# Stabilized Finite Element Multigrid Techniques for Space-Time Parallelism in Convection-Diffusion Problems

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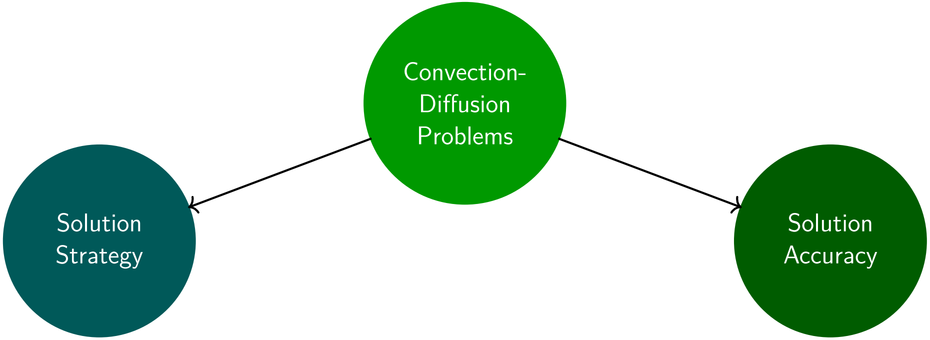
# Motivation




- **PinT methods** offer a pathway to exploit modern HPC system, but require solvers that are:
  - robust across varying diffusion coefficients and long time intervals
  - efficiently parallelizable in space *and* time

- Standard Galerkin methods can exhibit non-physical oscillations in **convection-dominated** regimes
- **Stabilization techniques** are required to improve numerical behavior and maintain physical fidelity

# Outline

# Model Problem

**$d$-dimensional convection-diffusion problem**

Find $u : \Omega \times (0,T) \to \mathbb{R}$ such that

$$\begin{aligned} \partial_t u(x,t) - \varepsilon \Delta u(x,t) + \nabla \cdot (\boldsymbol{v}(x,t) u(x,t)) &= f(x,t) && \text{in } \Omega \times (0,T), \\ u(x,t) &= 0 && \text{on } \partial\Omega \times (0,T), \\ u(x,0) &= u^0(x) && \text{in } \Omega, \end{aligned}$$

where $\Omega \subset \mathbb{R}^d, T > 0$, diffusion coefficient $\varepsilon > 0$ and velocity field $\boldsymbol{v}$.

- **Diffusion:** leads to a smoothing of the concentration distribution (high to low concentration)
- **Convection:** Transports the concentration with the flow (displacement without spreading in purely convective models)
- **Combined:** Diffusion smooths, while convection shifts the profile (spreading and transport), the balance between the two effects captured by: $Pe = \frac{vL}{\varepsilon}$

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# 1D Test Problem

**(Linearized) Burgers' Equation**

$$\begin{aligned} \partial_t u(x,t) - \varepsilon \partial_{xx} u(x,t) + \tfrac{1}{2}\partial_{xx} u(x,t)^2 &= f(x,t) \quad \text{in } (0,3)\times(0,T), \\ u(x,0) &= u^0(x) \quad \text{in } (0,3), \end{aligned}$$

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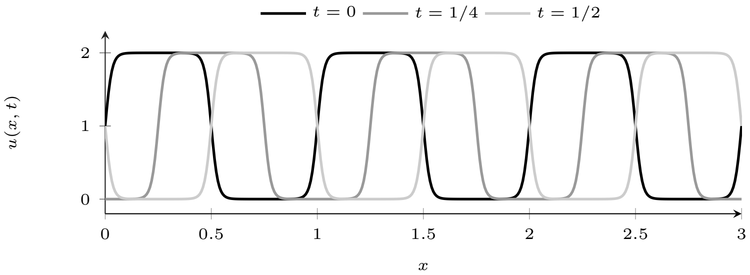


- "less" smooth solution: $u(x,t) = \frac{1}{\tanh(\eta)}\left(\tanh(\eta \sin(2\pi(x-t))) + \tanh(\eta)\right)$, where $\eta = 5$
- velocity field $v = u$ and corresponding source term $f$.

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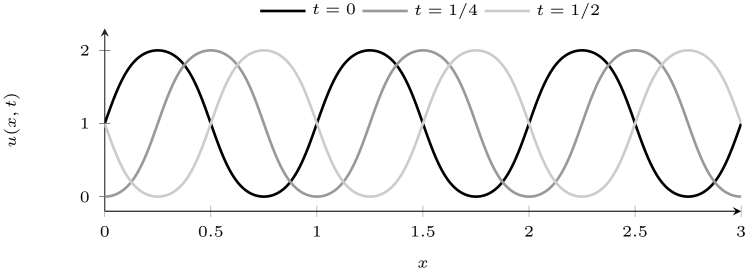


- "more" smooth solution: $u(x,t) = \frac{1}{\tanh(\eta)}\left(\tanh(\eta \sin(2\pi(x-t))) + \tanh(\eta)\right)$, where $\eta = 1$
- velocity field $v = u$ and corresponding source term $f$.

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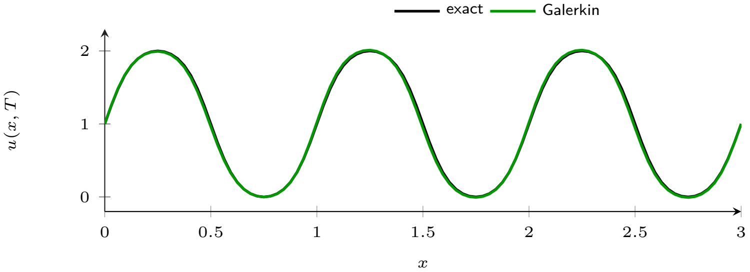
where $T > 0$, diffusion coefficient $\varepsilon = 10^{-1}$.

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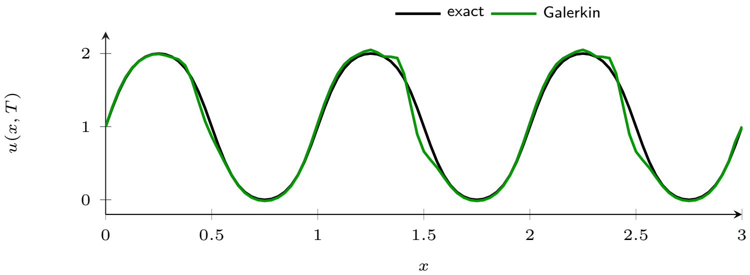
$$u(x,0) = u^0(x) \quad \text{in } (0,3),$$

where $T > 0$, diffusion coefficient $\varepsilon = 10^{-2}$.

