Preconditioning the Stage Equations of Implicit Runge-Kutta Methods

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Outline

- Introduction and Preliminaries
- Preconditioner
- Interaction with inexactness

Model problem

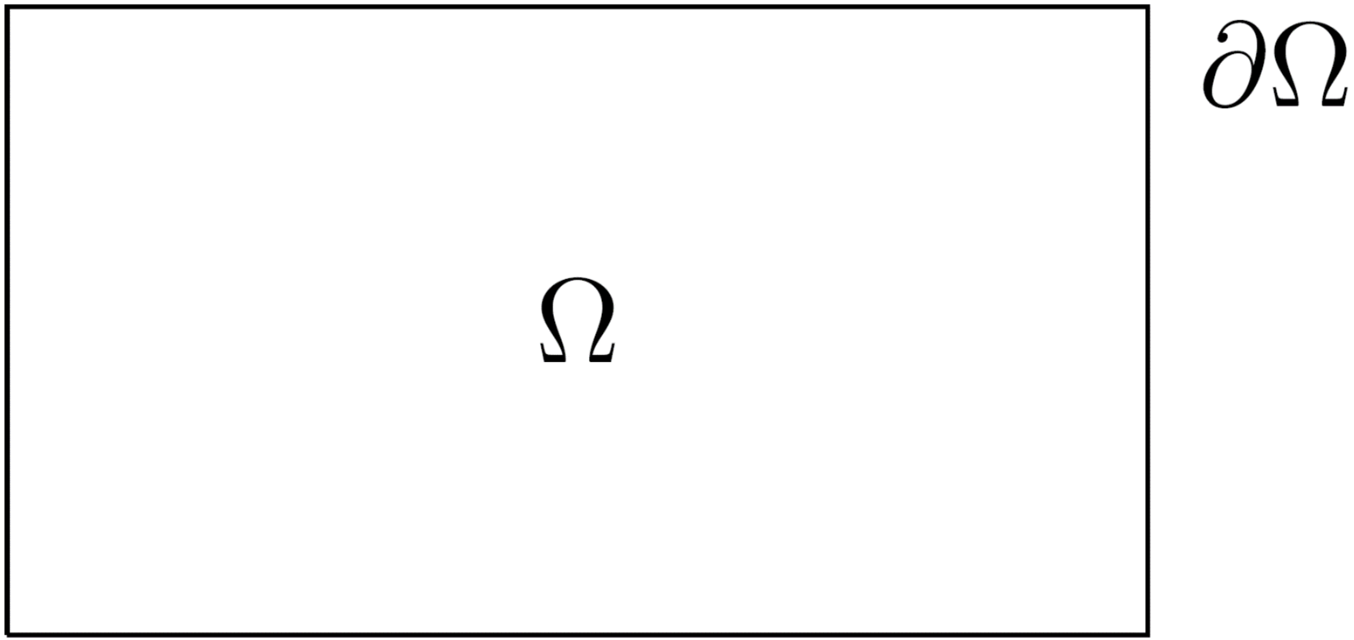
Model problem

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

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

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

Model problem



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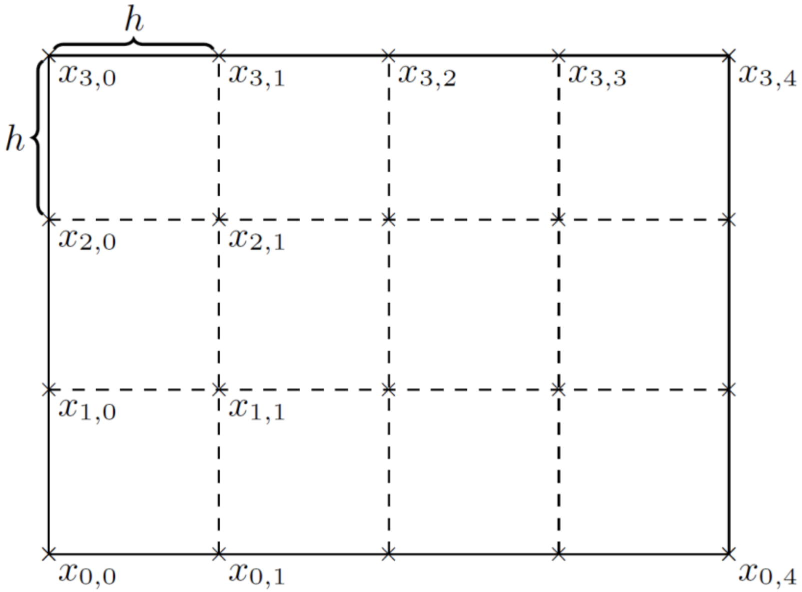

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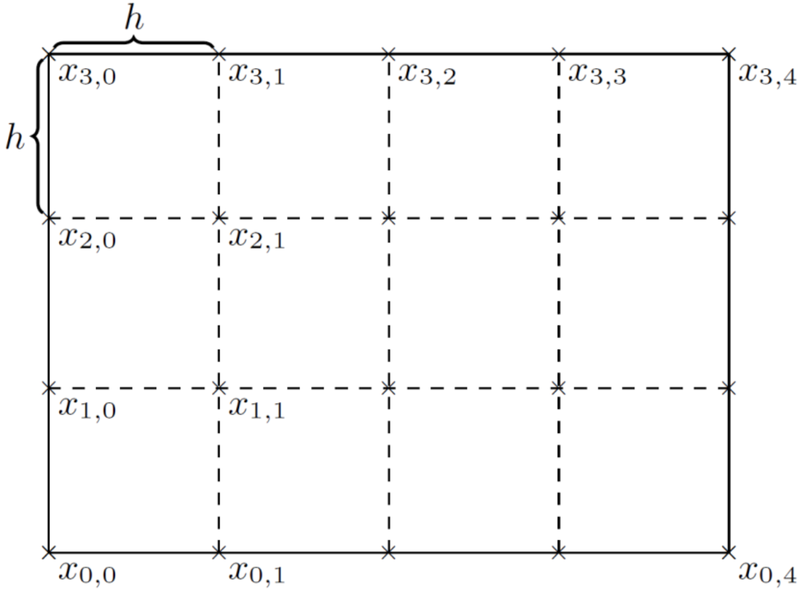

