Preconditioning the Stage Equations of Implicit Runge-Kutta Methods for Parabolic PDEs

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Outline

- Introduction and Preliminaries
- Preconditioner
- Optimization

Model problem

Model problem

$$\frac{\partial}{\partial t}u = \Delta u \quad \text{in } \Omega \times (0,T)$$

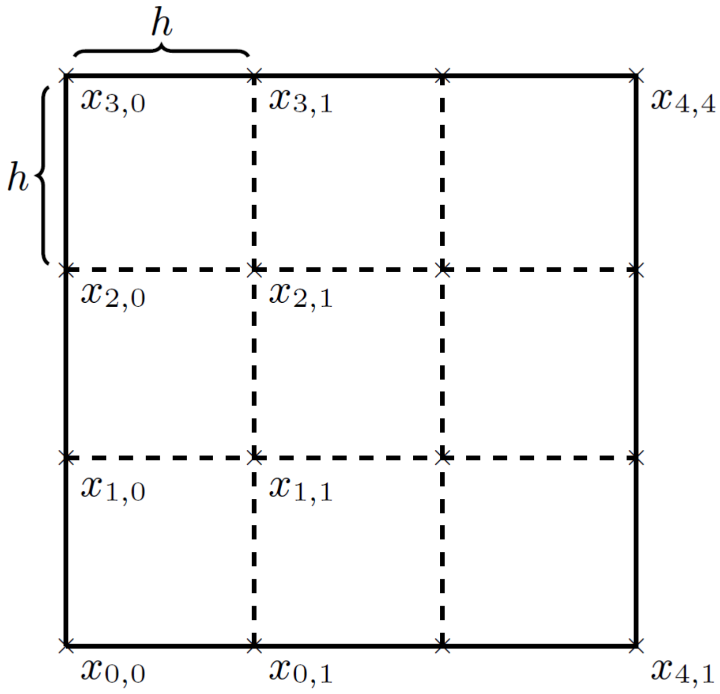
$$u = g \quad \text{on } \partial\Omega \times (0,T)$$