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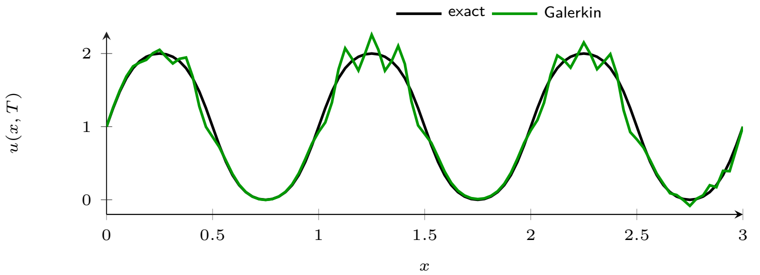


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- velocity field $v = u$ and corresponding source term $f$, $Pe_l \gg 1$.

# Galerkin Finite Elements and VMS Stabilization

- Problem at hand

$$\partial_t u - \varepsilon \Delta u + \nabla \cdot (\boldsymbol{v} u) = f \quad \text{in } \Omega \times (0,T)$$

- Semi-discrete variational problem

$$\begin{aligned} (\partial_t u_h, \varphi_h) + \varepsilon(\nabla u_h, \nabla \varphi_h) + (\nabla \cdot (\boldsymbol{v} u_h), \varphi_h) & \\ + \alpha_{\mathsf{VMS}}[(\nabla u_h, \nabla \varphi_h) - (\mathbf{g}_h, \nabla \varphi_h)] &= (f, \varphi_h), \quad \forall \varphi_h \in V_h \\ (\mathbf{g}_h - \nabla u_h, \boldsymbol{\psi}_h) &= 0 \qquad\qquad \forall \boldsymbol{\psi}_h \in (V_h)^d \end{aligned}$$

Variational multiscale (VMS) method[1]: add diffusive and compensation term with stabilization parameter $\alpha_{\mathsf{VMS}} \geq 0$

- higher order stabilization
- stabilization term vanishes in the continuous setting $\rightarrow$ consistence

[1] John, Kaya, Layton (2006); Lohmann et al. (2017).

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+\alpha_{\mathsf{VMS}}[(\nabla u_h, \nabla \varphi_h) - (\mathbf{g}_h, \nabla \varphi_h)] &= (f, \varphi_h), \quad \forall \varphi_h \in V_h \\
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# 1D Finite Differences Interpretation

- linear finite elements, uniform grid with mesh size $h$ and $N$ spatial unknowns, quadrature based mass-lumping, $v = 1$
- semi-discrete formulation in matrix form: $\boldsymbol{M} \sim$ id, $\boldsymbol{B} \sim$ grad, $\boldsymbol{B}^\top \sim$ div

$$\boldsymbol{M}\partial_t \boldsymbol{u}(t) + \varepsilon \boldsymbol{L}\boldsymbol{u}(t) + \boldsymbol{K}\boldsymbol{u}(t) + \alpha_{\mathsf{VMS}} \underbrace{(\boldsymbol{L} - \boldsymbol{B}^\top \boldsymbol{M}^{-1}\boldsymbol{B})}_{(=:\boldsymbol{W})} \boldsymbol{u}(t) = \boldsymbol{f}(t)$$

- Stabilization matrix $\boldsymbol{W}$ in FD

$$\boldsymbol{M}^{-1}\boldsymbol{L} \sim -\frac{1}{h^2}[1, -2, 1] \quad \rightsquigarrow \text{Taylor:} \quad \frac{1}{h^2}(h^2 u_{xx} + Ch^4 u_{xxxx} + O(h^6))$$

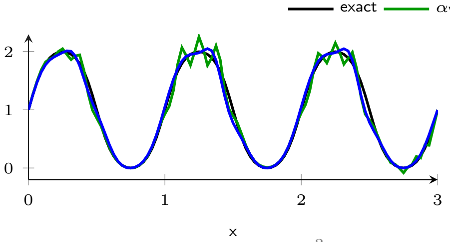
$$\boldsymbol{M}^{-1}\boldsymbol{B}^\top \boldsymbol{M}^{-1}\boldsymbol{B} \sim -\frac{1}{(2h)^2}[1, 0, -2, 0, 1] \quad \rightsquigarrow \text{Taylor:} \quad \frac{1}{4h^2}(4h^2 u_{xx} + 2^4 Ch^4 u_{xxxx} + O(h^6))$$

$$\Longrightarrow \quad \boldsymbol{M}^{-1}\boldsymbol{W} \sim \frac{1}{(2h)^2}[1, -4, 6, -4, 1] \quad \rightsquigarrow \text{Taylor:} \quad \tilde{C}h^2 u_{xxxx} + O(h^4)$$

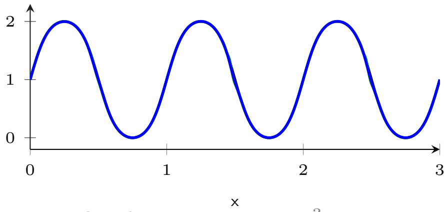
- Stabilization term corresponds to scaled biharmonic operator $\Rightarrow$ second order of accuracy

# VMS Stabilization in Convection-Dominated Cases

- **Non-phyiscal oscillations** may occur when diffusion decreases
  $\rightarrow$ can be **smoothed by stabilization** or by finer resolution




Level 5, $T = 3, \varepsilon = 10^{-3}$.




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

- Choose $\alpha_{\text{VMS}}$ fix or $\alpha_{\text{VMS}}(x,t) = 0.1 \frac{Pe_l}{1+Pe_l} v(x,t)$, where $Pe_l = \frac{hv(x,t)}{\varepsilon}$

| $h = \delta t$ | $\alpha_{\text{VMS}} = 0$ | $0.1$ | $\alpha_{\text{VMS}}(x,t)$ |
|---|---|---|---|
| $1/32$ | $1.9 \cdot 10^{-1}$ | $1.4 \cdot 10^{-1}$ | $3.1 \cdot 10^{-1}$ |
| $1/64$ | $8.6 \cdot 10^{-2}$ | $4.5 \cdot 10^{-2}$ | $1.2 \cdot 10^{-1}$ |
| $1/128$ | $2.1 \cdot 10^{-2}$ | $1.6 \cdot 10^{-2}$ | $4.2 \cdot 10^{-2}$ |
| $1/256$ | $5.3 \cdot 10^{-3}$ | $5.8 \cdot 10^{-3}$ | $1.5 \cdot 10^{-2}$ |
| $1/512$ | $1.3 \cdot 10^{-3}$ | $2.1 \cdot 10^{-3}$ | $4.9 \cdot 10^{-3}$ |