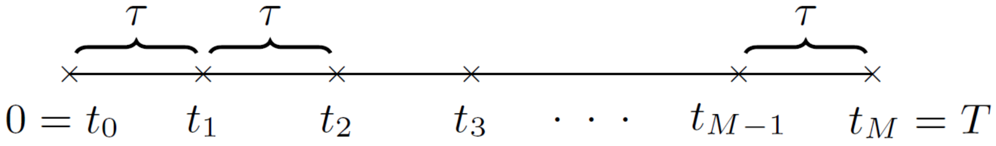

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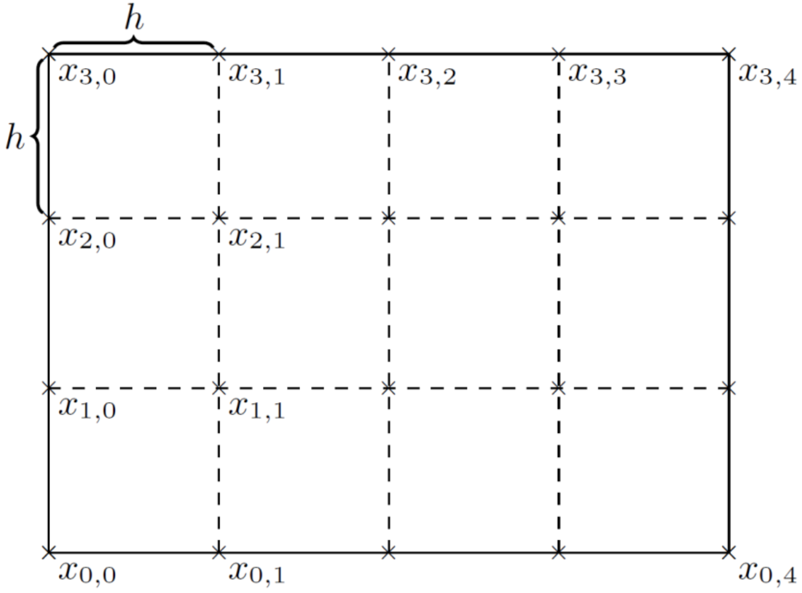
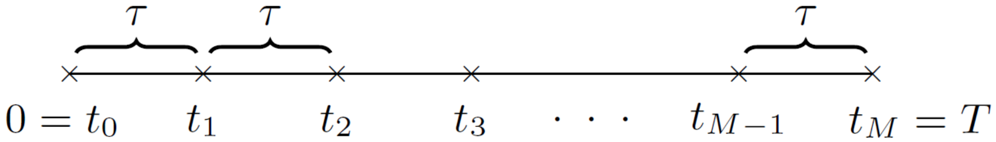
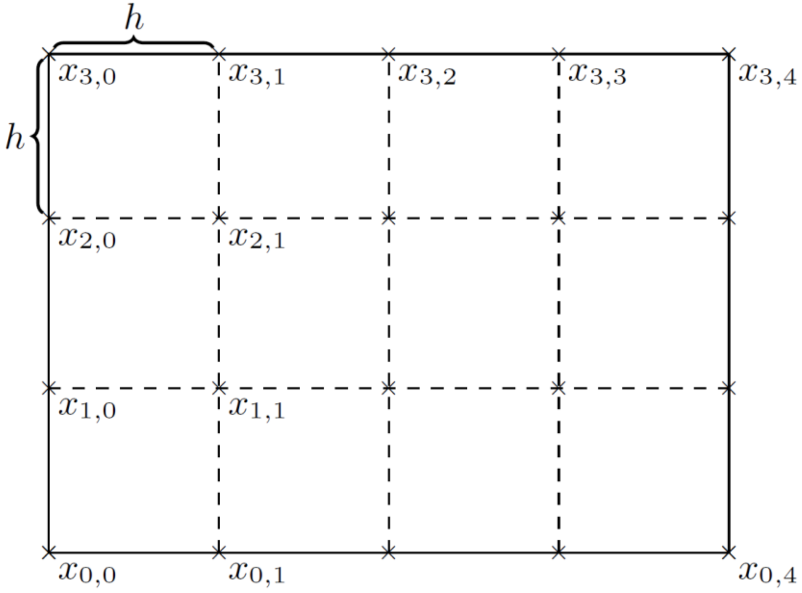
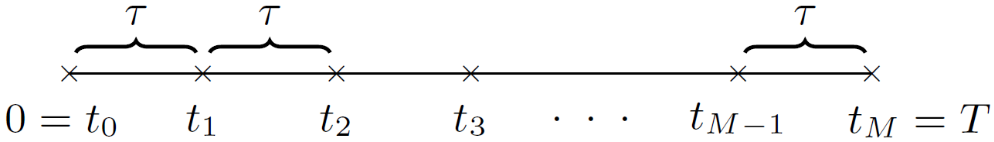




$$\mathbf{u}^m \approx u(t_m, x_{ij})$$

Model problem





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

$$\Delta \approx L$$

Runge-Kutta method

Runge-Kutta method

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

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

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

Runge-Kutta method

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

Runge-Kutta method

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

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

$$M$$

IRK preconditioners

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. *SIAM Journal on Scientific Computing*, 43(5):S475–S495, 2021.

IRK preconditioners

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

IRK preconditioners

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

IRK preconditioners

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

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

IRK preconditioners

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

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

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

Preconditioner analysis

sp.linalg.gmres

Preconditioner analysis

sp.linalg.gmres

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

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

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

Preconditioner analysis

Step I :

Preconditioner analysis

Step I :

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

Preconditioner analysis

Step I :

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

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

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

Preconditioner analysis

$$s = 2$$

Preconditioner analysis

Proposition. *Let* $s = 2$ *and* $a_{ij} \neq 0$. *Adopting the above notation and setting* $\mathrm{sp}(L) = \{\lambda_k\}_k$ *and* $\theta_k = \frac{\tau}{h^2}\lambda_k$ *we have* $\mathrm{sp}(M\left(P^{\mathrm{diag}}\right)^{-1}) = \zeta_{1,2}^{(k)}$ *with*

$$\zeta_{1,2}^{(k)} = 1 \pm \sqrt{\frac{a_{12}a_{21}}{(|\theta_k^{-1}| + a_{11})(|\theta_k^{-1}| + a_{22})}},$$

