Preconditioning the Stage Equations of Implicit Runge-Kutta Methods

Michal Outrata *and* Martin J. Gander
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Outline

- Introduction and Preliminaries
- Preconditioner
- Optimization
- Numerical examples

Model problem

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Model problem

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

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

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

Model problem

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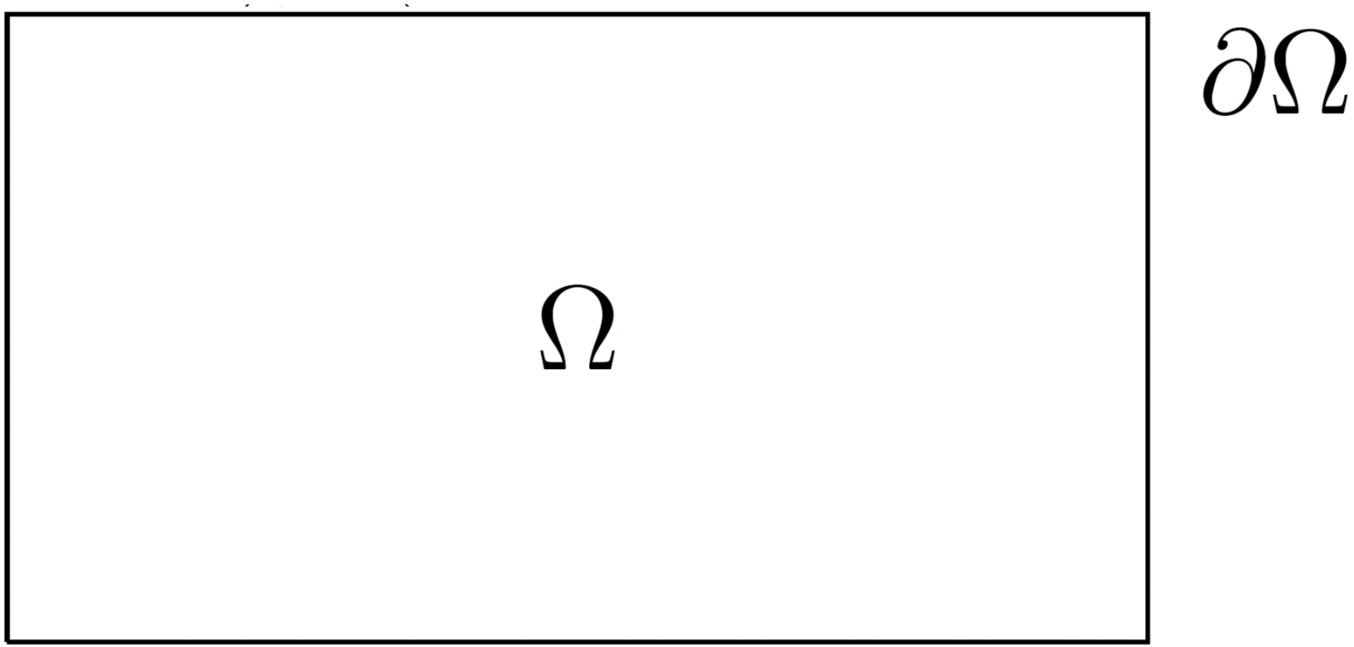

Discretization

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Discretization

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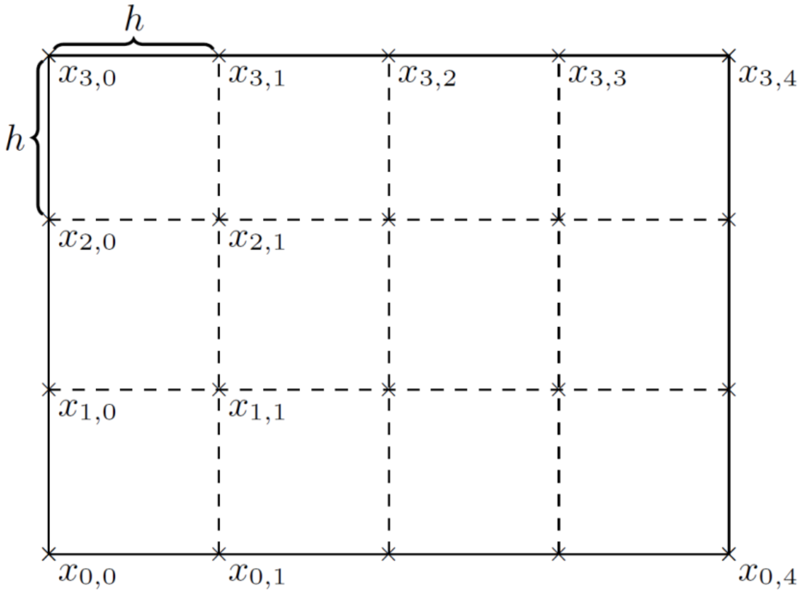

Discretization

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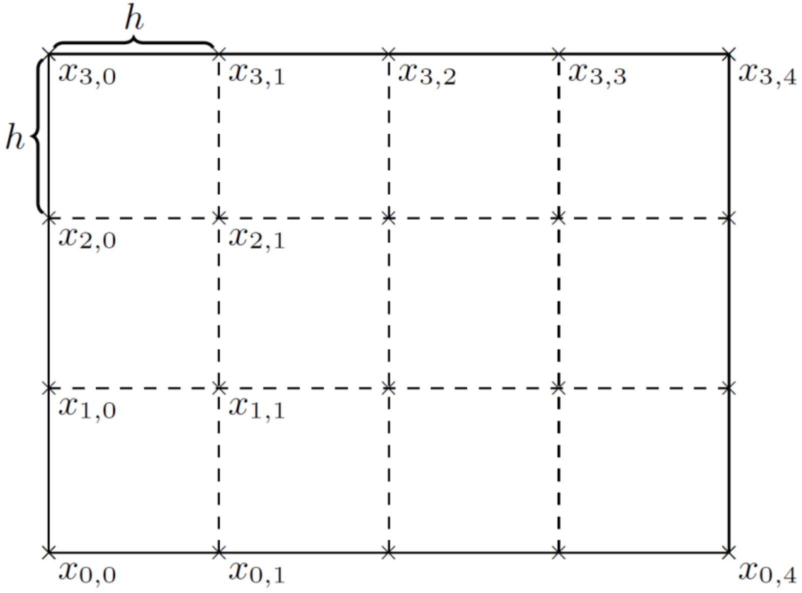

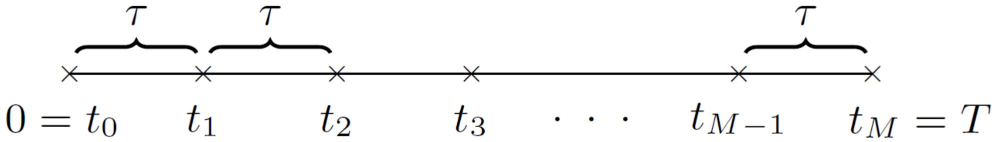

Discretization

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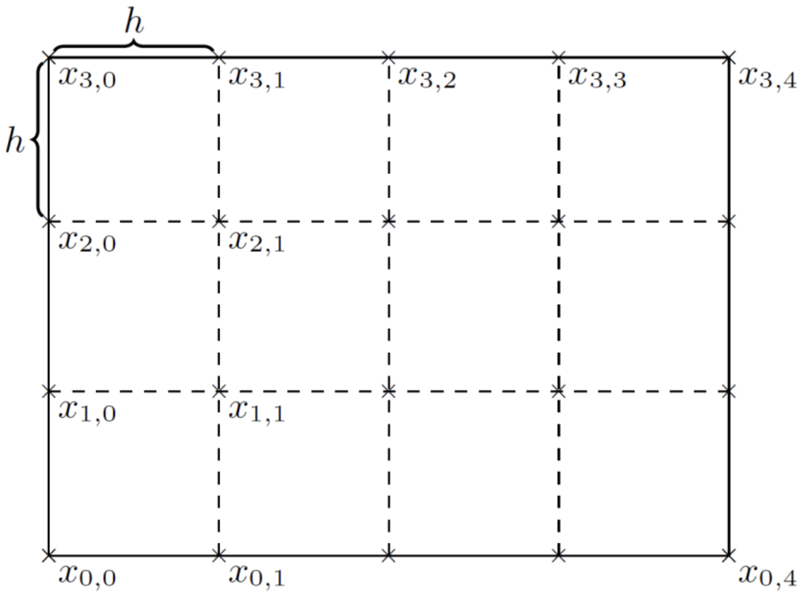

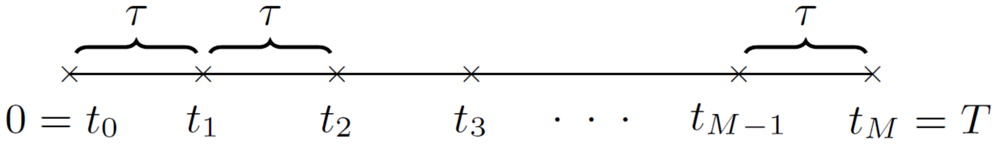

$$\mathbf{u}^m \approx u(t_m, x_{ij})$$

Discretization

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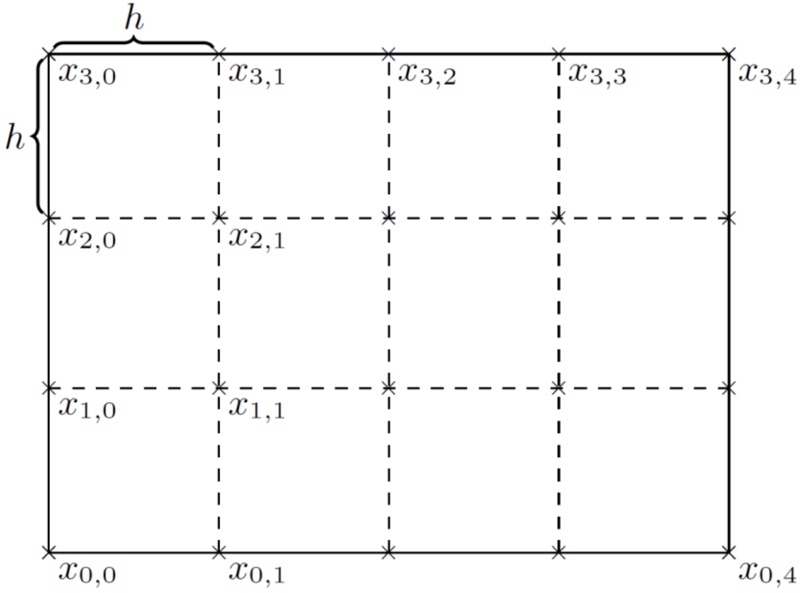