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

# Time Discretization

Implicit Theta scheme, $\theta \in (0,1]$, time steps $t^0, \ldots, t^K$, fixed time step size $\delta t$

$$\boldsymbol{A}\boldsymbol{u}^m + \boldsymbol{B}\boldsymbol{u}^{m-1} = \delta t \left( \theta \boldsymbol{f}^m + (1-\theta)\boldsymbol{f}^{m-1} \right) = \tilde{\boldsymbol{f}}^m, \quad m = 1, \ldots, K,$$

where $\quad \boldsymbol{A} := \boldsymbol{M} + \theta\delta t(\varepsilon \boldsymbol{L} + \boldsymbol{K}) + \delta t \alpha_{\mathsf{VMS}} \boldsymbol{W}, \quad \boldsymbol{B} := -\boldsymbol{M} + (1-\theta)\delta t(\varepsilon \boldsymbol{L} + \boldsymbol{K})$

Special characteristic: Fully implicit treatment of stabilization[2]

- considered for Crank-Nicolson scheme, i.e., $\theta = \frac{1}{2}$
- reduces computational effort
- no loss of accuracy (2nd order)
- very effective regarding the solver

[2] D., Turek, Lohmann (2024)

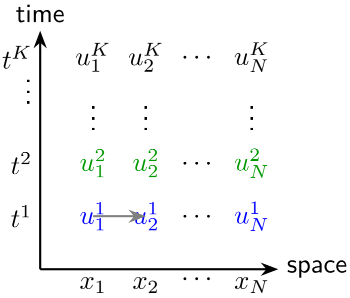
# Preliminaries

Blocking the unknowns in two different ways...

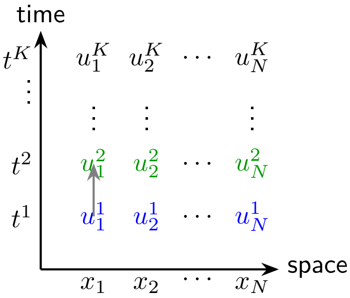
$N$ spatial nodes $x_1, \ldots, x_N$,
$K$ time steps $t^1, \ldots, t^K$

time-major ordering

space-major ordering



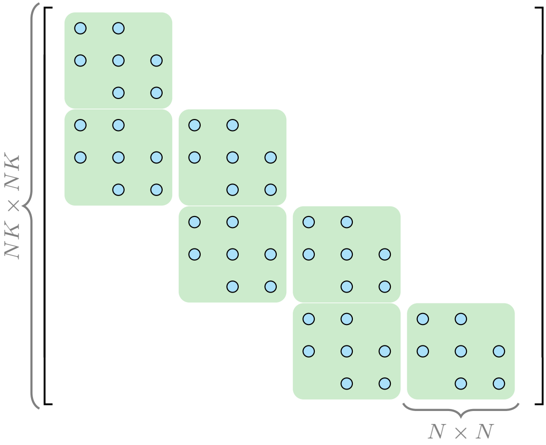

$$\tilde{\boldsymbol{u}} := \begin{bmatrix} u_1^1 \\ u_2^1 \\ \vdots \\ u_N^1 \\ u_1^2 \\ u_2^2 \\ \vdots \\ u_N^2 \\ \vdots \\ u_1^K \\ u_2^K \\ \vdots \\ u_N^K \end{bmatrix} \qquad \begin{bmatrix} u_1^1 \\ u_1^2 \\ \vdots \\ u_1^K \\ u_2^1 \\ u_2^2 \\ \vdots \\ u_2^K \\ \vdots \\ u_N^1 \\ u_N^2 \\ \vdots \\ u_N^K \end{bmatrix} =: \boldsymbol{u}$$

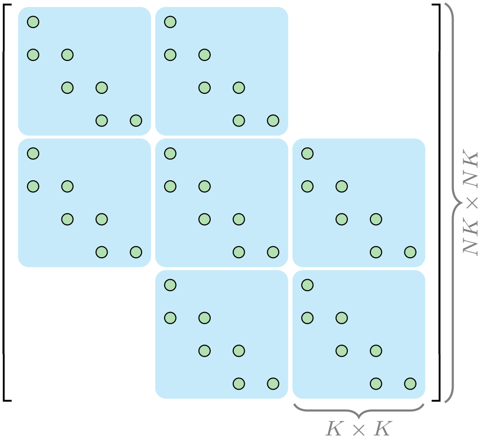


# Preliminaries II

...results in the following two global system matrix structures for $\alpha_{\mathsf{VMS}} = 0$ and 1D:

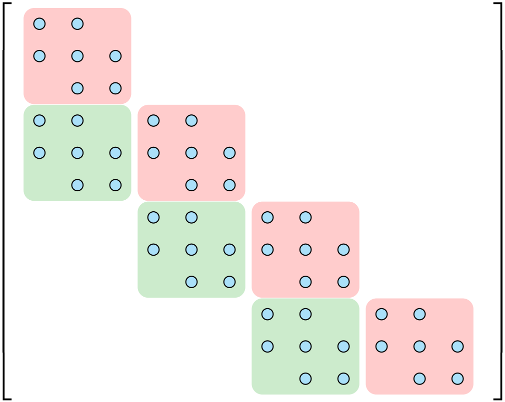
time-major ordering | space-major ordering



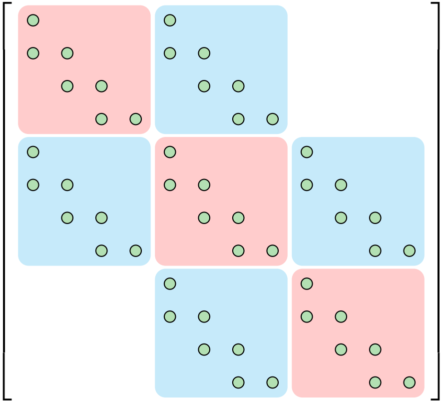



# Parallel-in-Time Multigrid Methods

**Space-Time Multigrid (STMG)**



**Multigrid Waveform Relaxation (WRMG)**



Smoothing: (damped) block Jacobi method: $\boldsymbol{x}^{(\nu)} = \boldsymbol{x}^{(\nu-1)} + \omega \boldsymbol{D}^{-1}(\boldsymbol{f} - \boldsymbol{S}\boldsymbol{x}^{(\nu-1)})$