and the condition number of the eigenbasis is given by

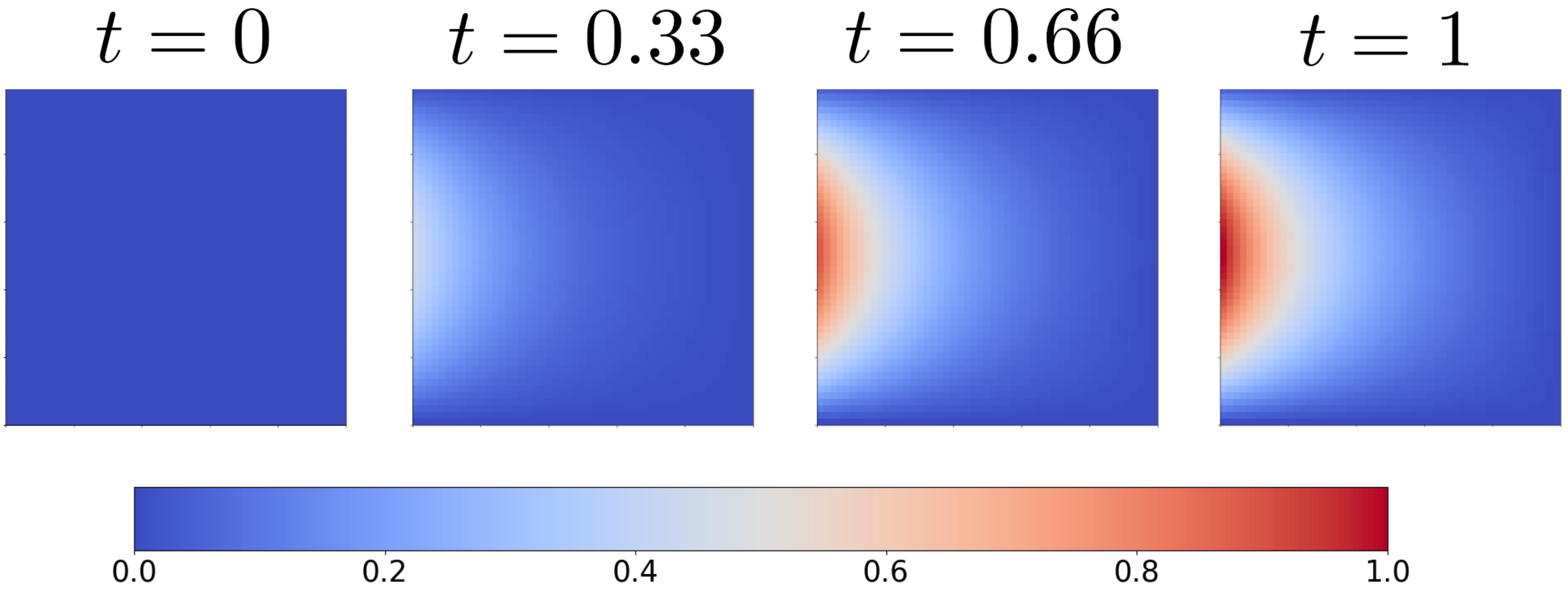
$$\kappa(S) = \max_{k=1,\dots,n} \sqrt{\frac{1 + \left|\frac{a_{21}(1+a_{22}|\theta_k|)}{a_{12}(1+a_{11}|\theta_k|)}\right| + \left|1 - \left|\frac{a_{21}(1+a_{22}|\theta_k|)}{a_{12}(1+a_{11}|\theta_k|)}\right|\right|}{1 + \left|\frac{a_{21}(1+a_{22}|\theta_k|)}{a_{12}(1+a_{11}|\theta_k|)}\right| - \left|1 - \left|\frac{a_{21}(1+a_{22}|\theta_k|)}{a_{12}(1+a_{11}|\theta_k|)}\right|\right|}}.$$

IRK preconditioners

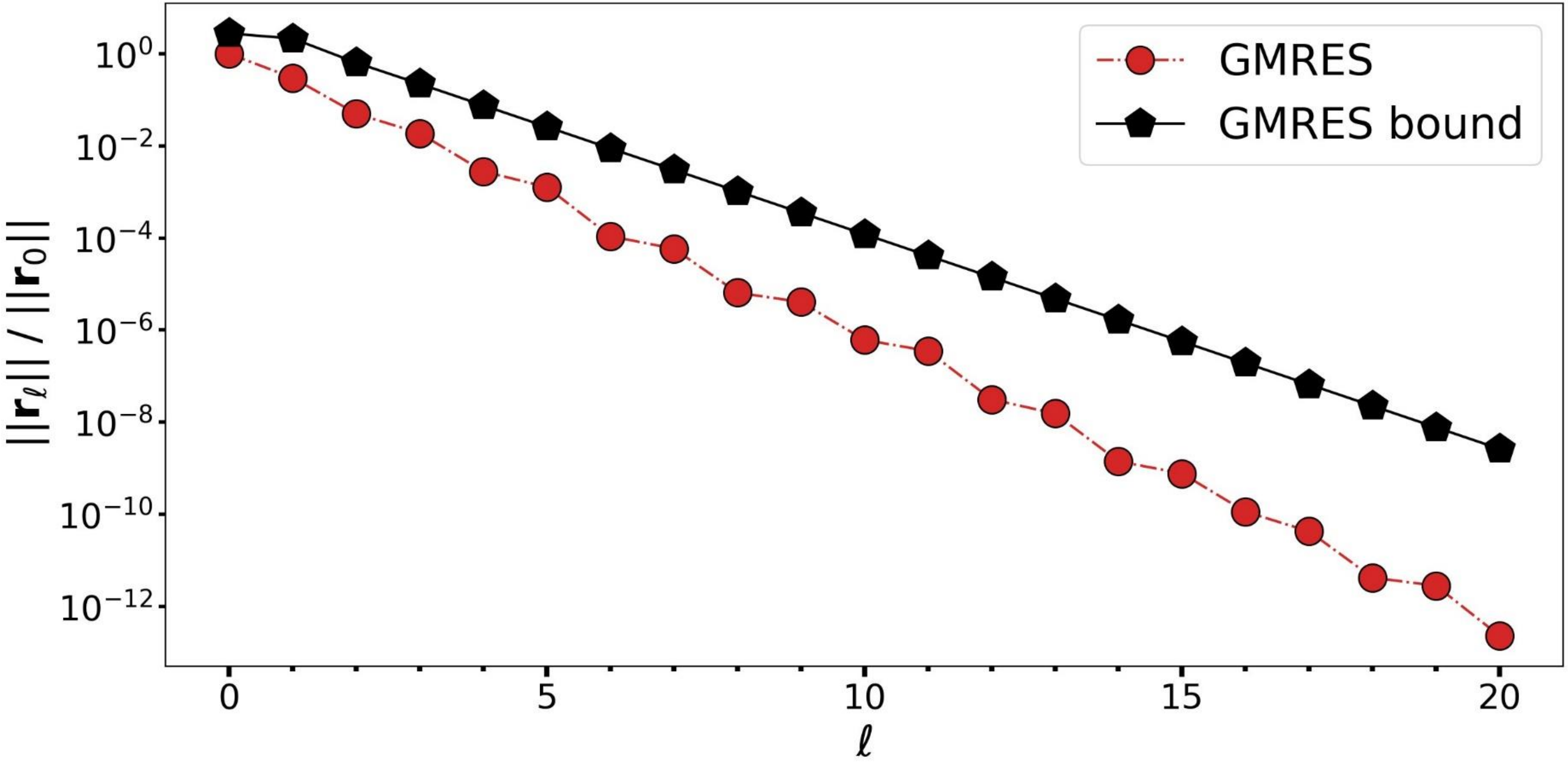
How much can we understand and predict ?