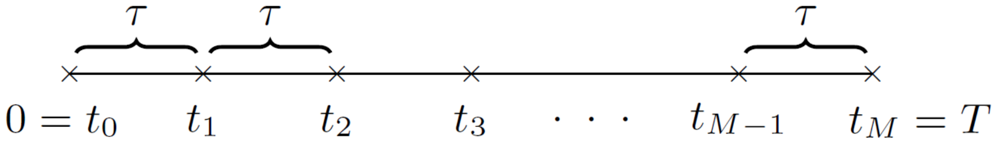

$$\mathbf{u}^m \approx u(t_m, x_{ij})$$

$$\Delta \approx L$$

Runge-Kutta method

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Runge-Kutta method

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$$
\begin{aligned}
\frac{\partial}{\partial t} u &= \Delta u \quad \text{in } \Omega \times (0, T) \\
u &= g \quad \text{on } \partial\Omega \times (0, T) \\
u &= u_0 \ \ \text{at } \partial\Omega \times \{0\}
\end{aligned}
$$

Runge-Kutta method

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

Runge-Kutta method

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

$$\mathbf{k}_1^m = \frac{1}{h^2} L\mathbf{u}^{m-1} + \frac{\tau}{h^2} \sum_{j=1}^{s} a_{1,j} L\mathbf{k}_j^m$$

$$\vdots$$

$$\mathbf{k}_s^m = \frac{1}{h^2} L\mathbf{u}^{m-1} + \frac{\tau}{h^2} \sum_{j=1}^{s} a_{s,j} L\mathbf{k}_j^m$$

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

Runge-Kutta methods

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$$\mathbf{k}_1^m = \frac{1}{h^2} L\mathbf{u}^{m-1} + \frac{\tau}{h^2} \sum_{j=1}^{s} a_{1,j} L\mathbf{k}_j^m$$

$$\vdots$$

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Runge-Kutta methods

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$$\mathbf{k}_1^m = \frac{1}{h^2} L\mathbf{u}^{m-1} + \frac{\tau}{h^2}\sum_{j=1}^{s} a_{1,j} L\mathbf{k}_j^m$$

$$\vdots$$

$$\mathbf{k}_s^m = \frac{1}{h^2} L\mathbf{u}^{m-1} + \frac{\tau}{h^2}\sum_{j=1}^{s} a_{s,j} L\mathbf{k}_j^m$$

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

Preconditioner – idea

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Preconditioner – idea

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

Preconditioner – idea

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

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

Preconditioner

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

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

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

Convergence Analysis

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sp.linalg.gmres

Convergence Analysis

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sp.linalg.gmres

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

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

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

Preconditioner – analysis

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Preconditioner – analysis

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Step I :

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Step I :

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

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Step I :

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

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

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Step II :

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Step II :

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

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

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

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

$$X \in \mathbb{R}^{ns \times ns} \qquad X_k \in \mathbb{R}^{s \times s}$$

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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* $\left(\mu_\ell^{(k)}, \boldsymbol{s}_\ell^{(k)} \otimes \boldsymbol{e}_k\right)$.

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$$s = 2$$

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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* $\mathrm{sp}(M\left(P^{\mathrm{triang}}\right)^{-1}) = \{1\} \cup_{k=1}^{n} \zeta_k$ *with*

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

Preconditioner – analysis

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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* $\mathrm{sp}(M\left(P^{\mathrm{triang}}\right)^{-1}) = \{1\} \cup_{k=1}^{n} \zeta_k$ *with*

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

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

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

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

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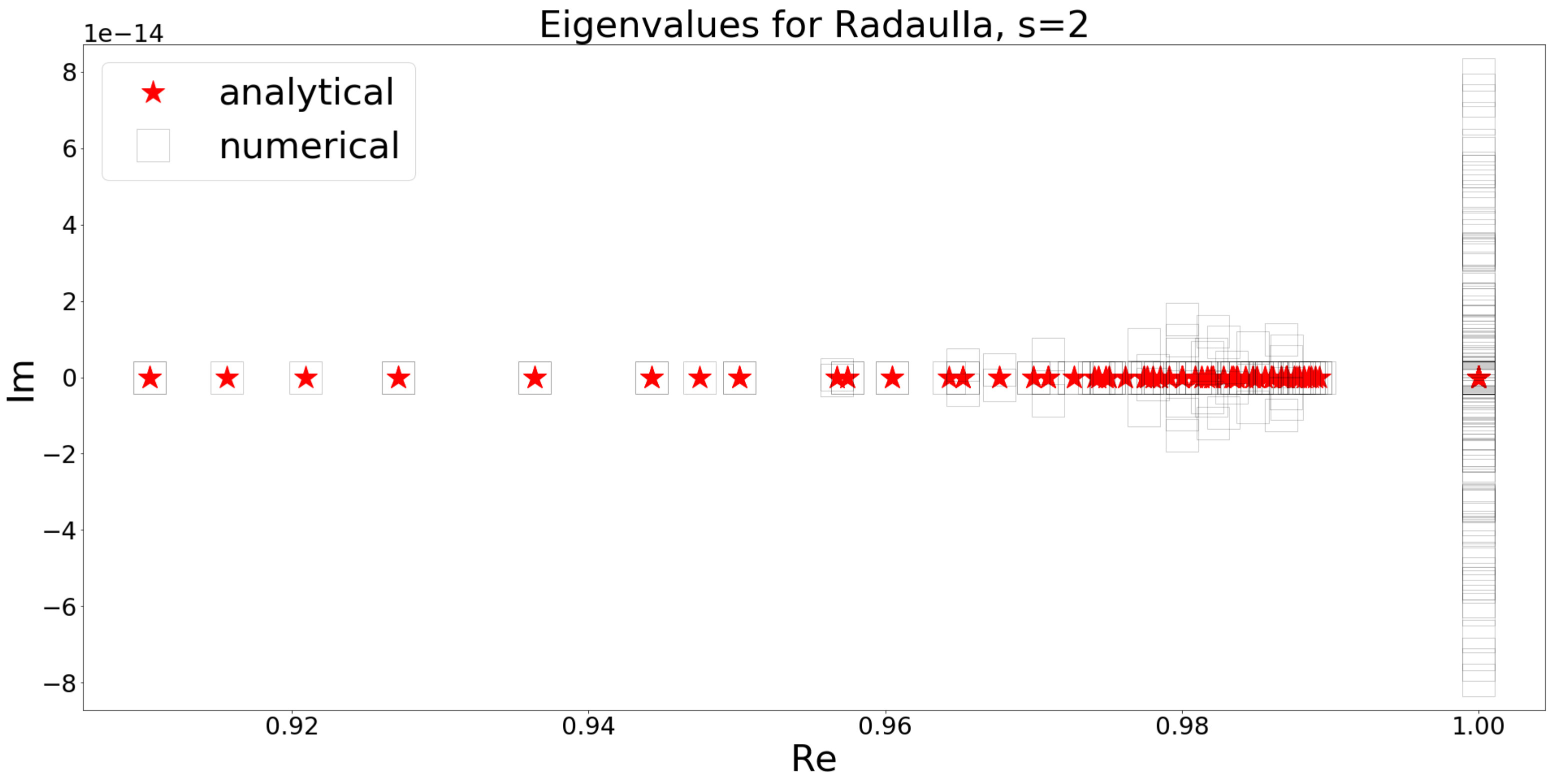

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Corollary. *Let* $s = 2$ *and notation and assumptions as above. Then*

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Corollary. *Let $s = 2$ and notation and assumptions as above. Then*

$$|\zeta_k - 1| = \left| \frac{\frac{a_{21}a_{12}}{a_{11}}\theta_k}{q_2(|\theta_k|)} \right|$$

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Corollary. *Let $s = 2$ and notation and assumptions as above. Then*

$$|\zeta_k - 1| = \left| \frac{\frac{a_{21}a_{12}}{a_{11}}\theta_k}{q_2(|\theta_k|)} \right| \quad \text{and} \quad \lim_{|\zeta_k - 1| \to 0} \kappa(S) = \text{n/a}.$$

Numerical examples

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Numerical examples

FD-IRK, 2 stages,
unit square, Dirichlet BC,
source at $\{x = 0\}$.

Numerical examples

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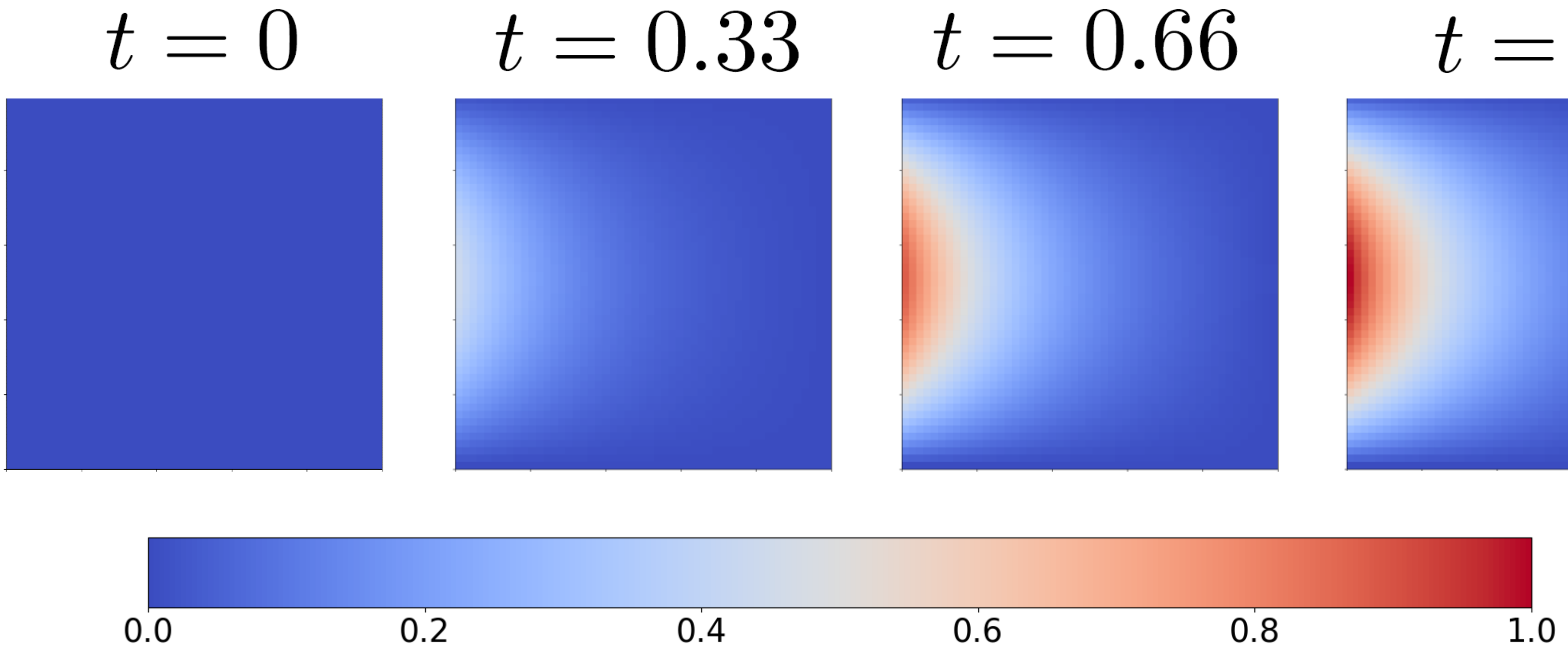