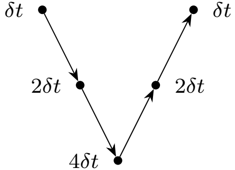
number of pre-smoothing and post-smoothing steps: $\nu_1$ and $\nu_2$

# Parallel-in-Time Multigrid Methods II

### Space-Time Multigrid (STMG)

- Gander & Neumüller (2016)
- Parallelization in time (and space)
- Solves the full space-time problem on a space-time grid
- Approximates $\boldsymbol{D}$ with multigrid in space ($\text{tol}_{\text{rel}} = 10^{-1}$)
- Coarsening per spatial node:

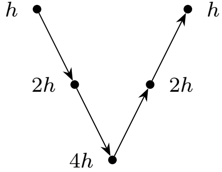
$$\boldsymbol{P}^{\delta t,h}_{2\delta t,h} = \boldsymbol{P}^{\delta t}_{2\delta t} \otimes \boldsymbol{I}_N, \quad \boldsymbol{R}^{2\delta t,h}_{\delta t,h} = (\boldsymbol{P}^{\delta t,h}_{2\delta t,h})^\top$$



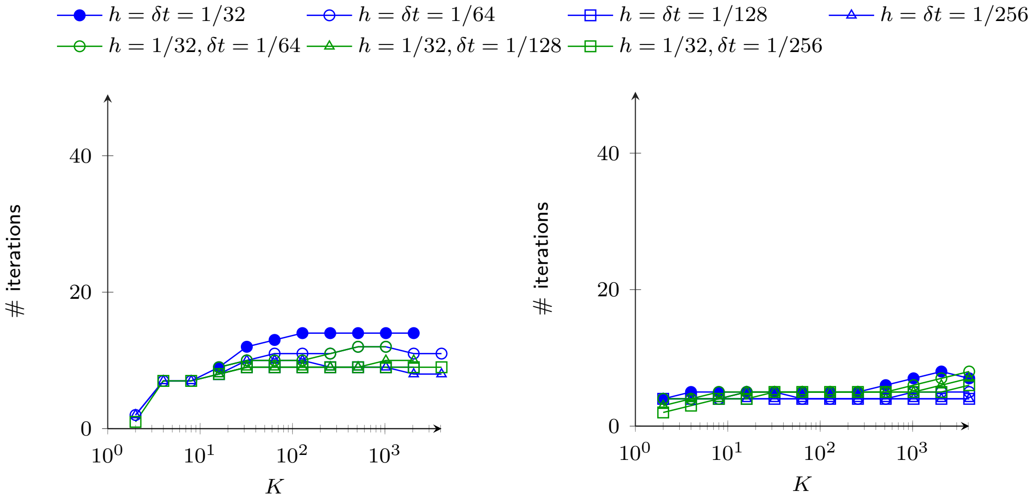

### Multigrid Waveform Relaxation (WRMG)

- Lubich & Ostermann (1987)
- Enhances parallelization in space
- Solves "space-only" problem with vector-valued unknowns for each spatial node → applied simultaneously across all time steps
- Standard coarsening in space for each time step:

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



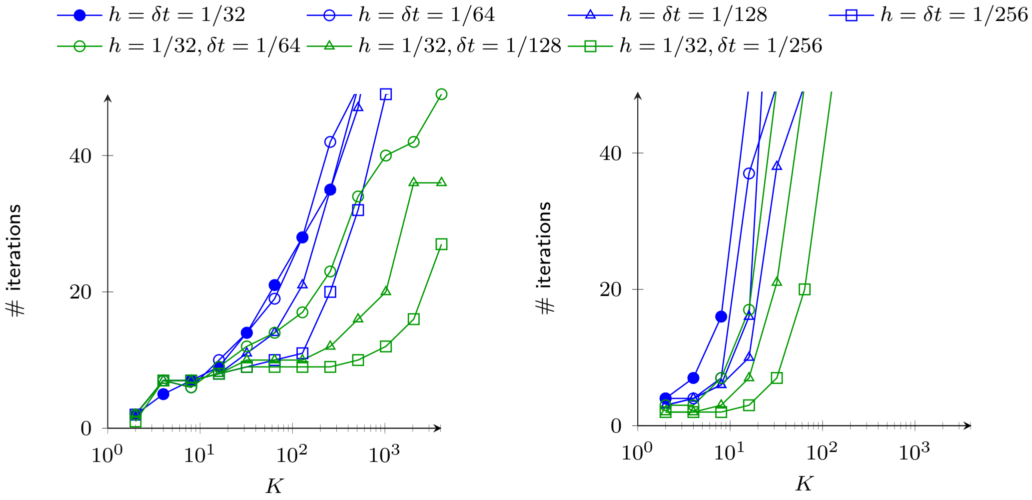
# Numerical Studies: $\alpha_{\mathsf{VMS}} = 0$




STMG, F-cycle, FGMRES(2+2), coarsening in time, $\varepsilon = 10^{-2}$.

WRMG, F-cycle, GMRES(2+2), coarsening in space, $\varepsilon = 10^{-1}$.

# Numerical Studies: $\varepsilon = 10^{-3}, \alpha_{\text{VMS}} = 0$




STMG, F-cycle, FGMRES(2+2), coarsening in time.

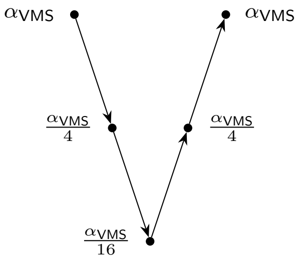
WRMG, F-cycle, GMRES(2+2), coarsening in space.

