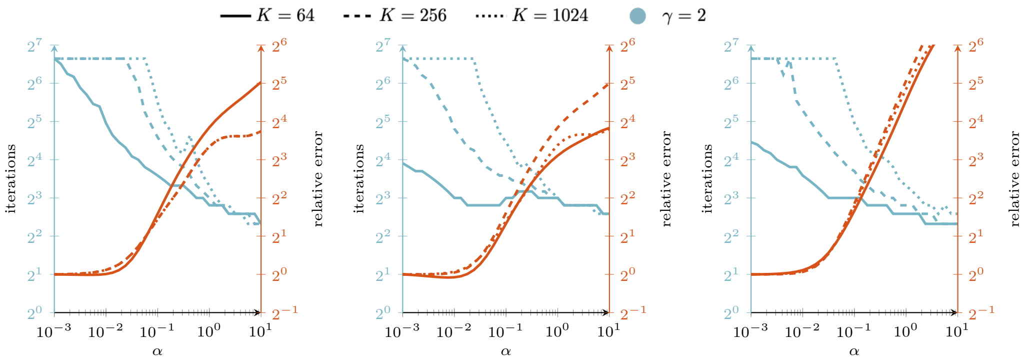
Stabilization multigrid, F-cycle, $\varepsilon = 10^{-3}$



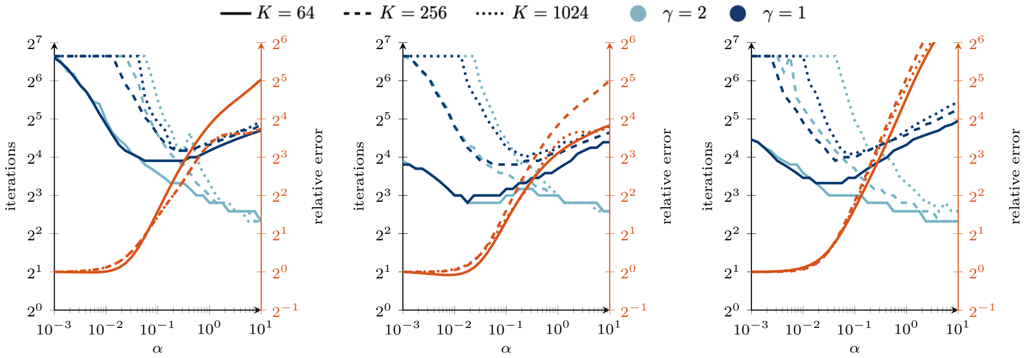
Level 5, $\delta t = \frac{1}{32}$. Level 5, $\delta t = \frac{1}{128}$. Level 7, $\delta t = \frac{1}{128}$.

Results:

- two-grid result can also be observed for multigrid
- but stabilization on coarse grid may not be enough for stable convergence rates
  $\alpha_{add} := \alpha \left(\frac{h_f}{h}\right)^\gamma \Rightarrow$ choosing $\gamma = 0$ or 1 can help!

MG algorithm:
maximum number of iterations: 100.

Stabilization multigrid, F-cycle, $\varepsilon = 10^{-3}$



Level 5, $\delta t = \frac{1}{32}$. Level 5, $\delta t = \frac{1}{128}$. Level 7, $\delta t = \frac{1}{128}$.

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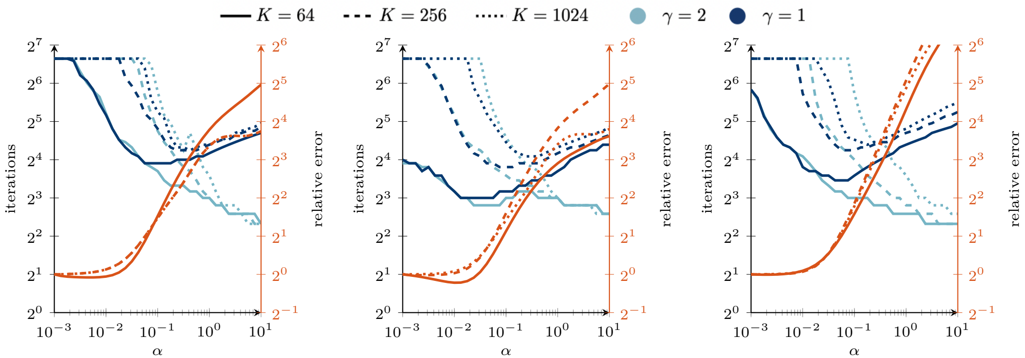
- but stabilization on coarse grid may not be enough for stable convergence rates
  $\alpha_{add} := \alpha \left(\frac{h_f}{h}\right)^{\gamma}$ $\Rightarrow$ choosing $\gamma = 0$ or 1 can help!

MG algorithm:
maximum number of iterations: 100.

Stabilization multigrid, F-cycle, $\varepsilon = 10^{-6}$



Level 5, $\delta t = \frac{1}{32}$.　　Level 5, $\delta t = \frac{1}{128}$.　　Level 7, $\delta t = \frac{1}{128}$.

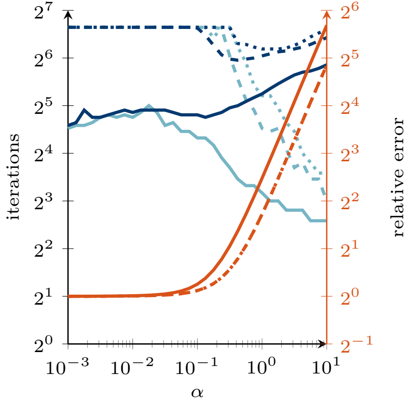
Results:

- without stabilization: ε-dependency
- with stabilization: similar results even for smallest ε

MG algorithm:
maximum number of iterations: 100.