Numerical examples

First GMRES solve for the stage functions of IRK

$$s = 2$$

Numerical examples

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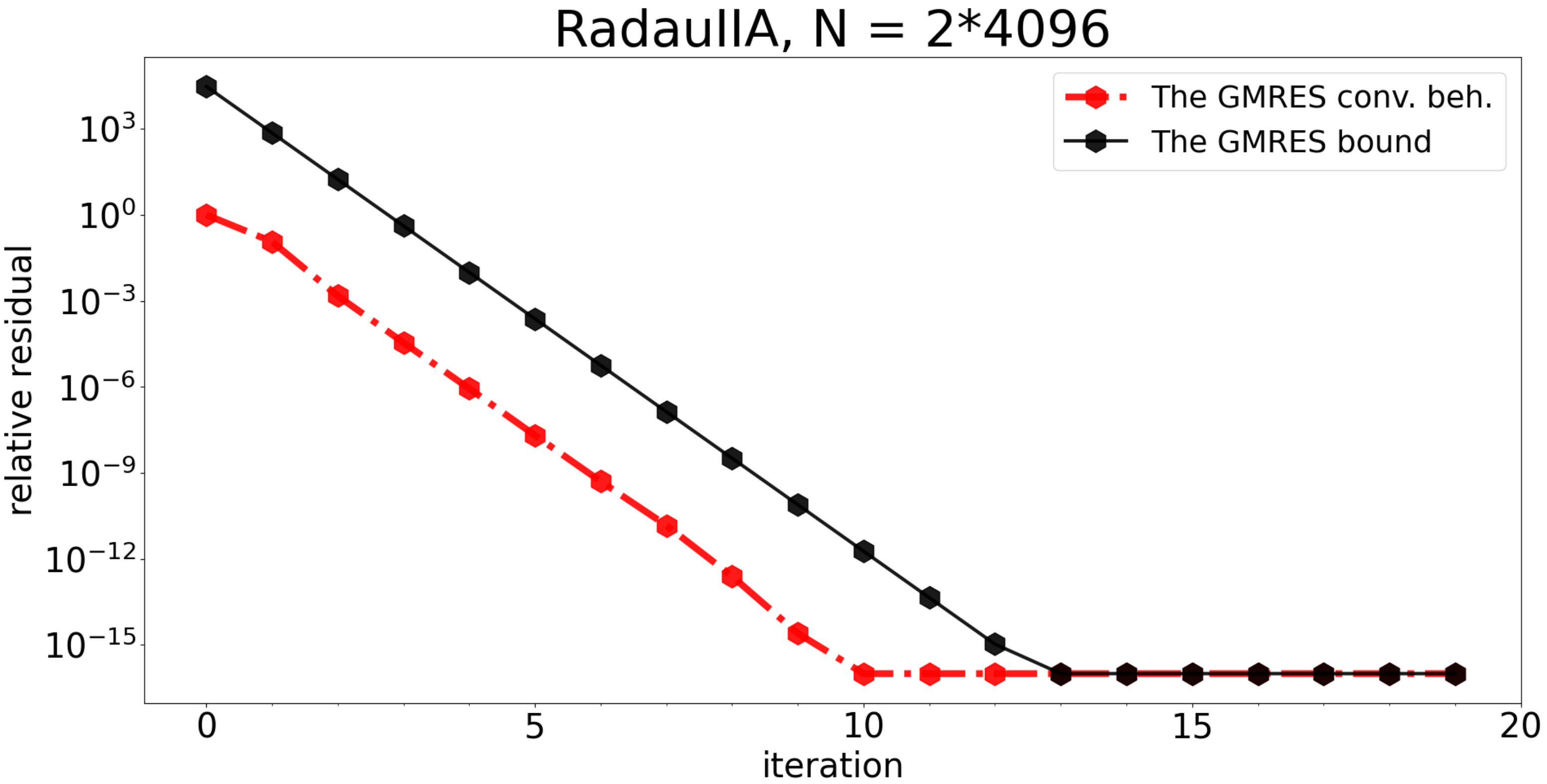

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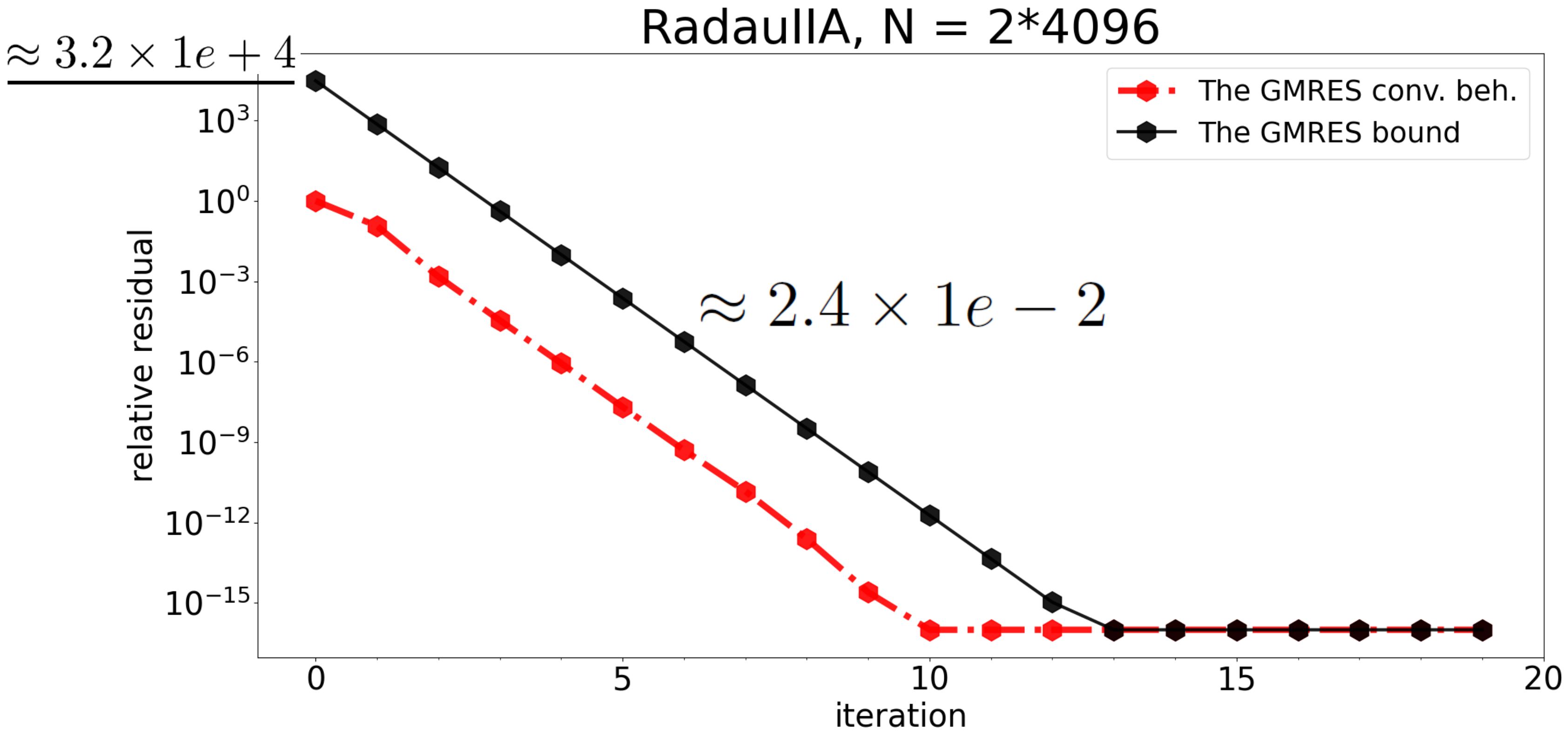