$$u = u_0 \;\; \text{at } \partial\Omega \times \{0\}$$

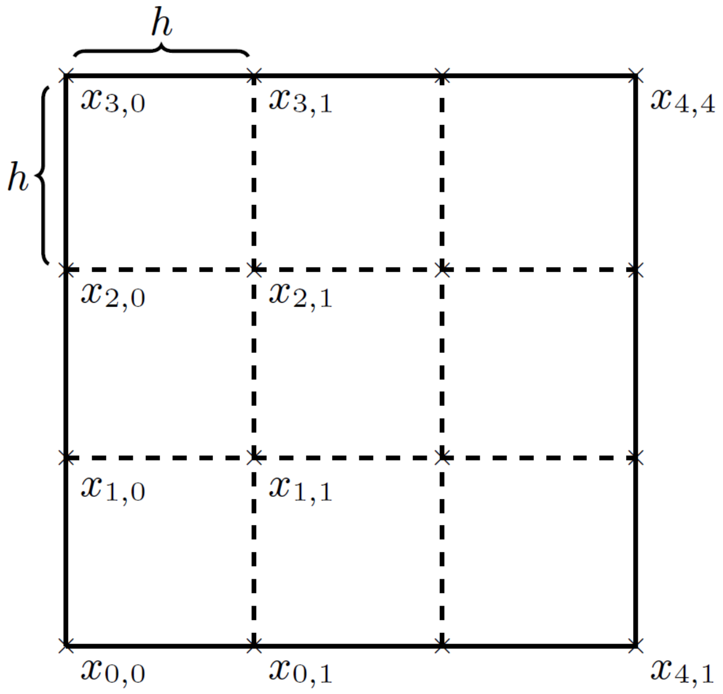
Model problem

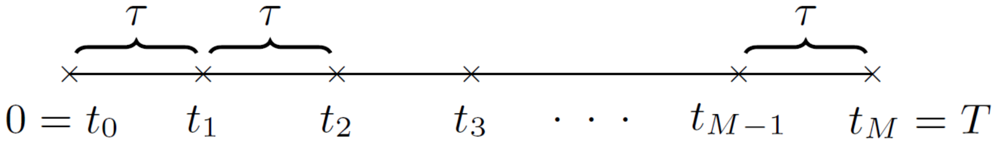
$$\Omega = (0,1) \times (0,1)$$

Discretization



Discretization





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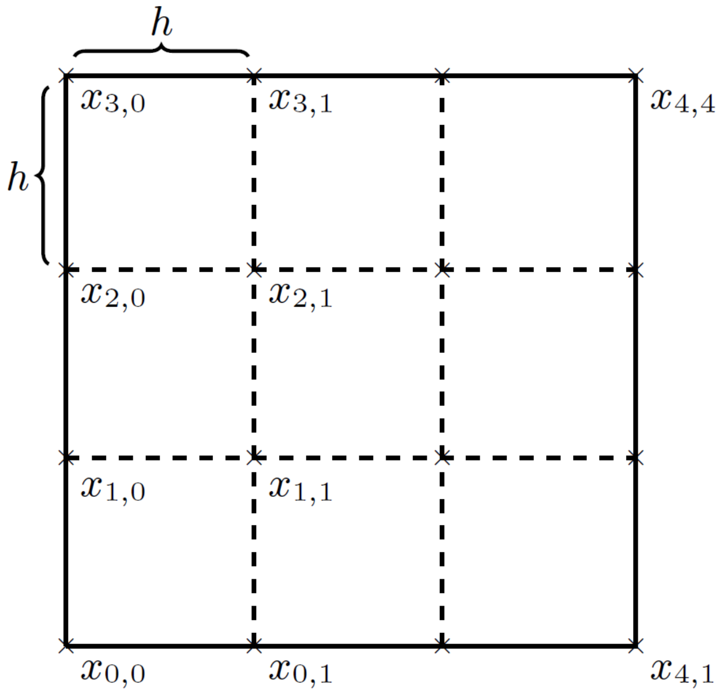
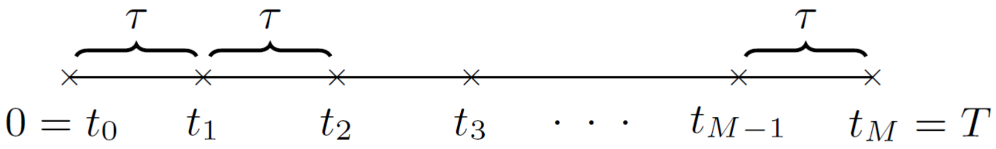
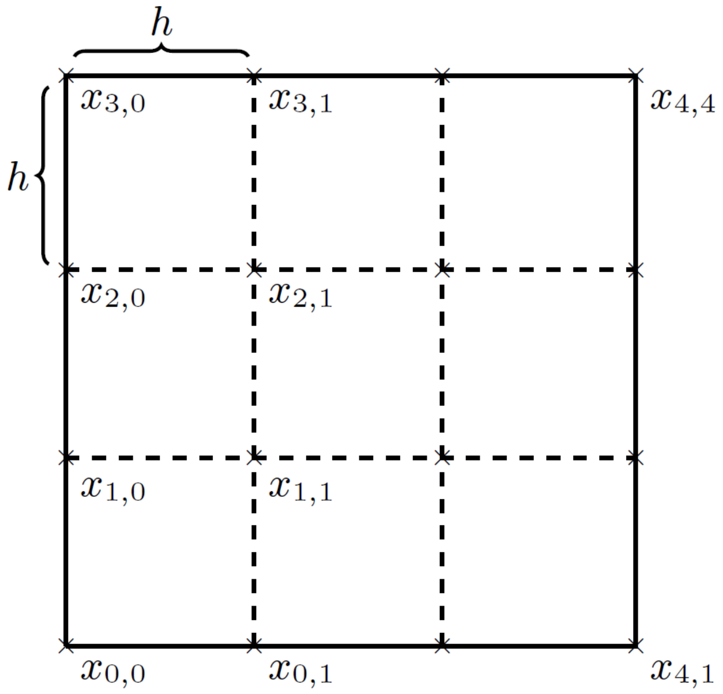
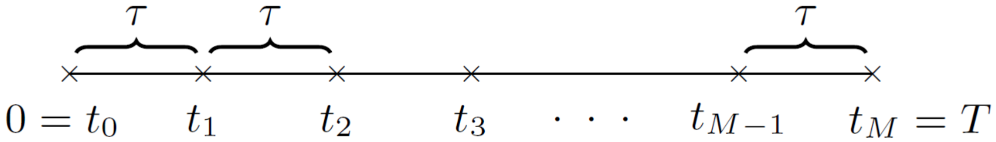




$$\mathbf{u}^m \approx u(t_m, x_{ij})$$

Discretization





$$\mathbf{u}^m \approx u(t_m, x_{ij})$$

$$\Delta \approx L$$

Runge-Kutta methods

Runge-Kutta methods

$$\mathbf{u}^m = \mathbf{u}^{m-1} + \tau \sum_{i=1}^{s} b_i \mathbf{k}_i^m$$

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$$\mathbf{u}^m = \mathbf{u}^{m-1} + \tau \sum_{i=1}^{s} b_i \mathbf{k}_i^m$$

$$\boxed{\left(I_s \otimes I_n - \frac{\tau}{h^2}(A \otimes L) \right)} \mathbf{k}^m = \frac{1}{h^2}(I_s \otimes L)\mathbf{u}^{m-1}$$

$$\boxed{M}$$

Preconditioner – idea

Preconditioner – idea

$$\hat{S} = M + \left(a_{2,2} - \frac{a_{1,2}a_{2,1}}{a_{1,1}}\right) hF$$

$$A \approx L\hat{U}$$

$$\begin{aligned} P_{triang} &= \hat{U} \\ &= \begin{bmatrix} M + a_{1,1}hF & a_{1,2}hF \\ & \hat{S} \end{bmatrix} \end{aligned}$$

Right-preconditioned GMRES: AP_{triang}^{-1}

Preconditioner – idea

M. M. Rana, V. E. Howle, K. Long, A. Meek, and W. Milestone. A New Block Preconditioner for Implicit Runge-Kutta Methods for Parabolic PDE Problems, 2021.

Preconditioner – idea

$$\text{factor}\left(I_s \otimes I_n - \frac{\tau}{h^2} A \otimes L\right)$$

Preconditioner – idea

$$\boxed{\text{factor}\left(I_s \otimes I_n - \frac{\tau}{h^2} A \otimes L\right)} \approx I_s \otimes I_n - \frac{\tau}{h^2} \boxed{\text{factor}\,(A)} \otimes L$$

Preconditioner – idea

$$\text{factor}\left(I_s \otimes I_n - \frac{\tau}{h^2} A \otimes L\right) \approx I_s \otimes I_n - \frac{\tau}{h^2}\,\text{factor}\,(A) \otimes L$$

$$\boxed{I_s \otimes I_n - \frac{\tau}{h^2} U_A \otimes L =: P^{\text{triang}}}$$

Preconditioner

$$I_s \otimes I_n - \frac{\tau}{h^2} U_A \otimes L =: P^{\text{triang}}$$

$$M \left(P^{\text{triang}}\right)^{-1}$$

$$\texttt{sp.linalg.gmres}\,(M, \text{rhs}, P^{\text{triang}})$$

Convergence analysis

sp.linalg.gmres

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sp.linalg.gmres

$$\frac{\|r_k\|}{\|r_0\|} \leq \min_{\substack{\varphi(0)=1 \\ \deg(\varphi)\leq k}} \|\varphi(M\left(P^{\text{triang}}\right)^{-1})\|$$

$$\frac{\|r_k\|}{\|r_0\|} \leq \kappa(S) \min_{\substack{\varphi(0)=1 \\ \deg(\varphi)\leq k}} \max_{\zeta_i \in \text{sp}(M(P^{\text{triang}})^{-1})} |\varphi(\zeta_i)|$$

$$\frac{\|r_k\|}{\|r_0\|} \leq \boxed{\kappa(S)} \boxed{\min_{\substack{\varphi(0)=1 \\ \deg(\varphi)\leq k}} \max_{\zeta \in \text{co}(sp(\cdots))} |\varphi(\zeta)|}$$

Preconditioner analysis

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Step I :

Preconditioner analysis

Step I :

$$M(P^{\text{triang}})^{-1} \sim \begin{bmatrix} X_{11} & \cdots & X_{1s} \\ \vdots & \ddots & \vdots \\ X_{s1} & \cdots & X_{ss} \end{bmatrix}$$