# Stabilization in WRMG

- Stabilization parameter in multigrid:

$$\alpha_{\mathsf{VMS}} \left(\frac{h}{H}\right)^2$$

$h$: mesh size of fine level, $H$: mesh size of current level



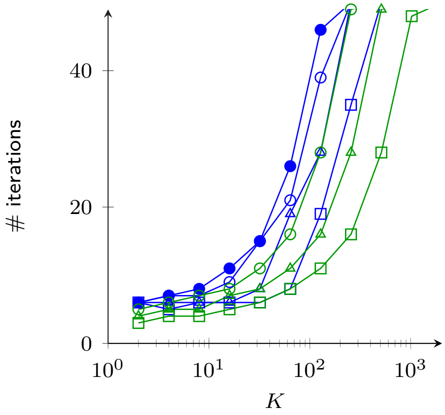

- Preferred choices: $\alpha_{\mathsf{VMS}} = 0.1$ fix or $\alpha_{\mathsf{VMS}}(x,t)$

- Solve the same continuous problem on each level, **but** less stabilization on coarser levels[3]

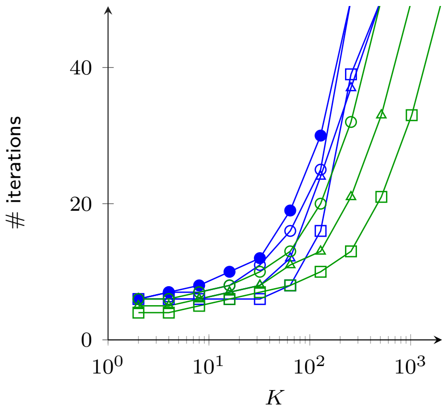
$$\alpha_{\mathsf{VMS}} \left(\frac{h}{H}\right)^2 \boldsymbol{M}^{-1}\boldsymbol{W}\boldsymbol{u} \sim \alpha_{\mathsf{VMS}} \left(\frac{h}{H}\right)^2 \tilde{C} H^2 u_{xxxx} = \alpha_{\mathsf{VMS}} h^2 \tilde{C} u_{xxxx}$$

[3] D., Turek, Lohmann (2023)

# Numerical Studies: $\varepsilon = 10^{-3}$




WRMG, F-cycle, GMRES(2+2), coarsening in space, $\alpha_{\text{VMS}} = 0.1$.

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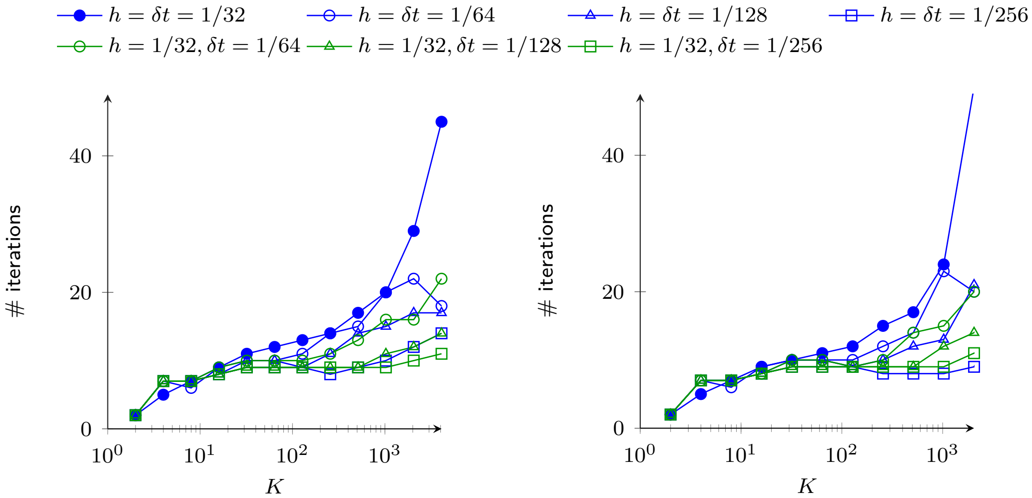


STMG, F-cycle, FGMRES(2+2), coarsening in time, $\alpha_{\text{VMS}} = 0.1$.

STMG, F-cycle, FGMRES(2+2), coarsening in time, $\alpha_{\text{VMS}}(x,t)$.

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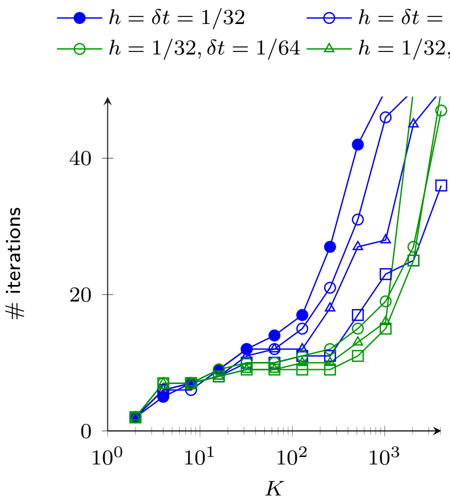
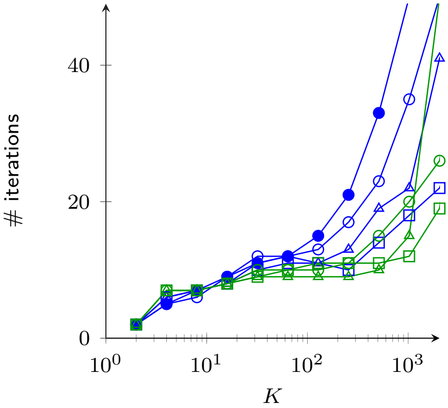



STMG, F-cycle, FGMRES(2+2),
coarsening in time and space, $\alpha_{\text{VMS}} = 0.1$.




STMG, F-cycle, FGMRES(2+2),
coarsening in time and space, $\alpha_{\text{VMS}}(x,t)$.

# Combined Approach: Space-Time Parallelization

STMG(t) and WRMG(s) offer powerful tools - but may be limited when used alone.

Challenges:

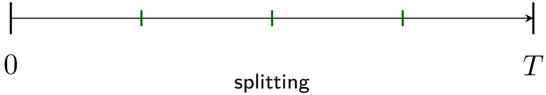
- small $\varepsilon$
- number of iterations low and bounded
- large time intervals

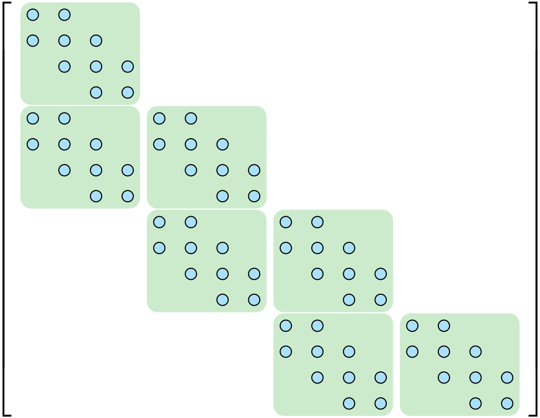
**Main idea and aims:**

- introduce **geometric multigrid in time** (and space), coupled with WRMG as an **inner block smoother** $\rightarrow$ enhanced space parallelism
- split time interval into subintervals for smoothing purposes $\rightarrow$ time parallelism by independent treatment of subintervals
- ensure **small coarse-grid problems** - via coarsening in both **space and time**
- scalable space-time parallelism to unlock more potential for extreme-scale computing