$$s = 2$$

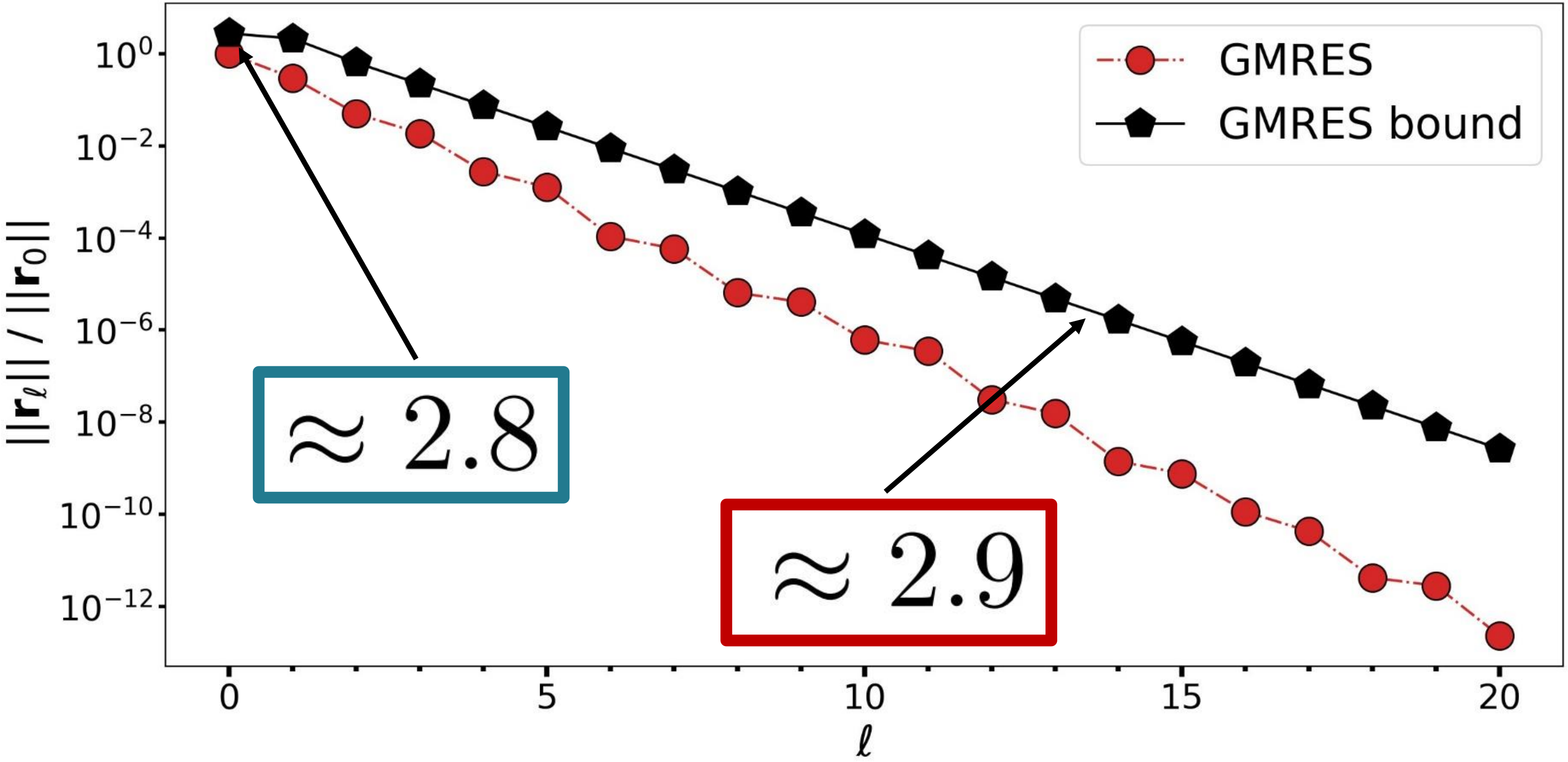
IRK preconditioners



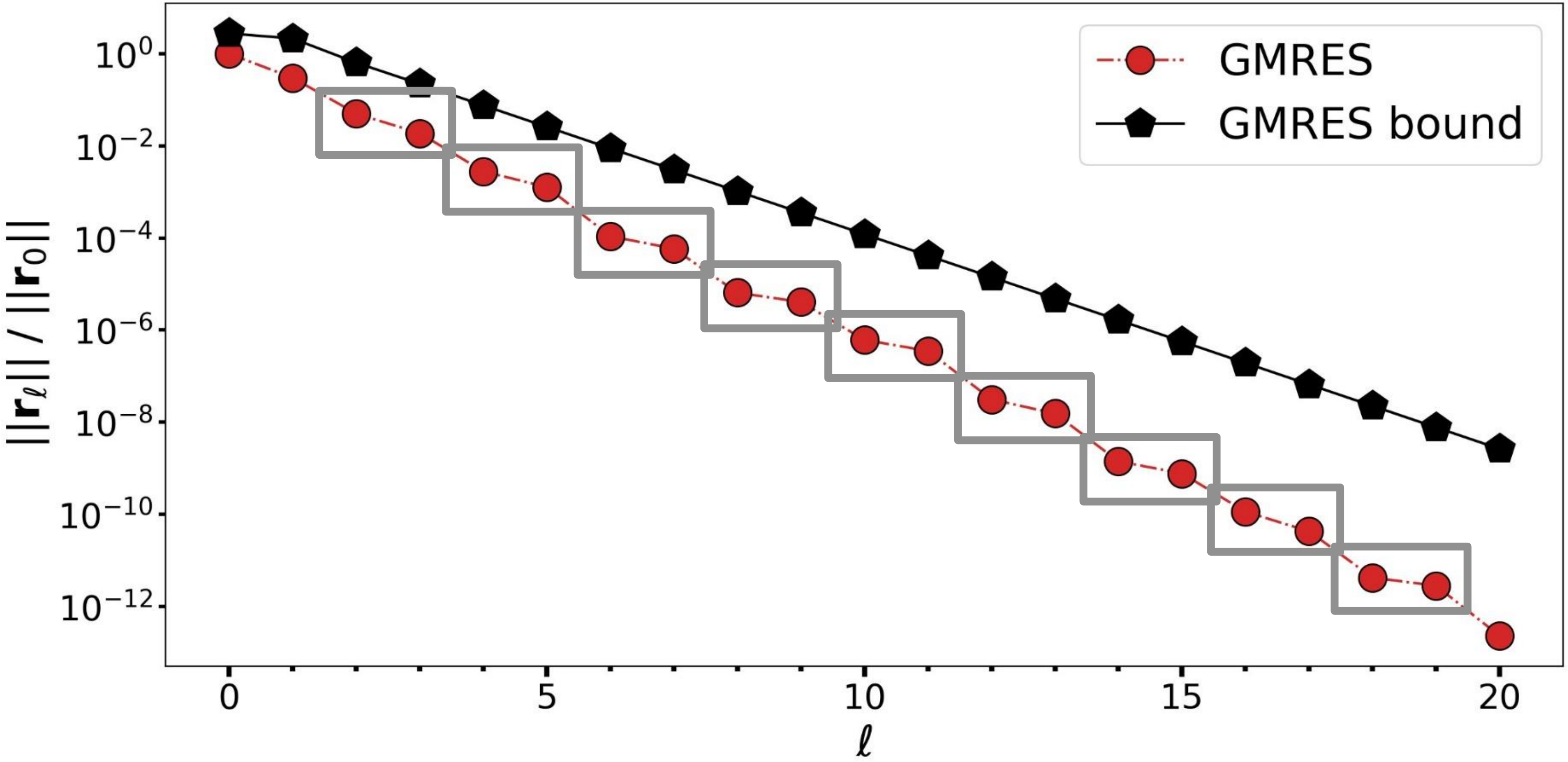
IRK preconditioners



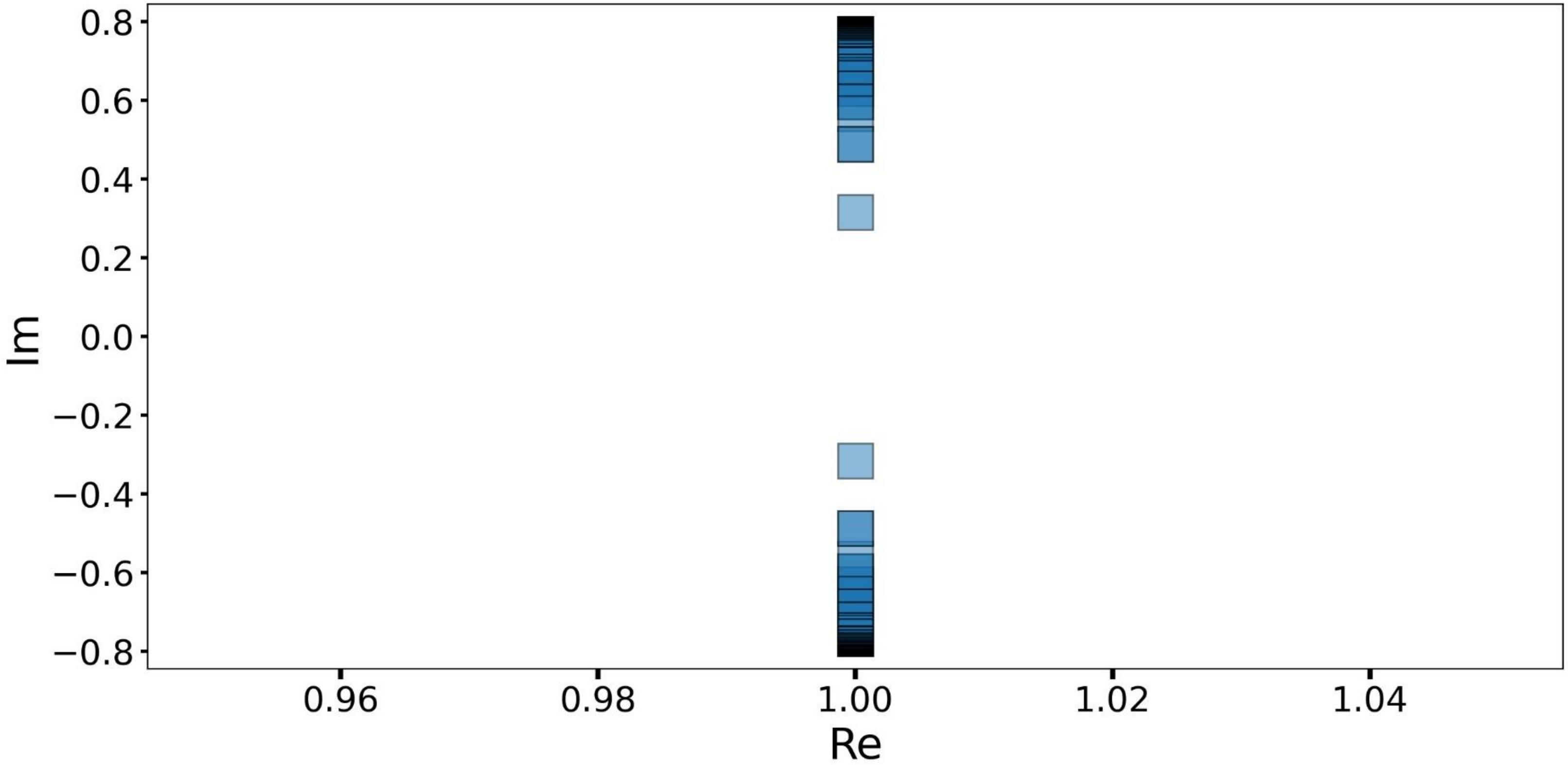
IRK preconditioners



IRK preconditioners



IRK preconditioners



IRK preconditioners

sp.linalg.gmres

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

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

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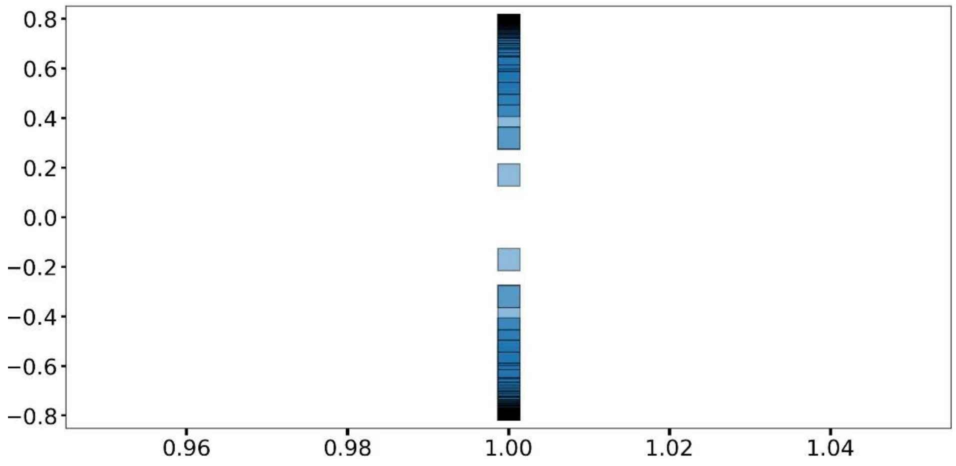