Numerical examples

First GMRES solve for the stage functions of IRK

$$s = 2$$

mesh refinement

Numerical examples

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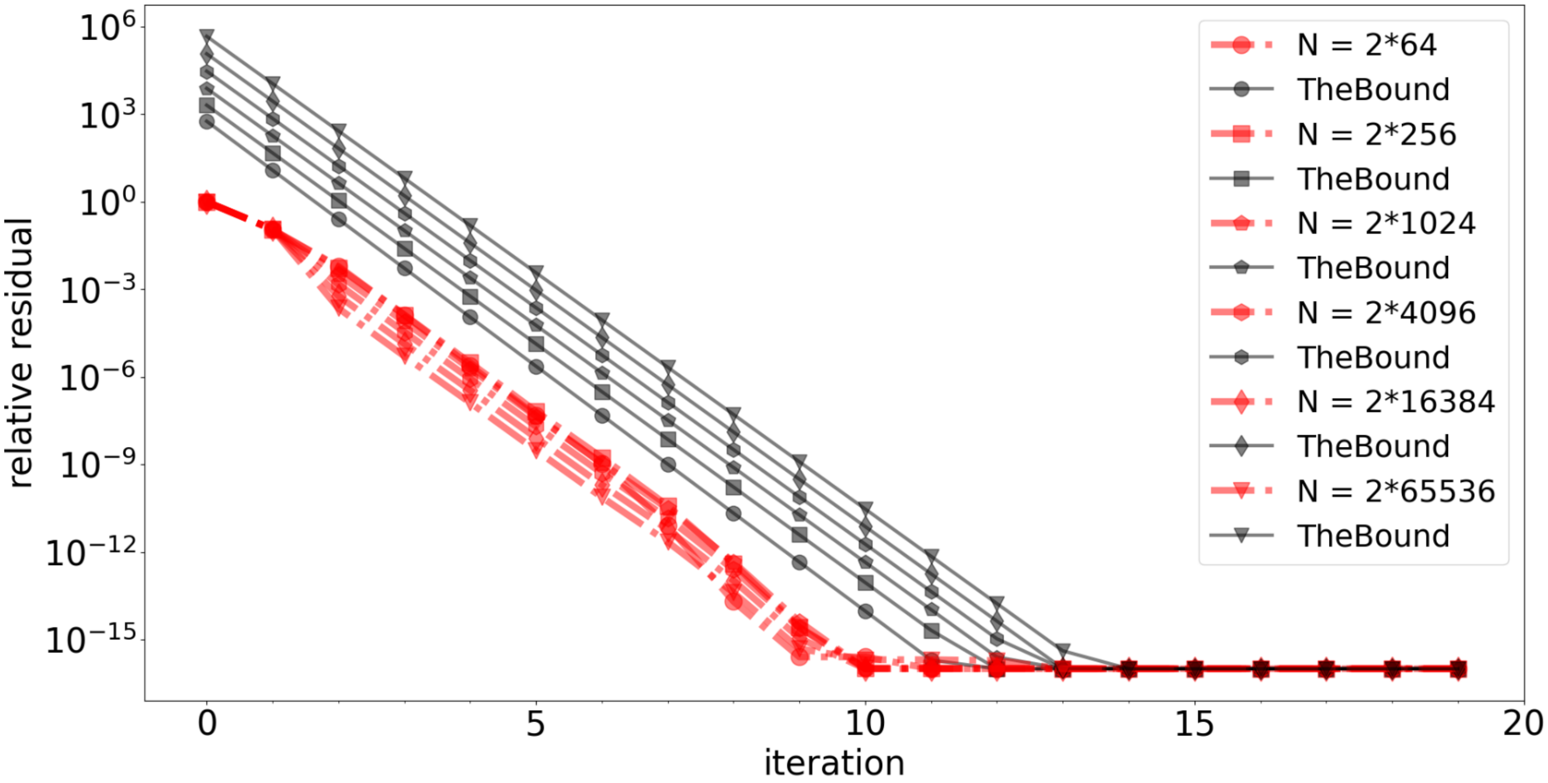

Numerical examples

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The overal IRK method - average #GMRES iteration

$$s = 2$$

Numerical examples

DoF	NoPrec	UpperTriang
$2 \cdot 64$	28	10
$2 \cdot 265$	85	11
$2 \cdot 1024$	84	11
$2 \cdot 4096$	84	11
$2 \cdot 16384$	85	11
$2 \cdot 65536$	85	12

Optimization of the method

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Optimization of the method

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

Optimization of the method

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

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

Optimization of the method

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

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Optimization of the method

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

- $$\frac{\|r_k\|}{\|r_0\|} \leq \kappa(S) \min_{\substack{\varphi(0)=1 \\ \deg(\varphi)\leq k}} \max_{\zeta\in[\zeta_{\min},\zeta_{\max}]} |\varphi(\zeta)|$$
- Order of convergence of RK
- Numerical stability (A, L)

Optimization of the method

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

- $\frac{\|r_k\|}{\|r_0\|} \leq \boxed{\kappa(S)} \min_{\substack{\varphi(0)=1 \\ \deg(\varphi)\leq k}} \max_{\boxed{\zeta \in [\zeta_{\min}, \zeta_{\max}]}} |\varphi(\zeta)|$
- Order of convergence of RK
- Numerical stability (A, L)

Numerical examples

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FD-IRK, 2 stages,
unit square, Dirichlet BC,
source at $\{x = 0\}$.

Numerical examples

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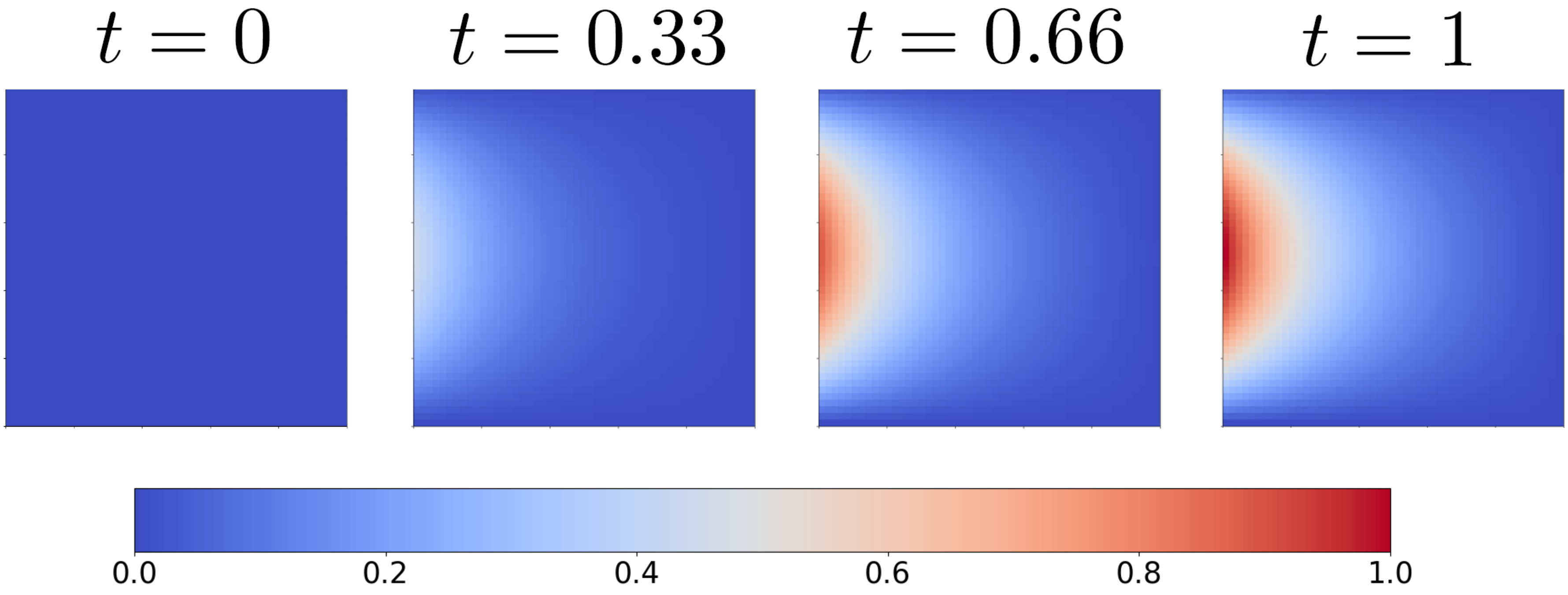

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First GMRES solve for the stage functions of IRK

$$s = 2$$

Numerical examples

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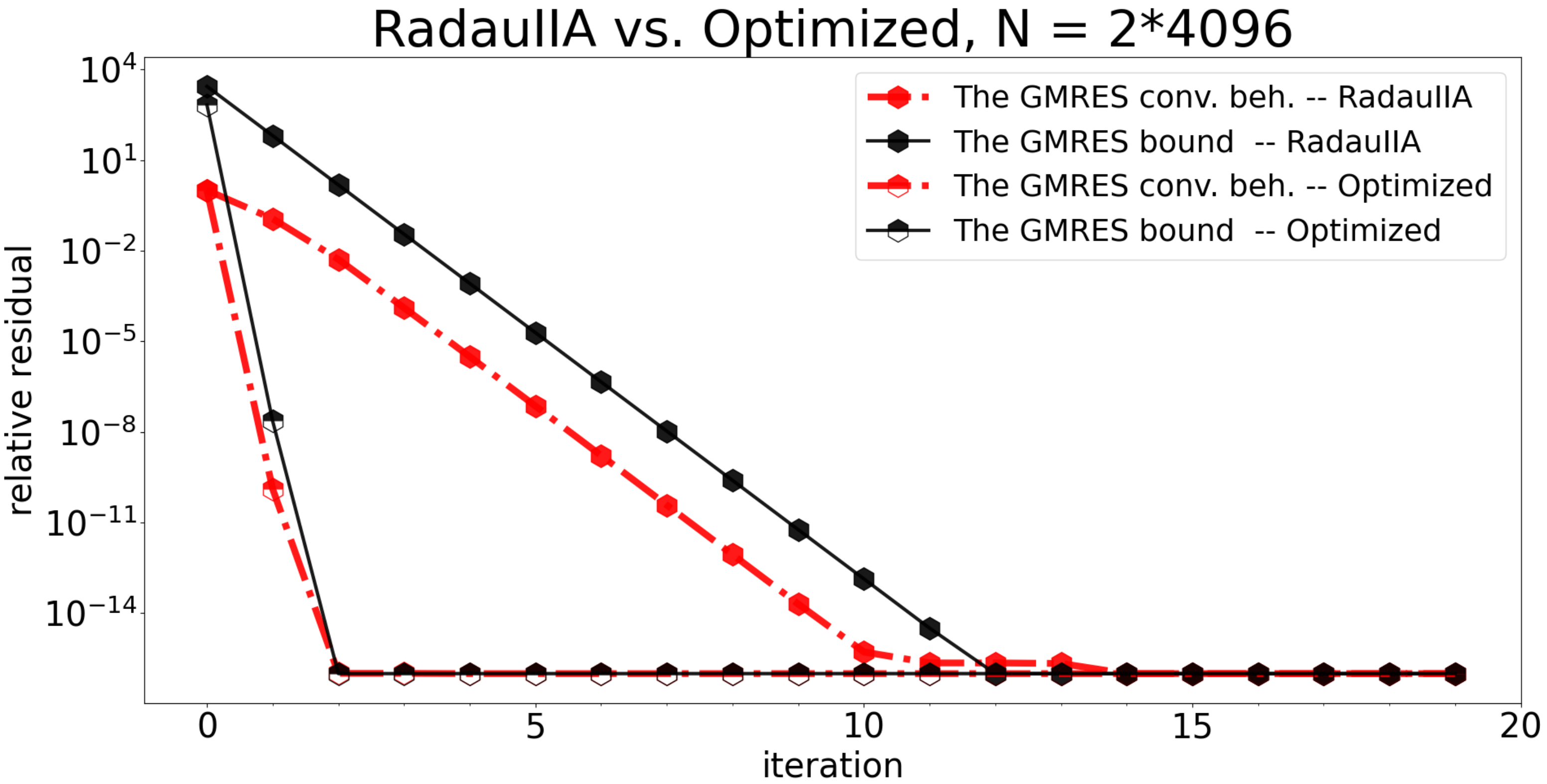