Preconditioner analysis

Step I :

$$M(P^{\text{triang}})^{-1} \sim \begin{bmatrix} X_{11} & \cdots & X_{1s} \\ \vdots & \ddots & \vdots \\ X_{s1} & \cdots & X_{ss} \end{bmatrix}$$

$$\text{with} \quad X_{ij} = \text{diag}\left(\xi_1^{(ij)}, \ldots, \xi_n^{(ij)}\right) \qquad \forall ij$$

Preconditioner analysis

Step II :

Preconditioner analysis

Step II :

$$X = \begin{bmatrix} X_{11} & \cdots & X_{1s} \\ \vdots & \ddots & \vdots \\ X_{s1} & \cdots & X_{ss} \end{bmatrix} \qquad \sim$$

$$\text{with} \quad X_{ij} = \operatorname{diag}\left(\xi_1^{(ij)}, \ldots, \xi_n^{(ij)}\right)$$

$$X \in \mathbb{R}^{ns \times ns}$$

Preconditioner analysis

Step II :

$$X = \begin{bmatrix} X_{11} & \dots & X_{1s} \\ \vdots & \ddots & \vdots \\ X_{s1} & \dots & X_{ss} \end{bmatrix} \quad \sim \quad X_k = \begin{bmatrix} \xi_k^{(11)} & \dots & \xi_k^{(1s)} \\ \vdots & \ddots & \vdots \\ \xi_k^{(s1)} & \dots & \xi_k^{(ss)} \end{bmatrix}$$

with $\quad X_{ij} = \operatorname{diag}\left(\xi_1^{(ij)}, \dots, \xi_n^{(ij)}\right)$

$$X_k \in \mathbb{R}^{s \times s}$$

$$X \in \mathbb{R}^{ns \times ns}$$

Preconditioner analysis

Lemma. *Let* $X \in \mathbb{R}^{ns \times ns}$ *and* $X_k \in \mathbb{R}^{s \times s}$ *be as above and set*

$$\text{eigenpair}\,(X_k) = \left(\mu_\ell^{(k)}, \boldsymbol{s}_\ell^{(k)}\right).$$

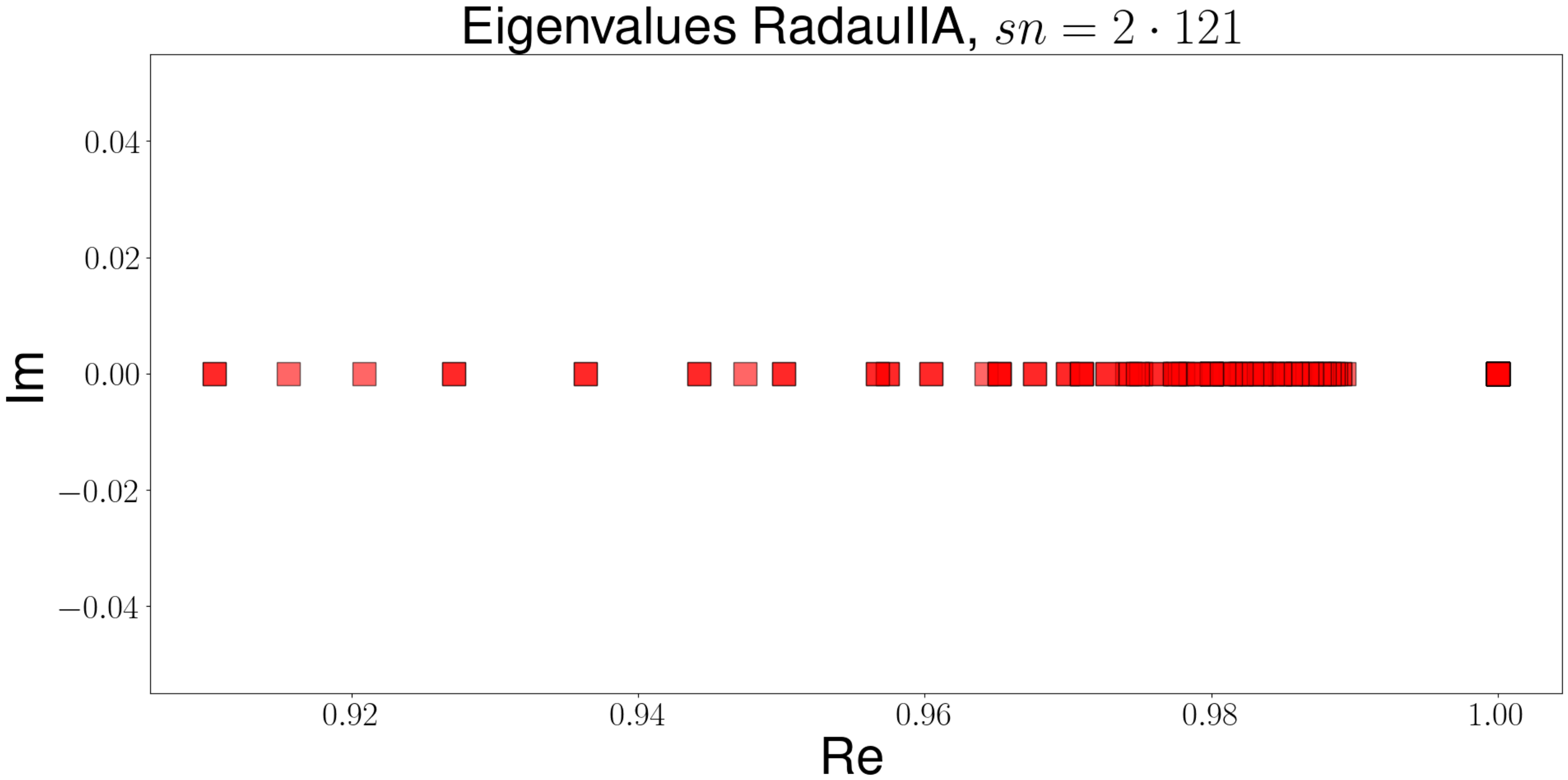
Then the eigenpairs of X *are equal to* $\left(\mu_\ell^{(k)}, \boldsymbol{s}_\ell^{(k)} \otimes \boldsymbol{e}_k\right)$.