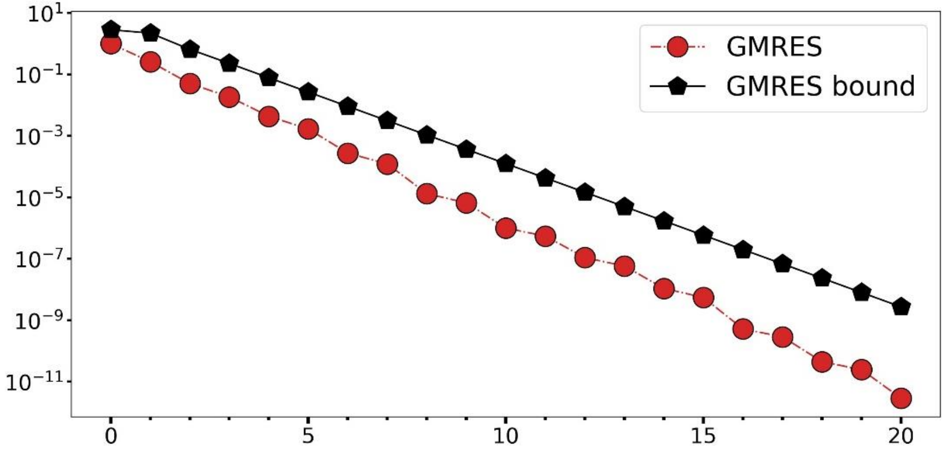
IRK preconditioners





Numerical aspects

Numerical aspects

The interaction of
GMRES and inexact solve

Numerical aspects

Each GMRES iteration

No preconditioner :

- 1 sparse mat-vec

Preconditioner :

- 1 sparse mat-vec
- 1 sparse solve

Numerical aspects

Each GMRES iteration

No preconditioner :

- 1 sparse mat-vec

Preconditioner :

- 1 sparse mat-vec