Numerical examples

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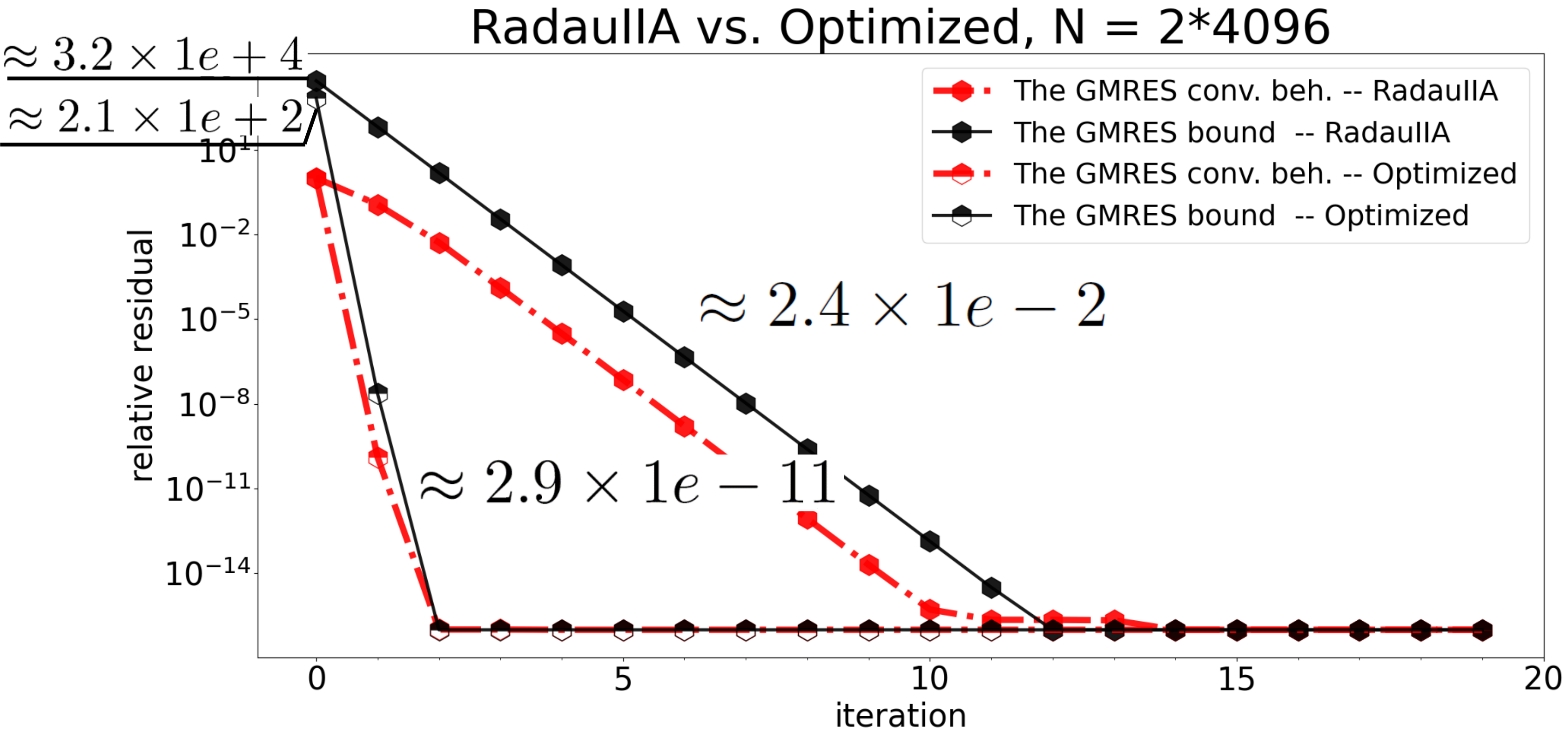

Numerical examples

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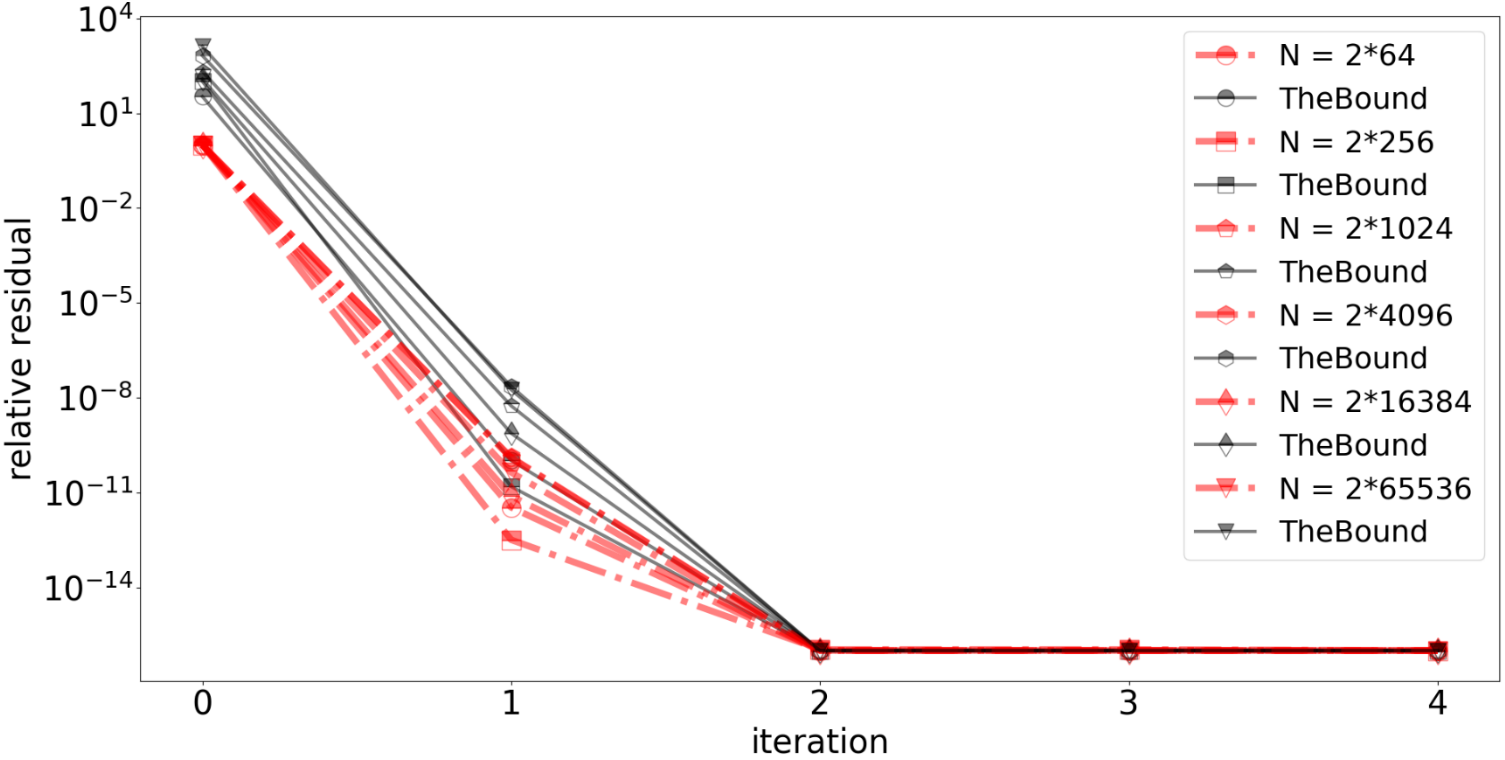
First GMRES solve for the stage functions of IRK

$$s = 2$$

mesh refinement

Numerical examples



Numerical examples

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The overal IRK method - average #GMRES iteration

$$s = 2$$

Numerical examples

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DoF	NoPrec	UpperTriang	UpperTriang opt
$2 \cdot 64$	28	10	1
$2 \cdot 265$	85	11	2
$2 \cdot 1024$	84	11	2
$2 \cdot 4096$	84	11	2
$2 \cdot 16384$	85	11	2
$2 \cdot 65536$	85	12	2

The overal IRK method – efficiency of the GMRES preconditioners

$$s = 2$$

Numerical examples

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Each GMRES iteration

No preconditioner :

Preconditioner :

Numerical examples

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Each GMRES iteration

No preconditioner :

- 1 sparse mat-vec

Preconditioner :

- 1 sparse mat-vec
- 1 sparse solve

Numerical examples

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Each GMRES iteration

No preconditioner :

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Numerical examples

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Each GMRES iteration

No preconditioner :

- 1 sparse mat-vec

Preconditioner :

- 1 sparse mat-vec
- 1 sparse solve

  → inexcat?