J. Liesen and Z. Strakoš. GMRES convergence analysis for a convection-diffusion model problem *SIAM Journal on Scientific Computing*, 26(6):1989–2009, 2005.

Preconditioner analysis

$$s = 2$$

Preconditioner analysis



Preconditioner analysis

Theorem. *Let* $s = 2$ *and* $a_{11}, \det(A) \neq 0$. *Adopting the above notation and setting* $\mathrm{sp}(L) = \{\lambda_k\}_k$ *and* $\theta_k = \frac{\tau}{h^2}\lambda_k$ *we have* $\mathrm{sp}(M\,(P^{\mathrm{triang}})^{-1}) = \{1\} \cup_{k=1}^{n} \zeta_k$ *with*

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$$\zeta_k = \frac{(1 - a_{22}\theta_k)(1 - a_{11}\theta_k) - a_{21}a_{12}\theta_k^2}{(1 - a_{11}\theta_k)\left(1 - \left(a_{22} - \frac{a_{21}a_{12}}{a_{11}}\right)\right)\theta_k}.$$

Preconditioner analysis

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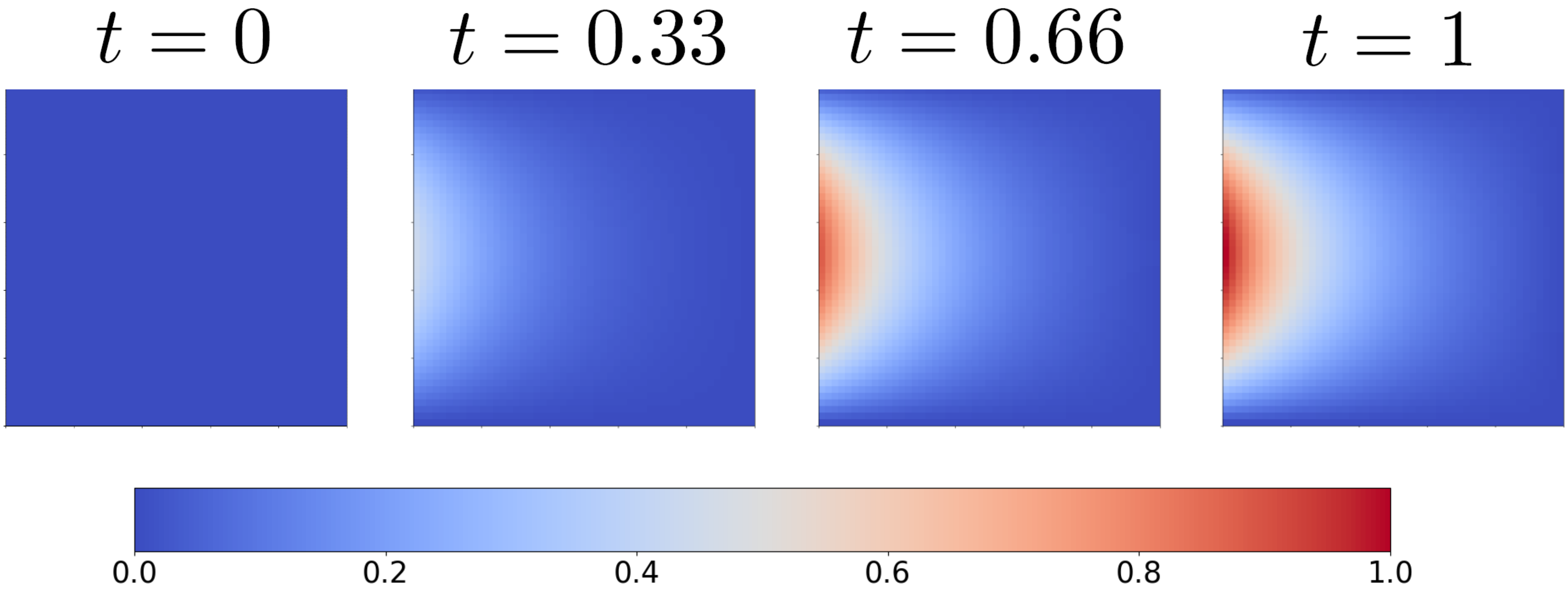
Moreover, assuming that $a_{21} \neq 0$ *it holds*

$$\kappa(S) = \max_{k\in\{1,\ldots,n\}} \kappa(S_k) = \max_{k\in\{1,\ldots,n\}} \sqrt{\frac{\sqrt{1+\alpha_k^2} + \alpha_k}{\sqrt{1+\alpha_k^2} - \alpha_k}}$$

$$\text{with} \quad \alpha_k = \frac{|a_{21}|}{\left|a_{11} - \theta_k^{-1}\right| \cdot |1 - \zeta_k|}$$