- 1 sparse solve

  → inexcat?

Numerical examples

Finite element method,
real-life geometry

Numerical examples

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

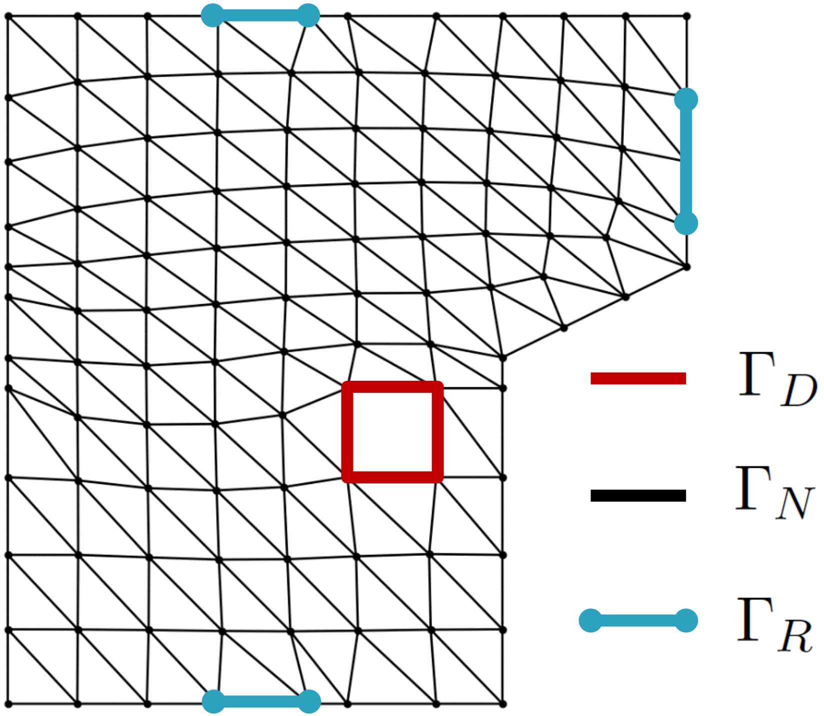
$$u = g \quad \text{on } \Gamma_D \times (0, T)$$

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

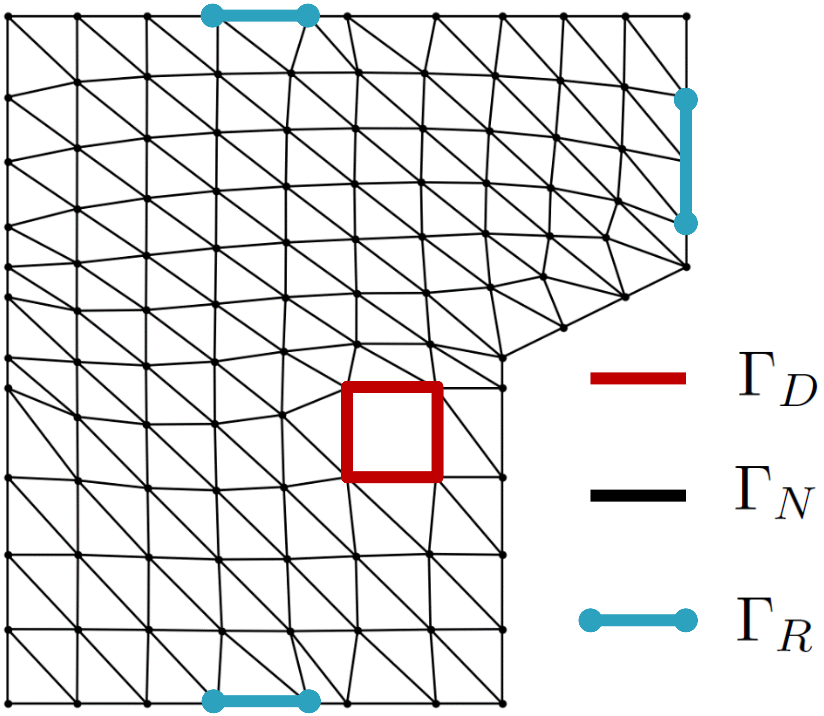
$$\frac{\partial u}{\partial \mathbf{n}} + pu = 0 \quad \text{on } \Gamma_R \times (0, T)$$