# Multigrid in Time: Smoothing

Split global time interval into $I$ subintervals



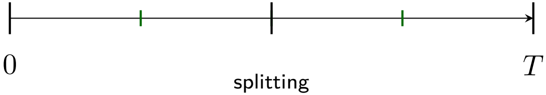



$$\boldsymbol{x}^{(\tilde{\nu})} = \boldsymbol{x}^{(\tilde{\nu}-1)} + \omega \tilde{M}^{-1}(\tilde{\boldsymbol{f}} - \tilde{S}\boldsymbol{x}^{(\tilde{\nu}-1)})$$

- compute residual $\tilde{\boldsymbol{r}} := (\tilde{\boldsymbol{f}} - \tilde{\boldsymbol{S}}\boldsymbol{x}^{(\tilde{\nu}-1)})$
- split global time interval into $I$ subintervals
- solve $M_i \boldsymbol{s}_i = \boldsymbol{r}_i, i = 1, ..., I$ on each subinterval, or, approximate $M_i$ with **WRMG**($\text{tol}_{\text{rel}} = 10^{-1}$)
- correction $\quad \boldsymbol{x}^{(\tilde{\nu})} = \boldsymbol{x}^{(\tilde{\nu}-1)} + \omega \tilde{\boldsymbol{s}}$

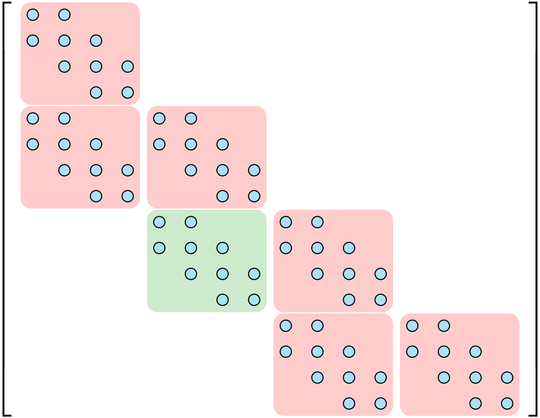
# Multigrid in Time: Smoothing

Split global time interval into $I$ subintervals

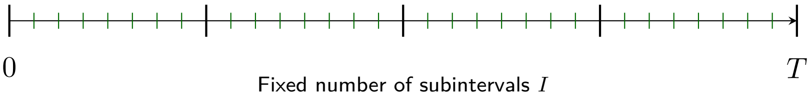



$$\boldsymbol{x}^{(\tilde{\nu})} = \boldsymbol{x}^{(\tilde{\nu}-1)} + \omega \tilde{M}^{-1}(\tilde{\boldsymbol{f}} - \tilde{S}\boldsymbol{x}^{(\tilde{\nu}-1)})$$

- compute residual $\tilde{\boldsymbol{r}} := (\tilde{\boldsymbol{f}} - \tilde{\boldsymbol{S}}\boldsymbol{x}^{(\tilde{\nu}-1)})$
- split global time interval into $I$ subintervals
- solve $M_i \boldsymbol{s}_i = \boldsymbol{r}_i, i = 1, ..., I$ on each subinterval, or, approximate $M_i$ with **WRMG**($\text{tol}_{\text{rel}} = 10^{-1}$)
- correction $\boldsymbol{x}^{(\tilde{\nu})} = \boldsymbol{x}^{(\tilde{\nu}-1)} + \omega \tilde{\boldsymbol{s}}$



# Multigrid in Time (and in Space): Coarsening




- Restriction (forward in time) and prolongation:

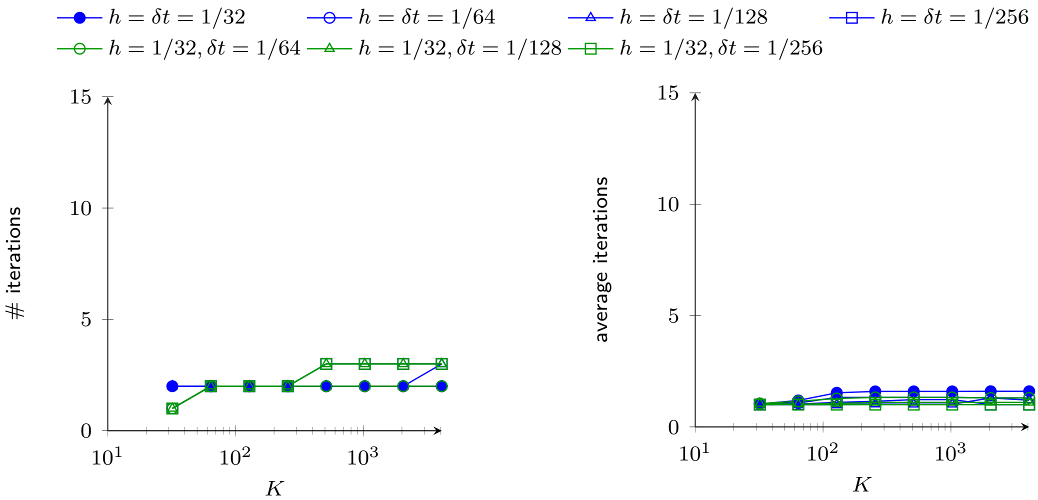
$$\boldsymbol{R}_{\delta t,h}^{2\delta t,h} = \boldsymbol{R}_{\delta t}^{2\delta t} \otimes \boldsymbol{I}_N, \quad \boldsymbol{P}_{2\delta t,h}^{\delta t,h} = (\boldsymbol{R}_{\delta t,h}^{2\delta t,h})^\top$$

- **Pro:** Processors correspond to fixed subintervals $\rightarrow$ reduces communication costs
- **Con:** Maximum number of levels depends on the number of time steps per sub interval on the fine level

In numerical studies: $32$ time steps per subinterval on fine level $\rightarrow$ computing time of coarse grid solver $< 1\%$