Numerical examples

Numerical examples

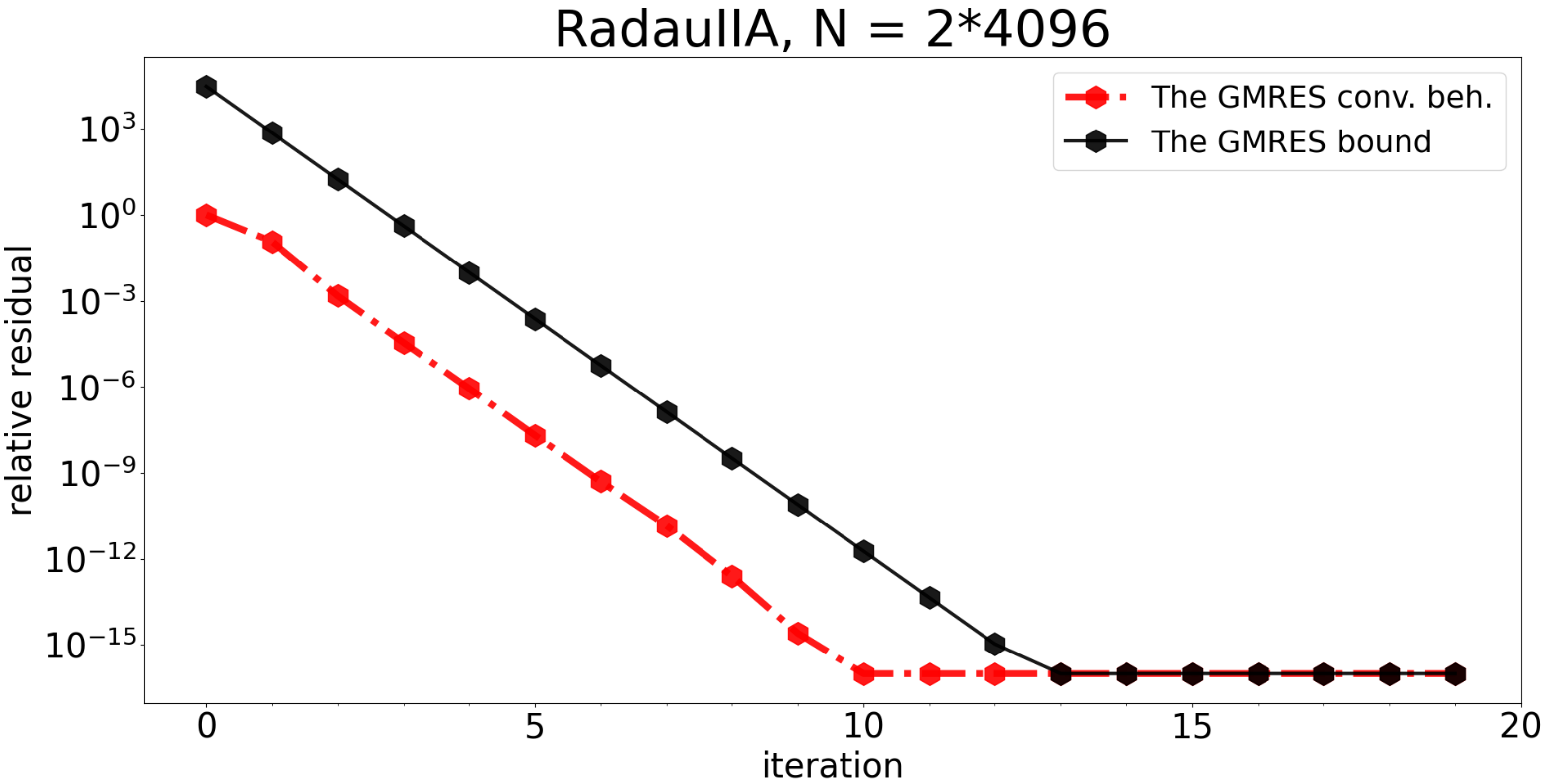


Numerical examples

First GMRES solve for the stage functions of IRK

$$s = 2$$

Numerical examples



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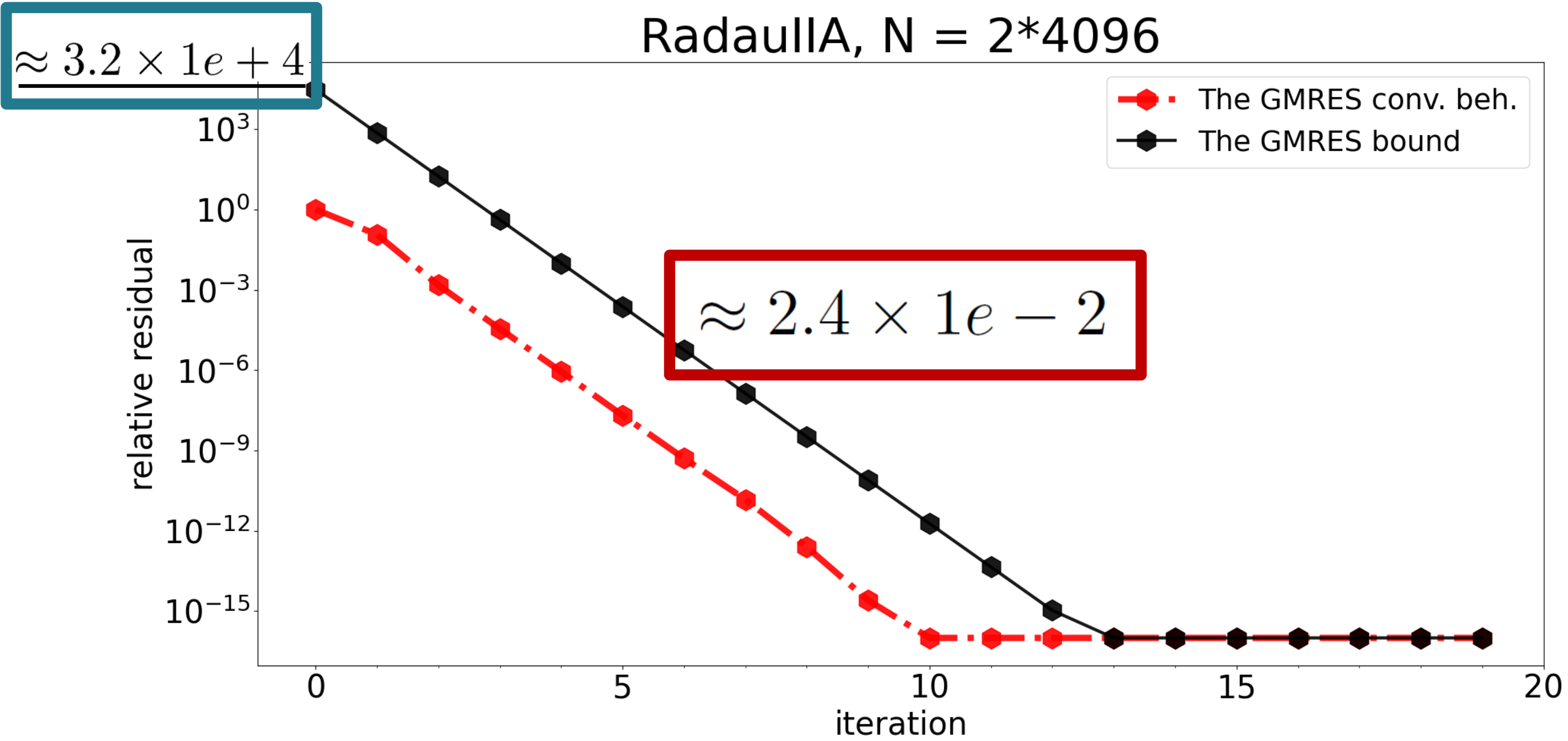