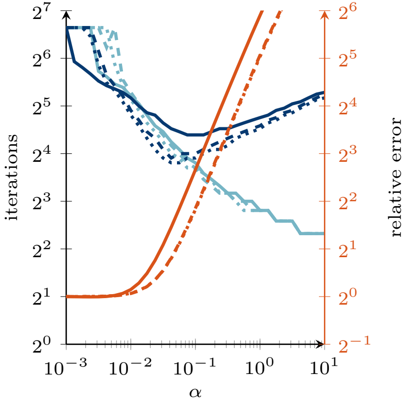
Difficulties and practical relevance

time step size $\delta t >$ fine mesh size



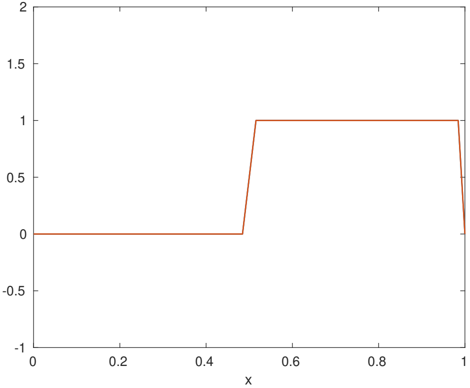
Level 9, $\delta t = \frac{1}{32}, \varepsilon = 10^{-3}$.

fixed final time T

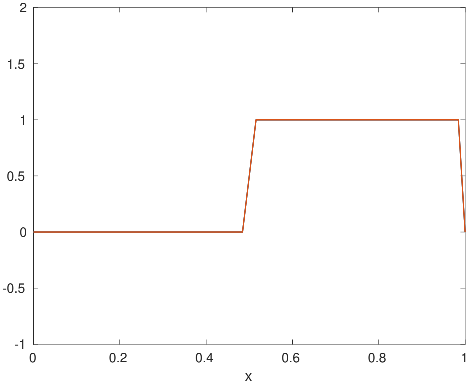


$T = 2$, Level 7, $\varepsilon = 10^{-3}$.

From another point of view: Heaviside step function



No stabilization.



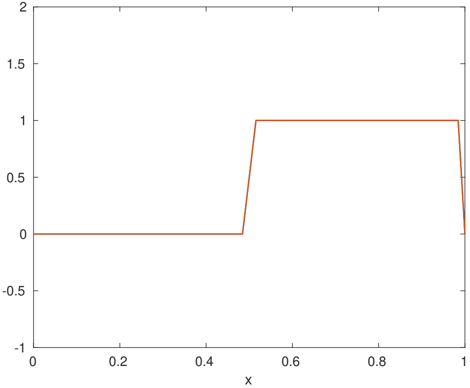
Stabilization with $\alpha = 0.01$.

- Level 6, $\delta t = \frac{1}{128}$
- oscillations in the numerical solution

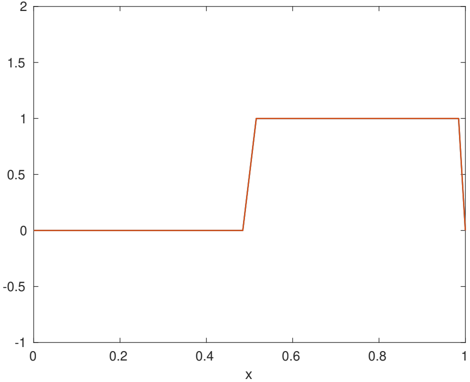
- small α can lead to a smoother numerical solution
- too large α can make it worse

$\rightarrow$ trade-off: solution vs. convergence behavior

From another point of view: Heaviside step function



No stabilization.



Stabilization with $\alpha = 0.1$.

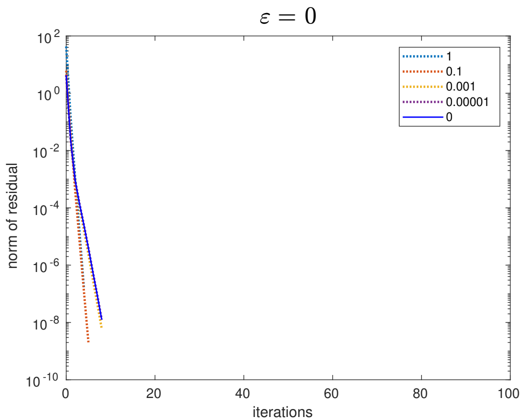
	δt	$1/32$	$1/128$	$1/512$
$\alpha = 0$	$K = 256$	100	100	100
	$K = 512$	100	100	100
	$K = 1024$	100	100	100
$\alpha = 0.1$	$K = 256$	18	14	10
	$K = 512$	24	15	12
	$K = 1024$	28	19	14

Level 7, $\varepsilon = 0$.

- small α can lead to a smoother numerical solution
- too large α can make it worse

$\rightarrow$ trade-off: solution vs. convergence behavior

Conclusion



Convergence behavior with stabilization.

Summary

- presented multigrid algorithm works fine for convection-diffusion equation if diffusion parameter is sufficiently large
- difficulties with convection-dominated problems $\rightarrow$ stabiliziation can help!
- choice of stabilization parameter is crucial

Outlook and more aspects

- extension to 2D and 3D problems
- studies on the reduction of the computational efficiency
- stabilization in time using u_{tttt}
- combination of this time-simultaneous algorithm and other parallel-in-time methods

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