**Note:** Fixing the number of time steps $= 1$ per interval when coarsening leads to STMG.

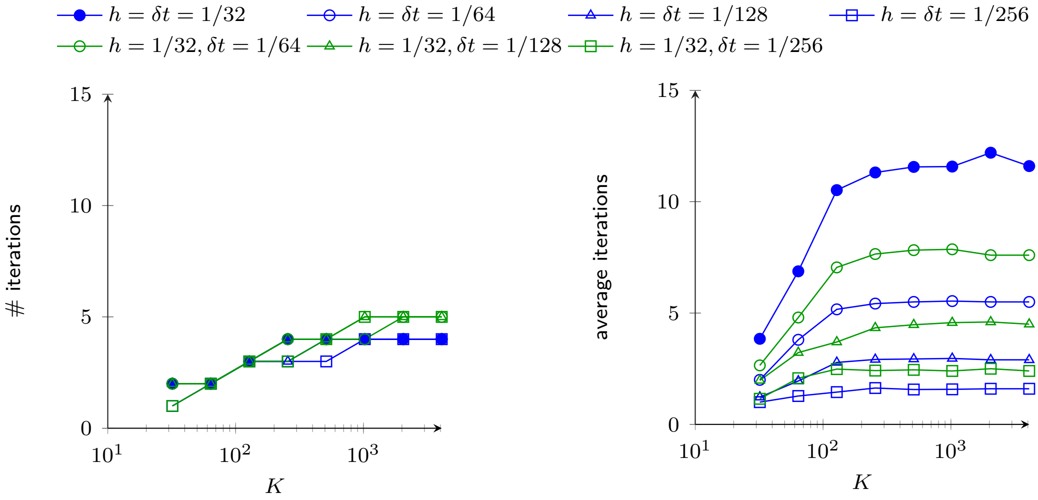
# Numerical Studies: $\varepsilon = 10^{-1}, \alpha_{\text{VMS}} = 0.$




MG, V-cycle, FGMRES(2+2) coarsening in time.

Inner WRMG, V-cycle, GMRES(2+2), coarsening in space.

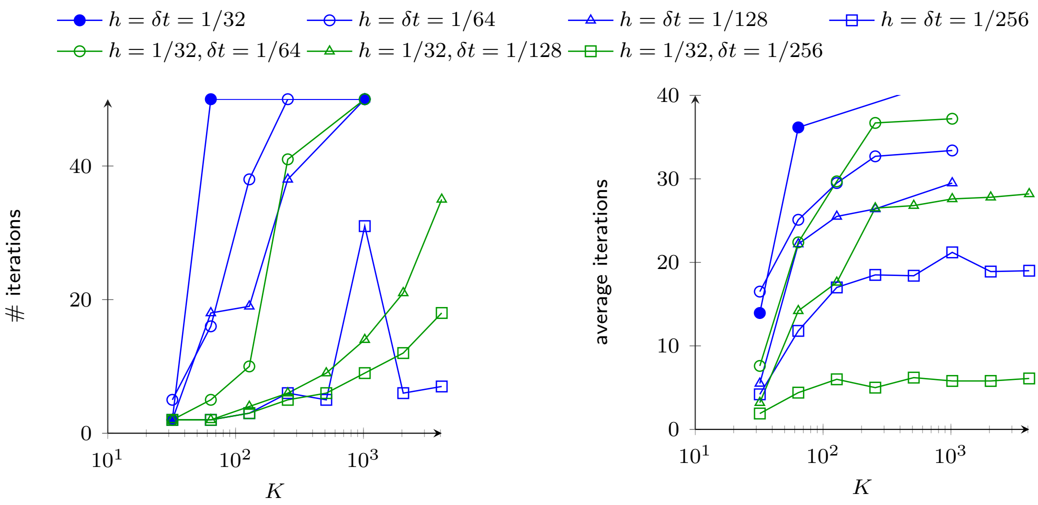
# Numerical Studies: $\varepsilon = 10^{-2}, \alpha_{\text{VMS}} = 0$




MG, V-cycle, FGMRES(2+2) coarsening in time.

Inner WRMG, V-cycle, GMRES(2+2), coarsening in space.

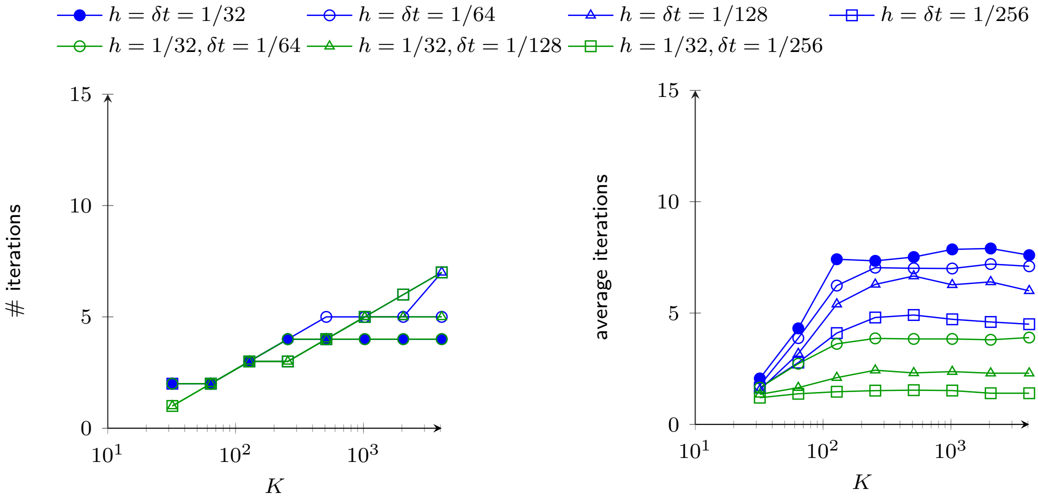
# Numerical Studies: $\varepsilon = 10^{-3}, \alpha_{\mathsf{VMS}} = 0$




MG, V-cycle, FGMRES(2+2) coarsening in time.

Inner WRMG, V-cycle, GMRES(2+2), coarsening in space.

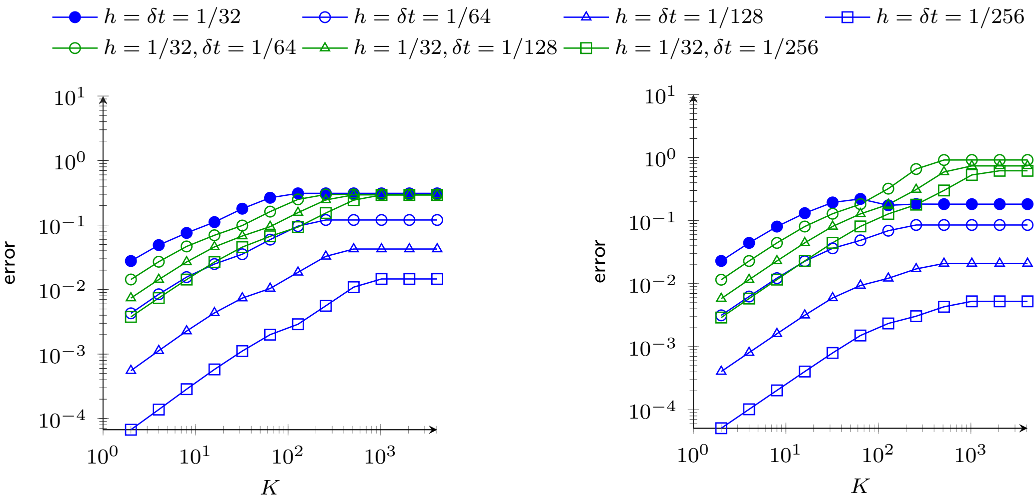
# Numerical Studies: $\varepsilon = 10^{-3}, \alpha_{\text{VMS}}(x,t)$




MG, V-cycle, FGMRES(2+2)
**coarsening in time and space**.