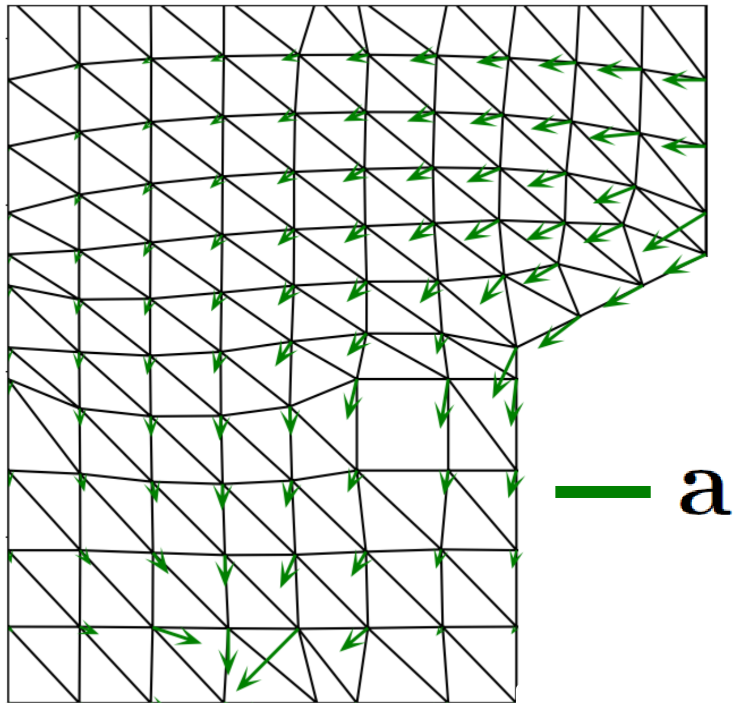
$$u = u_0 \ \text{ at } \partial\Omega \times \{0\}$$

Numerical examples



Numerical examples





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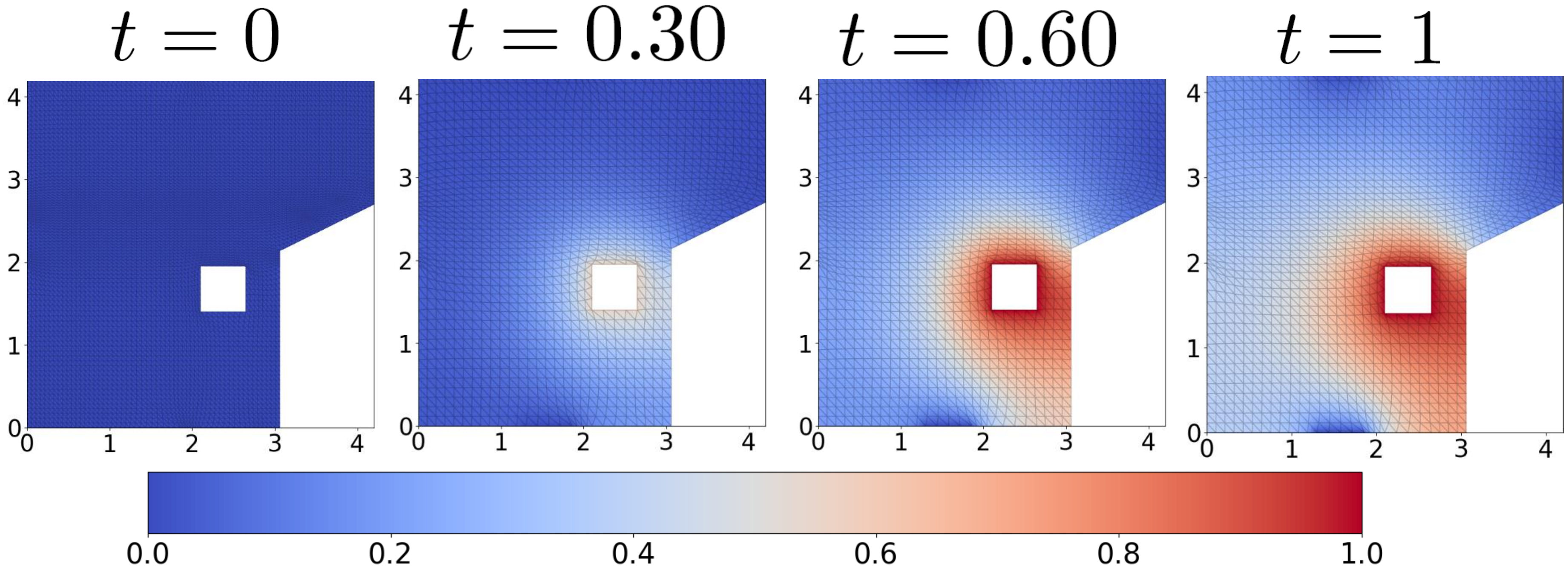
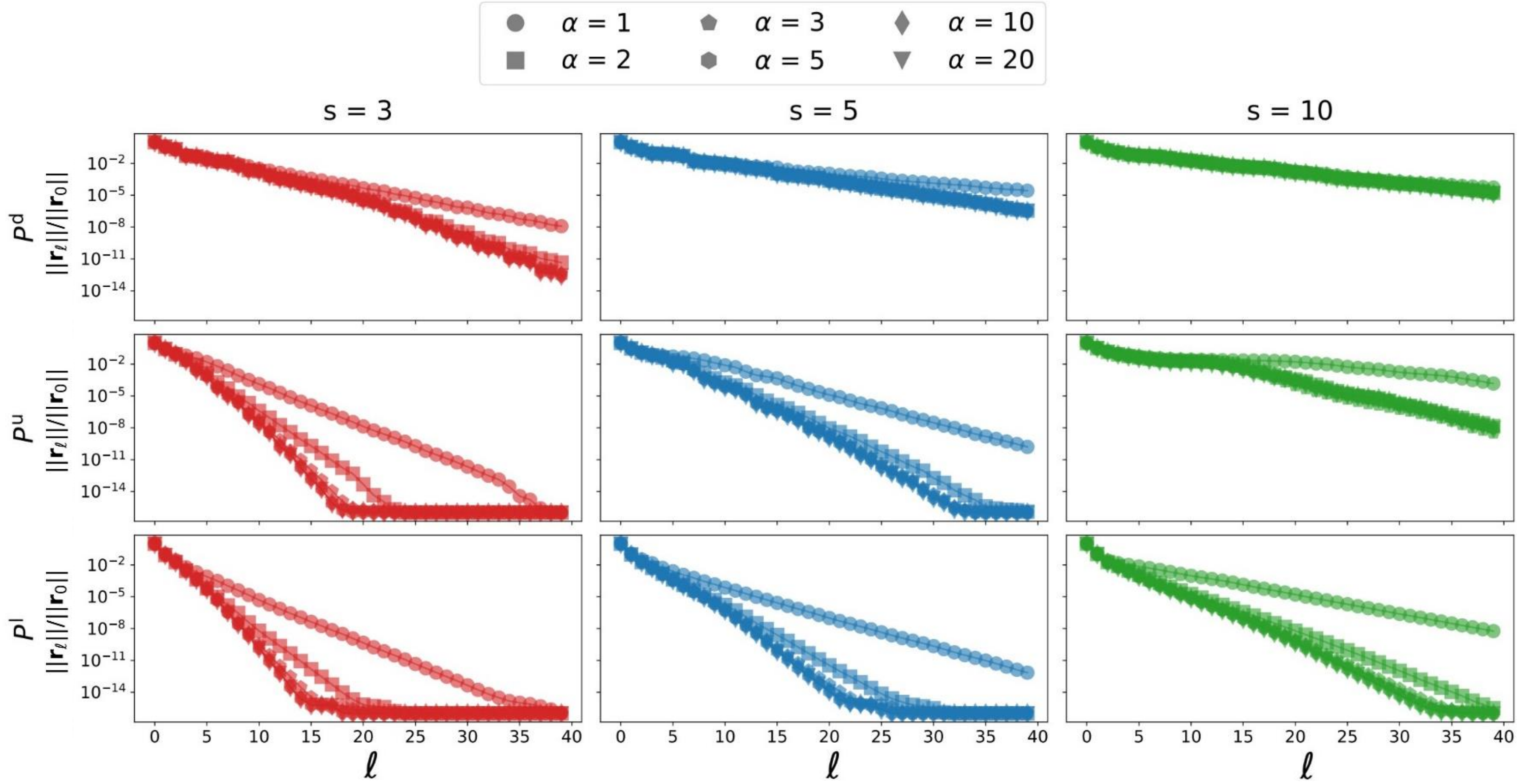