Numerical examples

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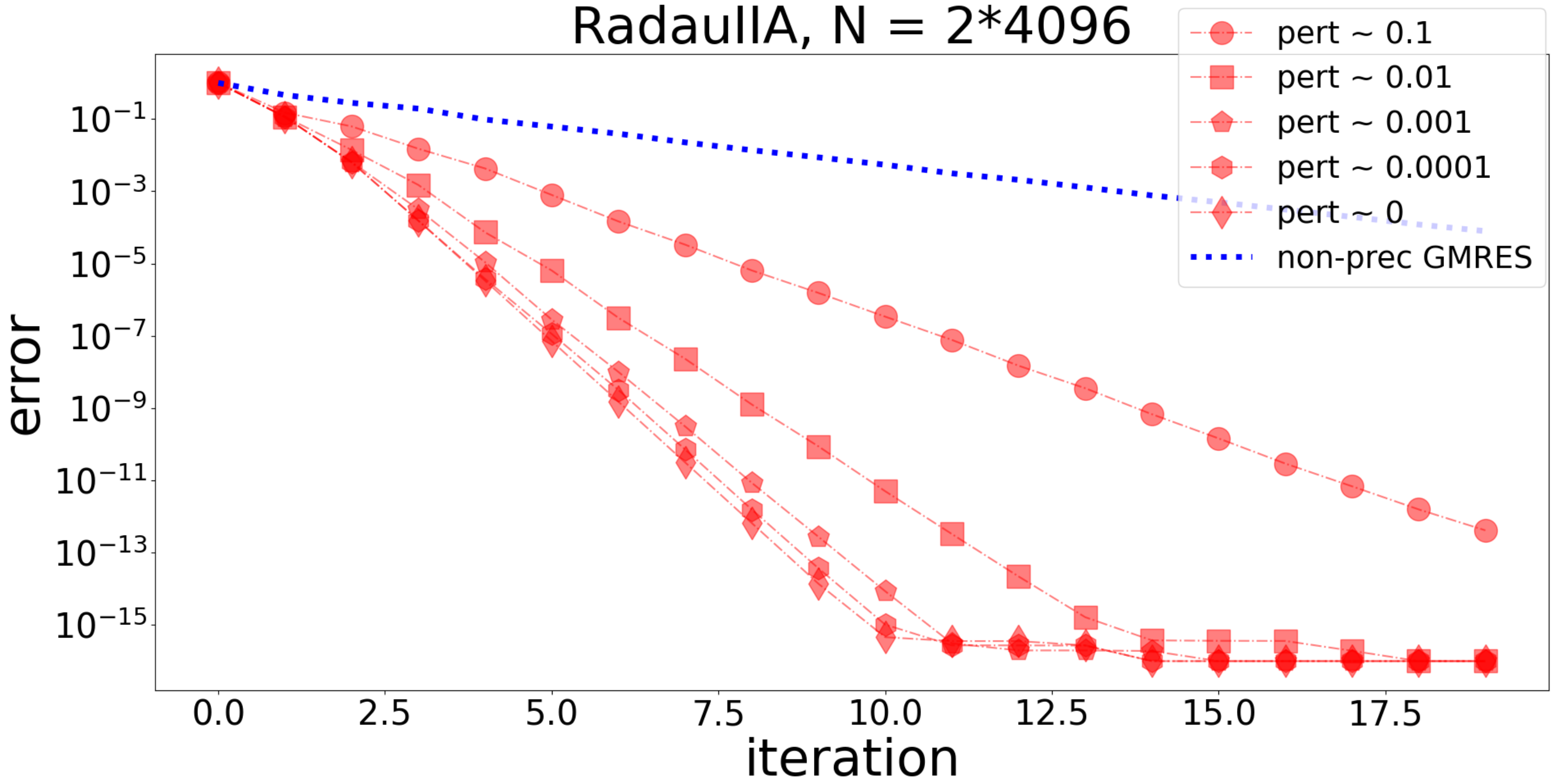

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Numerical examples

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Finite element method,
real-life geometry

$$s = 2$$

Model problem

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$$
\begin{aligned}
\left(\frac{\partial}{\partial t} - \nu\Delta + \mu(\mathbf{a},\nabla)\right) u &= f \quad \text{in } \Omega \times (0,T) \\
u &= g \quad \text{on } \Gamma_D \times (0,T) \\
\frac{\partial u}{\partial \mathbf{n}} &= 0 \quad \text{on } \Gamma_N \times (0,T) \\
\frac{\partial u}{\partial \mathbf{n}} + pu &= 0 \quad \text{on } \Gamma_R \times (0,T) \\
u &= u_0 \;\; \text{at } \partial\Omega \times \{0\}
\end{aligned}
$$

Model problem

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Model problem

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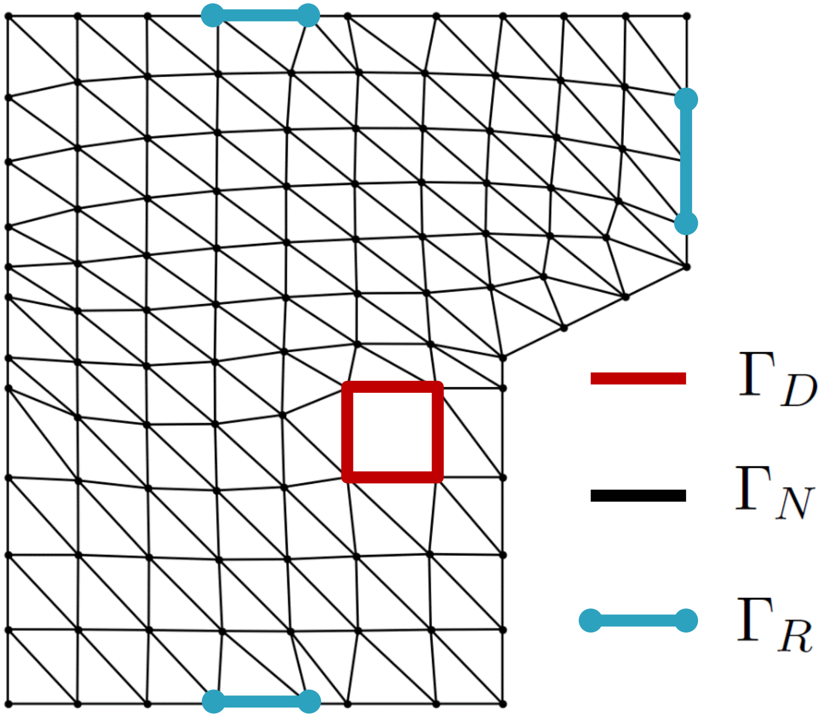

Model problem

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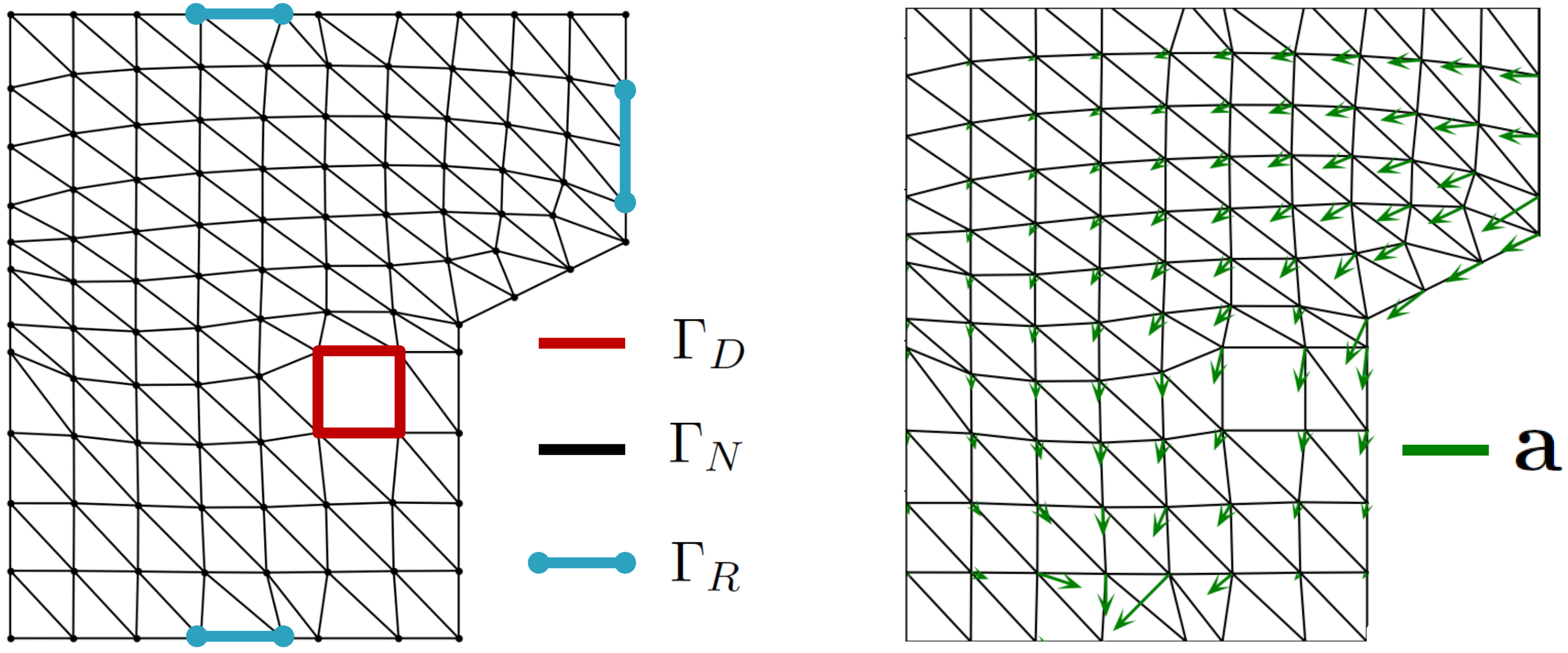
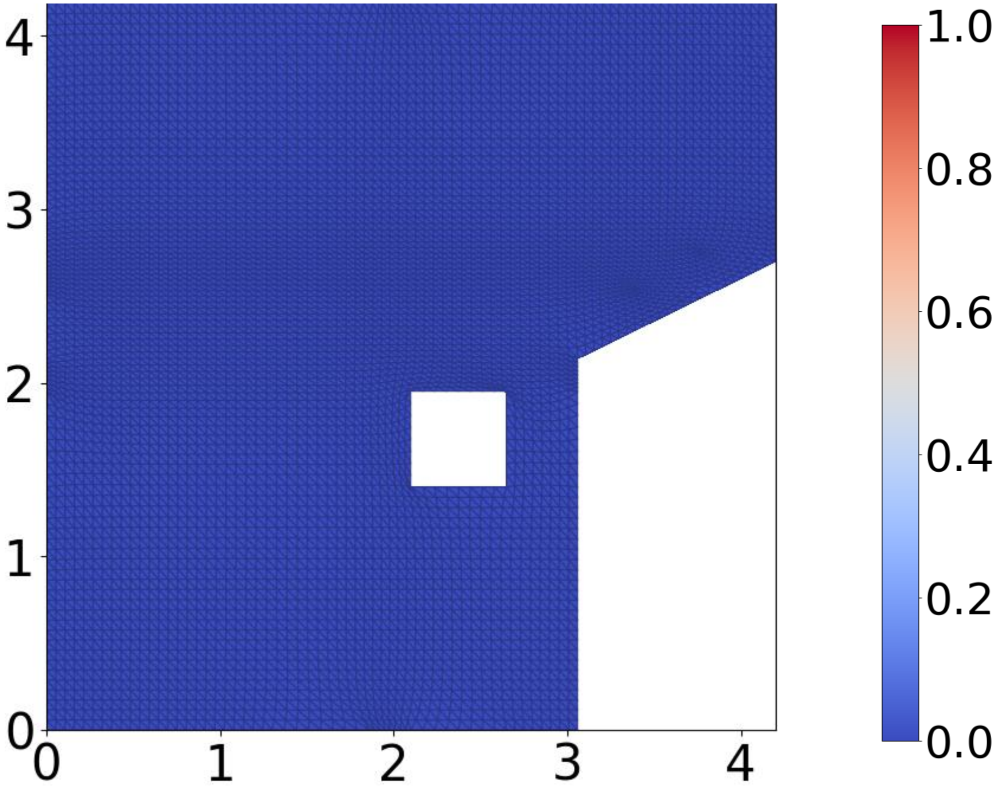