Results & Generalizations

Results & Generalizations

- \- Spectral focus jusification
- ± Multiple stages ($s \geq 3$)
- ± 2D spatial spectrum
- \+ Other preconditioners
- \+ Other Butcher tabs

Optimization of the method

Optimization of the method

$$
\begin{array}{c|ccc}
c_1 & a_{1,1} & \dots & a_{1,s} \\
\vdots & \vdots & \ddots & \vdots \\
c_s & a_{s,1} & \dots & a_{s,s} \\
\hline
 & b_1 & \dots & b_s
\end{array}
$$

Optimization of the method

$$\begin{array}{c|ccc} c_1 & a_{1,1} & \dots & a_{1,s} \\ \vdots & \vdots & \ddots & \vdots \\ c_s & a_{s,1} & \dots & a_{s,s} \\ \hline & b_1 & \dots & b_s \end{array}$$

- GMRES convergence
- Order of convergence of RK
- Numerical stability (A, L)

Optimization of the method

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\begin{array}{c|ccc}
c_1 & a_{1,1} & \dots & a_{1,s} \\
\vdots & \vdots & \ddots & \vdots \\
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 & b_1 & \dots & b_s
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$$

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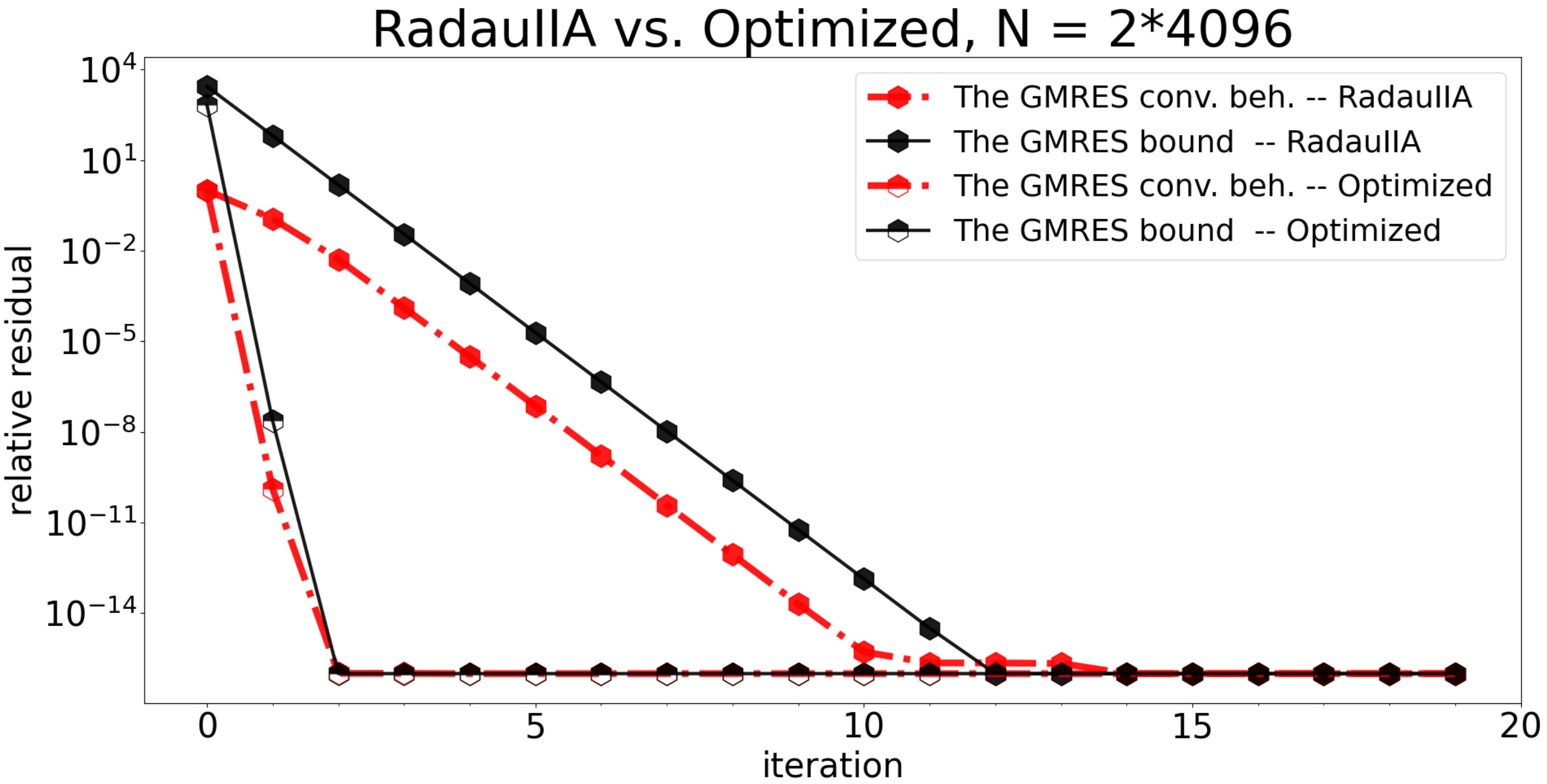