Inner WRMG, V-cycle, GMRES(2+2),
coarsening in space.

# Numerical Studies: $\varepsilon = 10^{-3}$



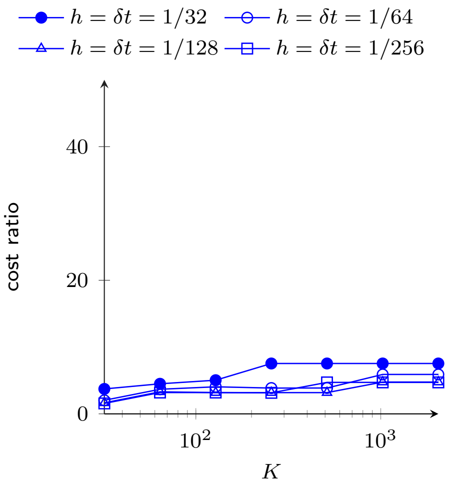

Discrete $L_2$-error at final time $T = \delta t K$, $\alpha_{\mathsf{VMS}}(x,t)$.

Discrete $L_2$-error at final time $T = \delta t K$, $\alpha_{\mathsf{VMS}} = 0$.

# Conclusion and More Aspects

- Stabilization can improve solution accuracy and solver performance in convection-dominated scenarios
- Combined method shows encouraging results for various $\varepsilon$ and large time intervals

- Extension to 2D and 3D problems
- Studies on computational and parallel efficiency




Cost ratio estimation: sequential vs. MG, V-cycle, FGMRES(2+2), $\varepsilon = 10^{-1}$, coarsening in space and time.

# Conclusion and More Aspects

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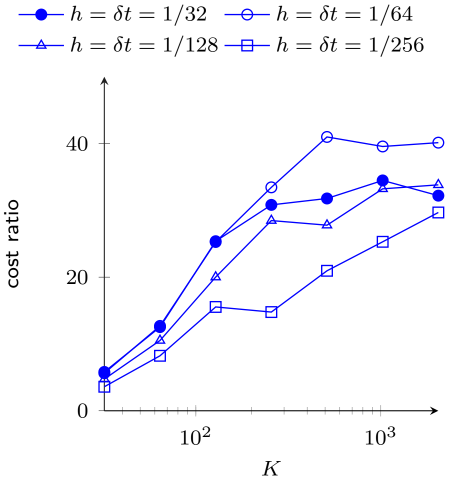


Cost ratio estimation: sequential vs. MG, V-cycle, FGMRES(2+2), $\varepsilon = 10^{-3}$, $\alpha_{\mathsf{VMS}}(x,t)$, coarsening in space and time.

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# Backup: Fully Implicit Treatment of Stabilization

- stabilization matrix $\boldsymbol{W} := \boldsymbol{L} - \boldsymbol{B}^\top \boldsymbol{M}^{-1} \boldsymbol{B}$
- stabilized FE discretization of problem at hand

$$\boldsymbol{A}\boldsymbol{u}^m + \boldsymbol{B}\boldsymbol{u}^{m-1} = \tilde{\boldsymbol{f}}^m$$

where

$$\begin{aligned} \boldsymbol{A} &:= \quad (\boldsymbol{M} + \alpha_{\mathsf{VMS}} \tfrac{\delta t}{2} \boldsymbol{W}) + \tfrac{\delta t}{2} (\varepsilon \boldsymbol{L} + \boldsymbol{K} + \alpha_{\mathsf{VMS}} \boldsymbol{W}), \\ \boldsymbol{B} &:= -(\boldsymbol{M} + \alpha_{\mathsf{VMS}} \tfrac{\delta t}{2} \boldsymbol{W}) + \tfrac{\delta t}{2} (\varepsilon \boldsymbol{L} + \boldsymbol{K} + \alpha_{\mathsf{VMS}} \boldsymbol{W}). \end{aligned}$$

- corresponds to the CN discretization of

$$\begin{aligned} &(\boldsymbol{M} + \alpha_{\mathsf{VMS}} \tfrac{\delta t}{2} \boldsymbol{W}) \partial_t \boldsymbol{u}(t) + (\varepsilon \boldsymbol{L} + \boldsymbol{K} + \alpha_{\mathsf{VMS}} \boldsymbol{W}) \boldsymbol{u}(t) = \boldsymbol{f}(t) \\ \Leftrightarrow \quad &\boldsymbol{M} \partial_t \boldsymbol{u}(t) + (\varepsilon \boldsymbol{L} + \boldsymbol{K}) \boldsymbol{u}(t) + \alpha_{\mathsf{VMS}} \boldsymbol{W} (\tfrac{\delta t}{2} \partial_t \boldsymbol{u}(t) + \boldsymbol{u}_h(t)) = \boldsymbol{f}(t) \end{aligned}$$

- variational formulation of VMS stabilization in $d$ dimensions

$$\begin{aligned} &(\partial_t u_h, \varphi_h) + \varepsilon(\nabla u_h, \nabla \varphi_h) + \nabla \cdot (\boldsymbol{v} u_h, \varphi_h) \\ &\qquad + \alpha_{\mathsf{VMS}} [(\nabla [u_h + \tfrac{\delta t}{2} \partial_t u_h], \nabla \varphi_h) - (\mathbf{g}_h, \nabla \varphi_h)] = (f_h, \varphi_h) \quad \forall \varphi_h \in V_h, \\ &\qquad (\mathbf{g}_h - \nabla [u_h + \tfrac{\delta t}{2} \partial_t u_h], \boldsymbol{\psi}_h) = 0 \quad \forall \boldsymbol{\psi}_h \in (V_h)^d \end{aligned}$$