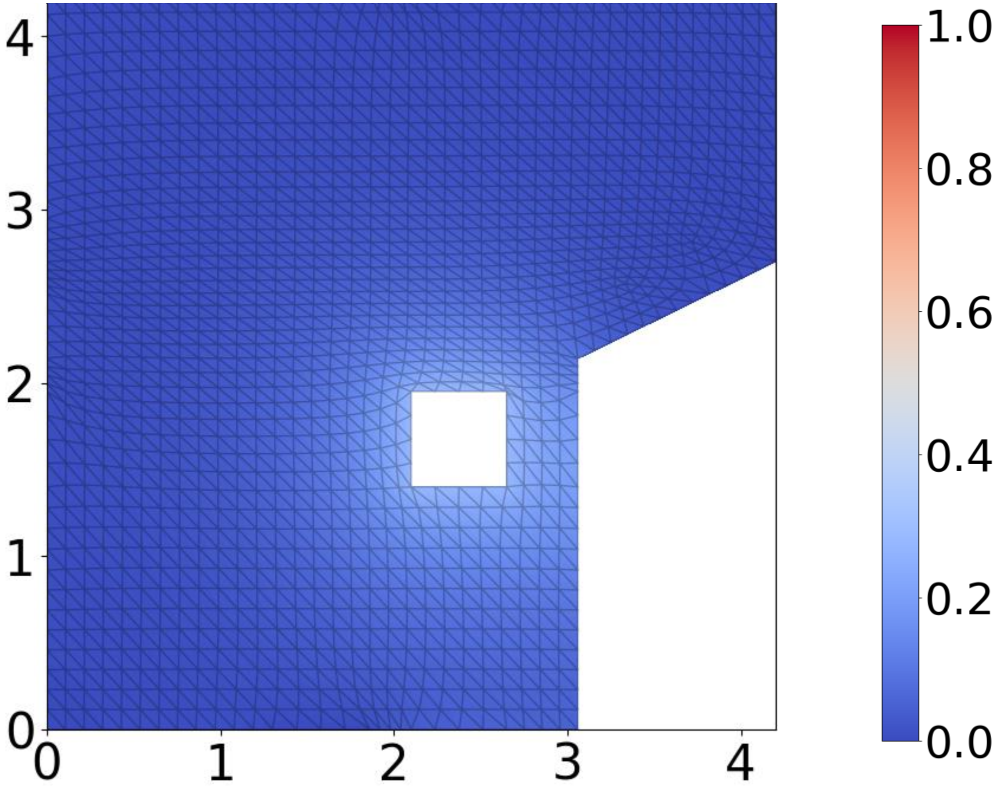
Numerical examples

$$t = 0$$



Numerical examples

$$t = 0.15$$



Numerical examples

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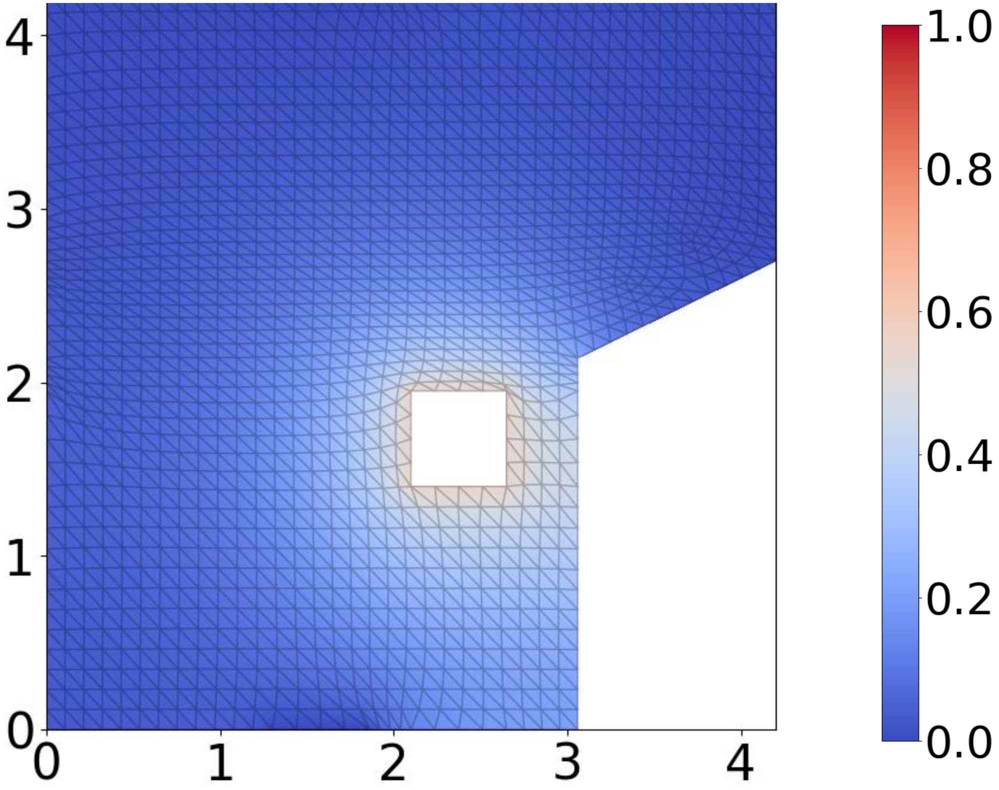
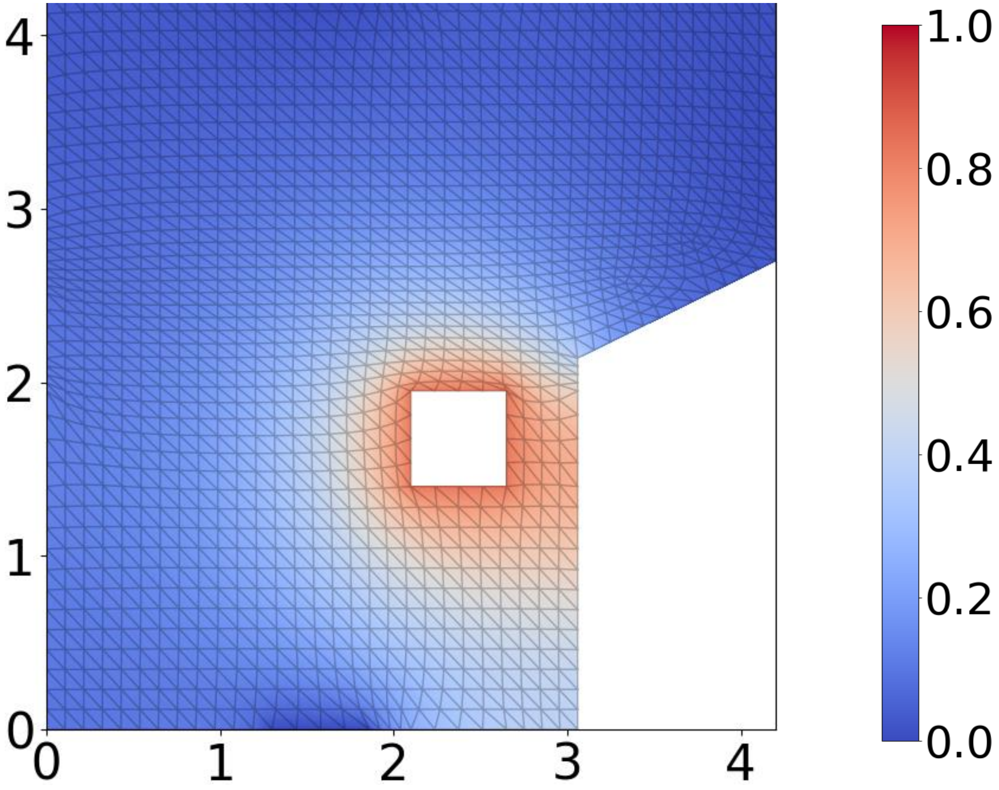
$$t = 0.30$$