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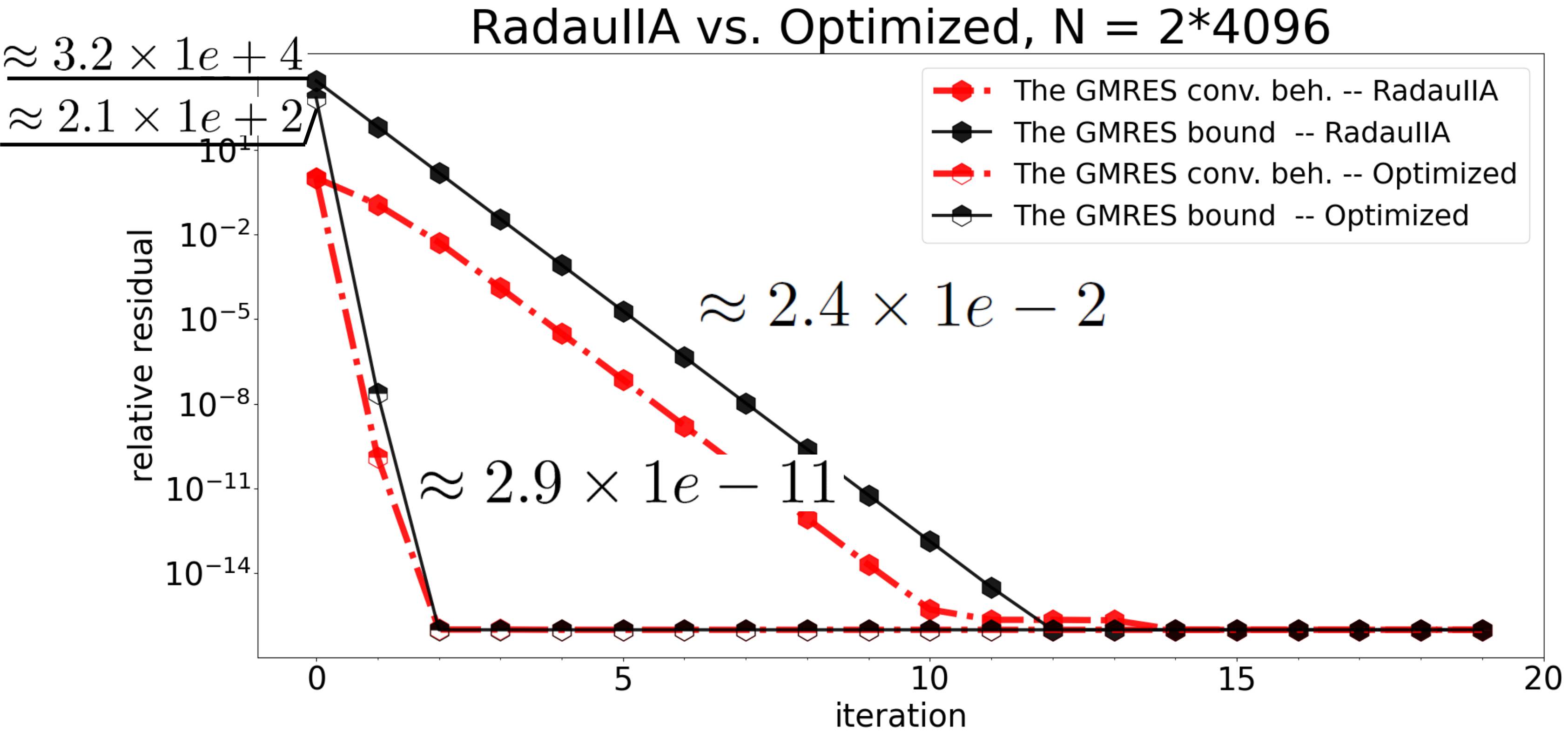


Numerical examples

Finite element method,
real-life geometry

$$s = 2$$

Model problem

$$\left(\frac{\partial}{\partial t} - \nu\Delta + \mu(\mathbf{a}, \nabla)\right) u = f \quad \text{in } \Omega \times (0, T)$$

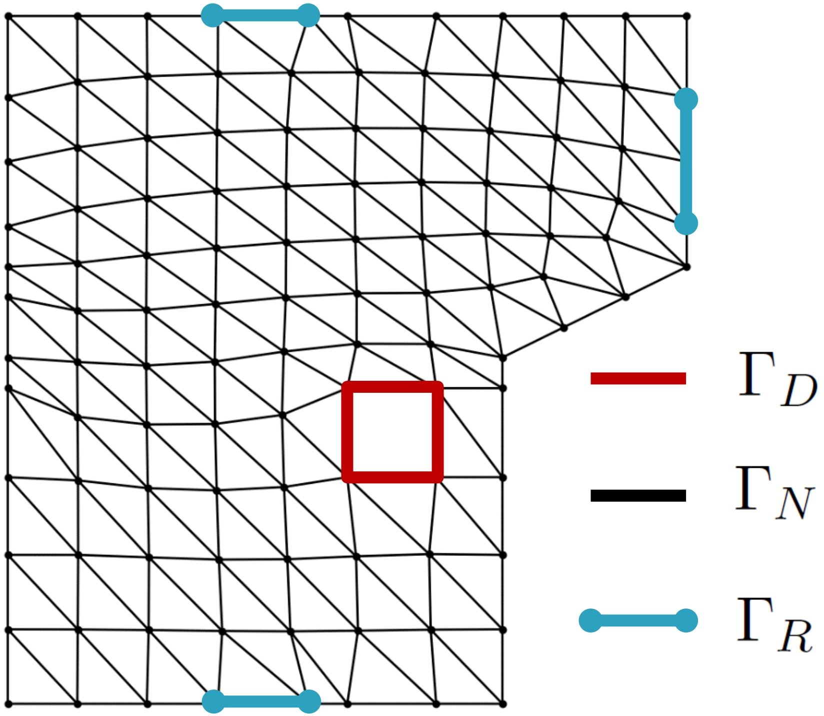
$$u = g \quad \text{on } \Gamma_D \times (0, T)$$

$$\frac{\partial u}{\partial \mathbf{n}} = 0 \quad \text{on } \Gamma_N \times (0, T)$$

$$\frac{\partial u}{\partial \mathbf{n}} + pu = 0 \quad \text{on } \Gamma_R \times (0, T)$$