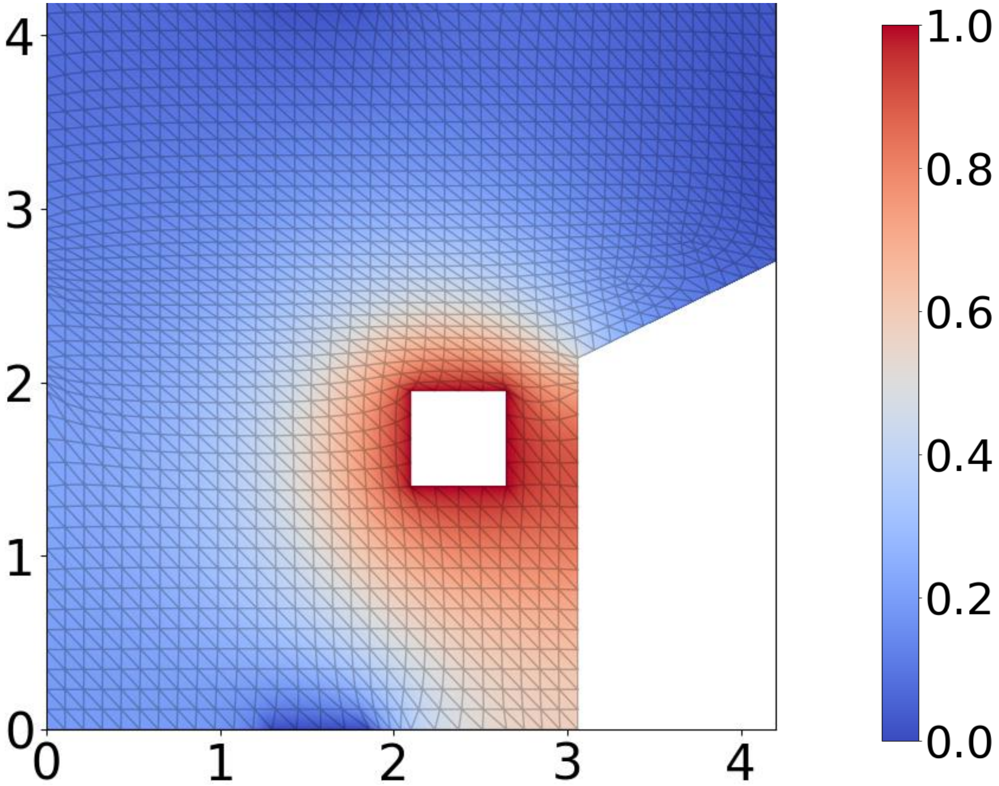
Numerical examples

$t = 0.45$



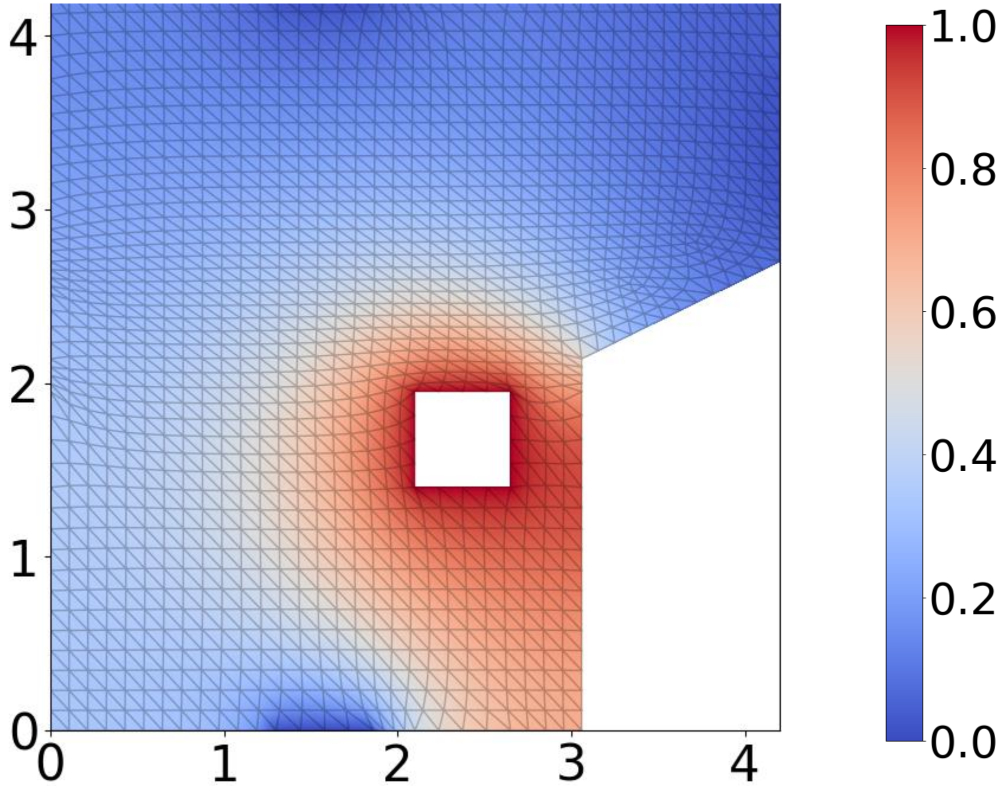
Numerical examples

$t = 0.60$



Numerical examples

$t = 0.85$



Numerical examples

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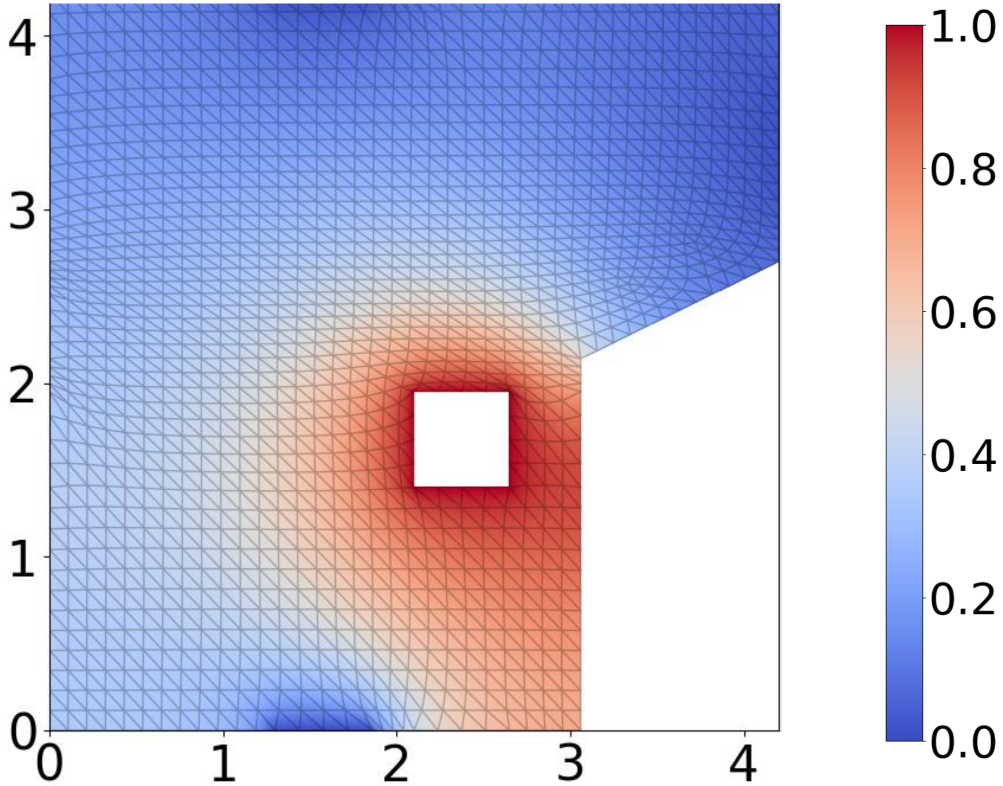
$t = 0.90$



Numerical examples

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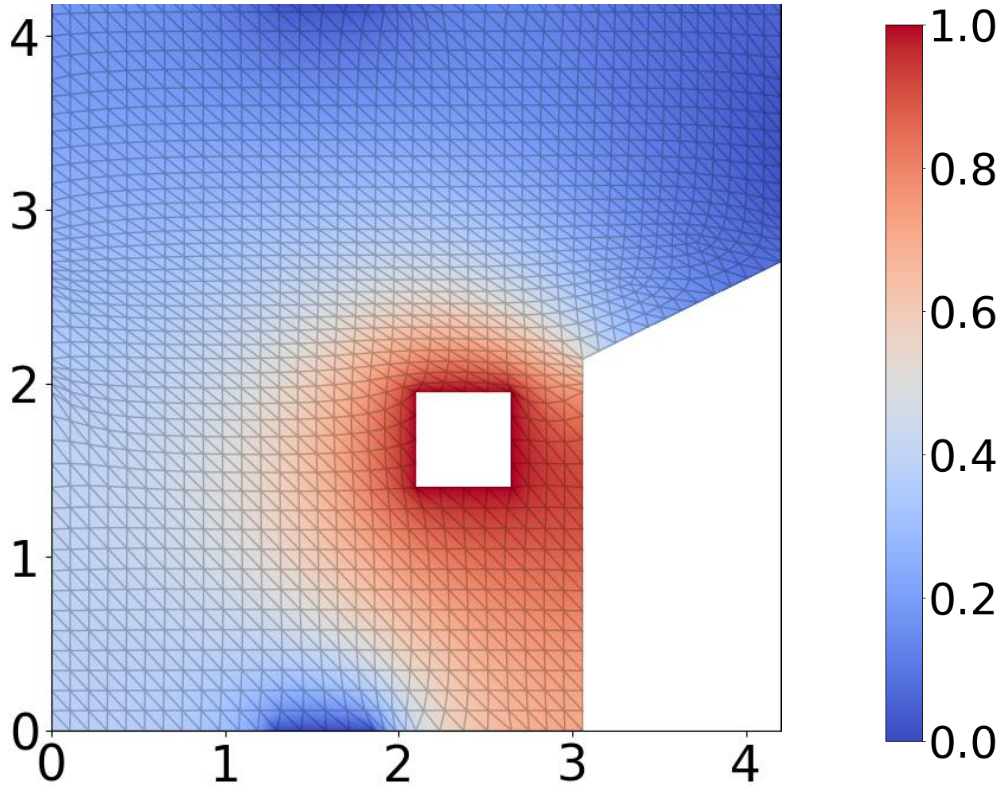
$$t = 1$$



Numerical examples

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The overal IRK method - average #GMRES iteration

$$s = 2$$

Numerical examples

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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

Conclusion

Results & Generalizations

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- Transformed system (M. Neytcheva)
- Multiple stages ($s \geq 3$)
- Other preconditioners (LU, diag, mtrx split., …)
- FEM discretization
- Limit analysis for τ and h

Future work

- Other preconditioners
- Analysis for difficult problems
- Analysis for multiple stages (with simplifications)
- Descriptive complex bounds (Joukowski/ FoV)
- No spectrum, only bounds (complex case)

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.

M. Neytcheva and O. Axelsson. Numerical Solution Methods for Implicit Runge-Kutta Methods of Arbitrarily High Order. In *Proceedings of ALGORITHMY 2020*, 2020.

G. Wanner, S. P. Nørsett, and E. Hairer. *Solving Ordinary Differential Equations I : Non-Stiff Problems*. Springer Berlin-Heidelberg, 1987.

G. Wanner and E. Hairer. *Solving Ordinary Differential Equations II : Stiff and Differential-Algebraic Problems*. Springer Berlin-Heidelberg, 1996.

R. A. Horn and C. R. Johnson. *Topics in Matrix Analysis*. Cambridge University Press, 1994.

Thank you for your attention