$$u = u_0 \quad \text{at } \partial\Omega \times \{0\}$$

Model problem



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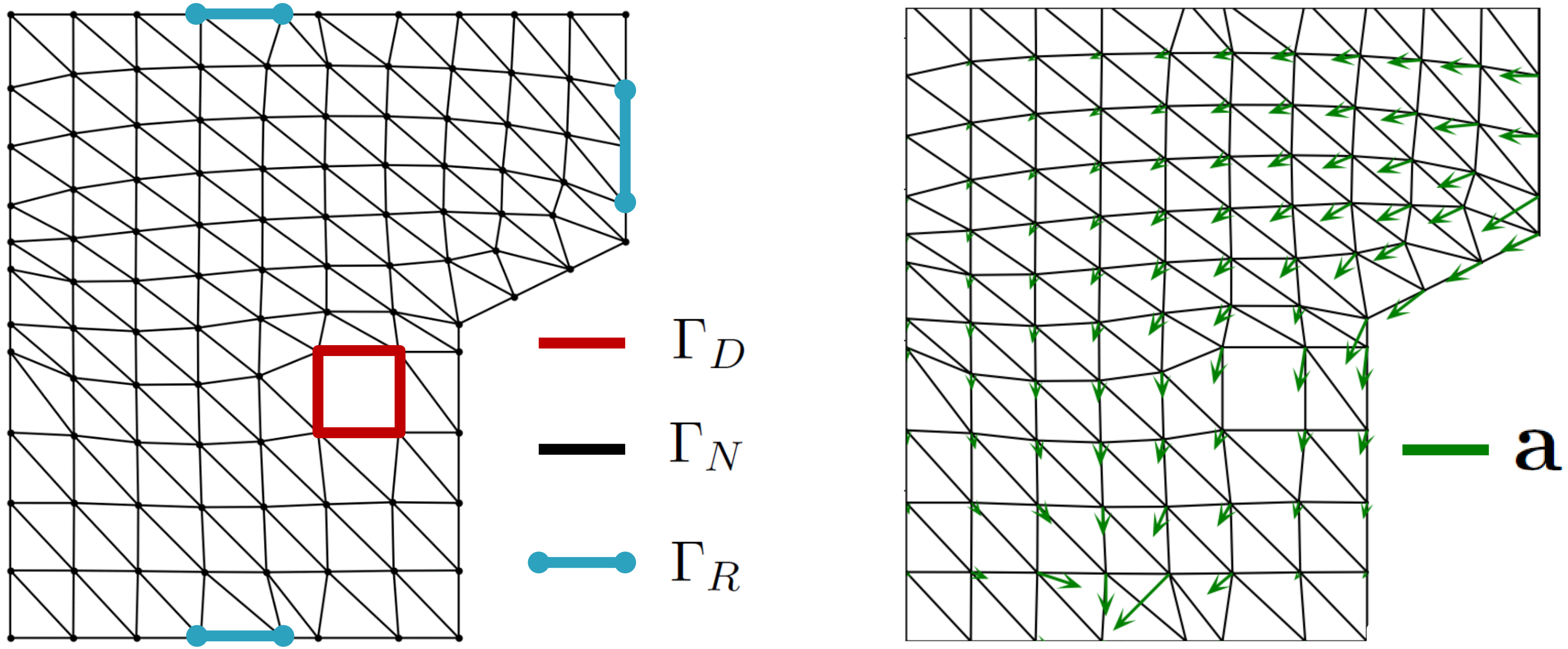
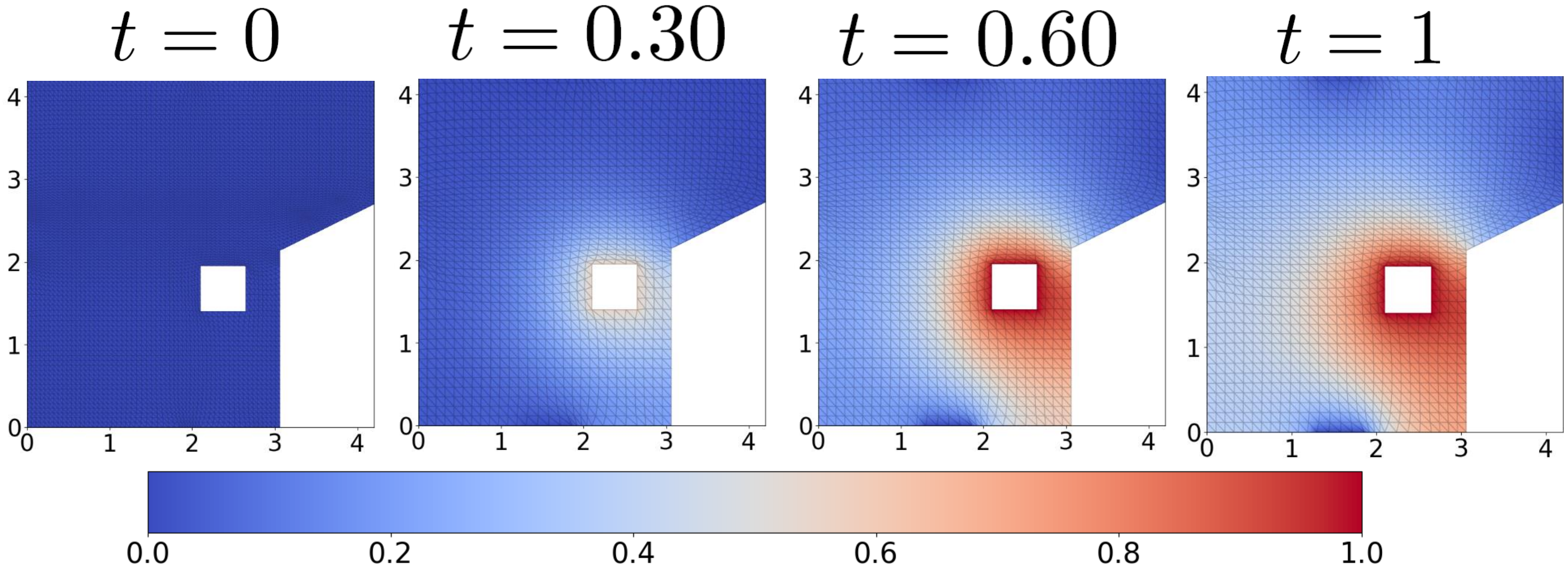


Numerical examples



Numerical examples

The overal IRK method - average #GMRES iteration

$$s = 2$$

Numerical examples

DoF	NoPrec	UpperTriang	UpperTriang opt
$2 \cdot 324$	42	10	2
$2 \cdot 1384$	45	10	2
$2 \cdot 5712$	42	10	2
$2 \cdot 23200$	42	10	2
$2 \cdot 93504$	42	11	3

Results & Generalizations

Results & Generalizations

- \- 2D spatial spectrum
- \+ Multiple stages ($s \geq 3$)
- \+ Stability (A, L) (& non-normality ?)
- \+ Other/New Butcher tabs (and preconditioners)
- \+ Efficiency

References

M. M. Rana, V. E. Howle, K. Long, A. Meek, and W. Milestone. A New Block Preconditioner for Implicit Runge-Kutta Methods for Parabolic PDE Problems, 2021.

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Thank you for your attention

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