Numerical examples



Conclusion

Thank you for your attention

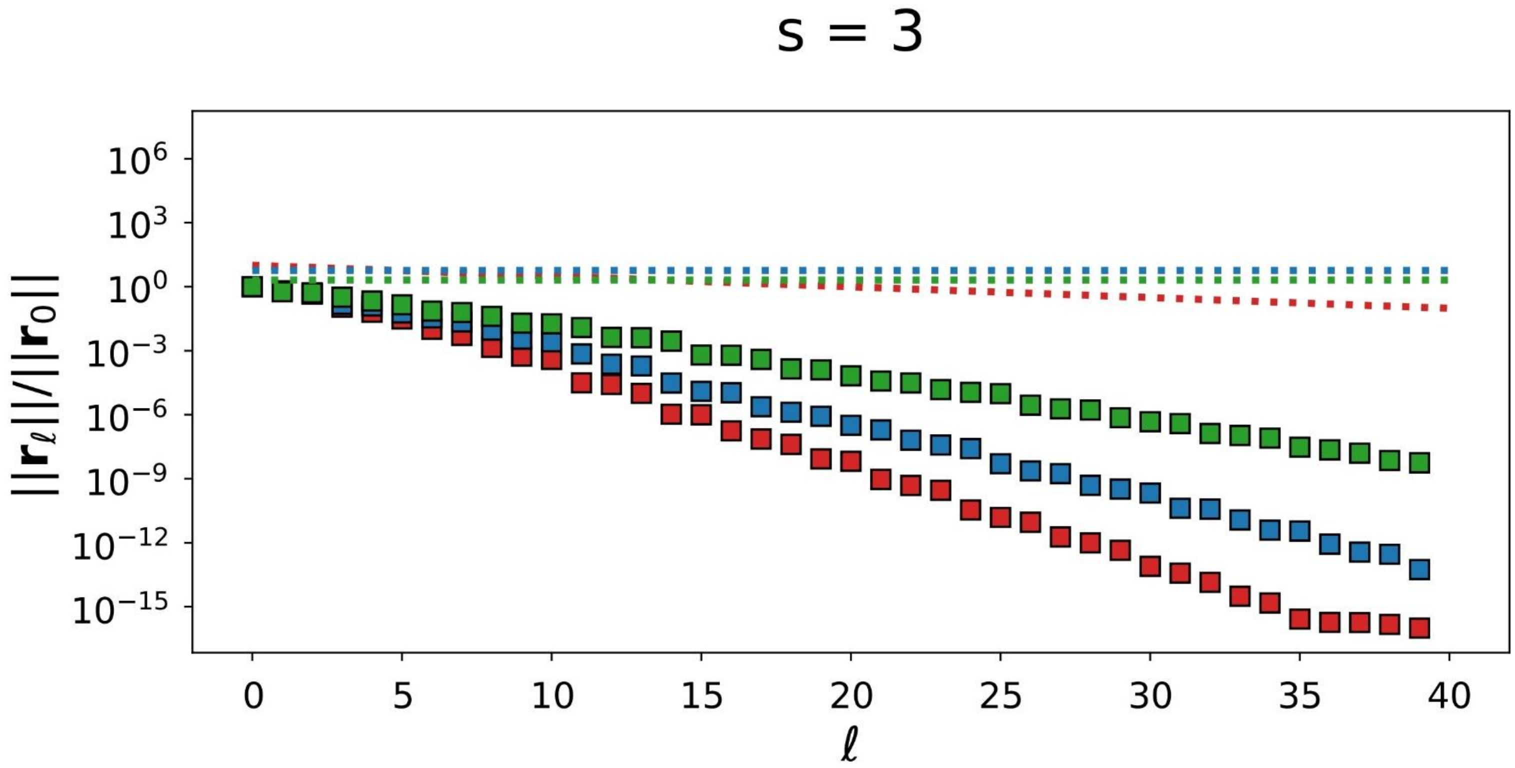
IRK preconditioners

How about

$$s \geq 2$$

Gauss | RadauIIA | LobattoIIIC

IRK preconditioners



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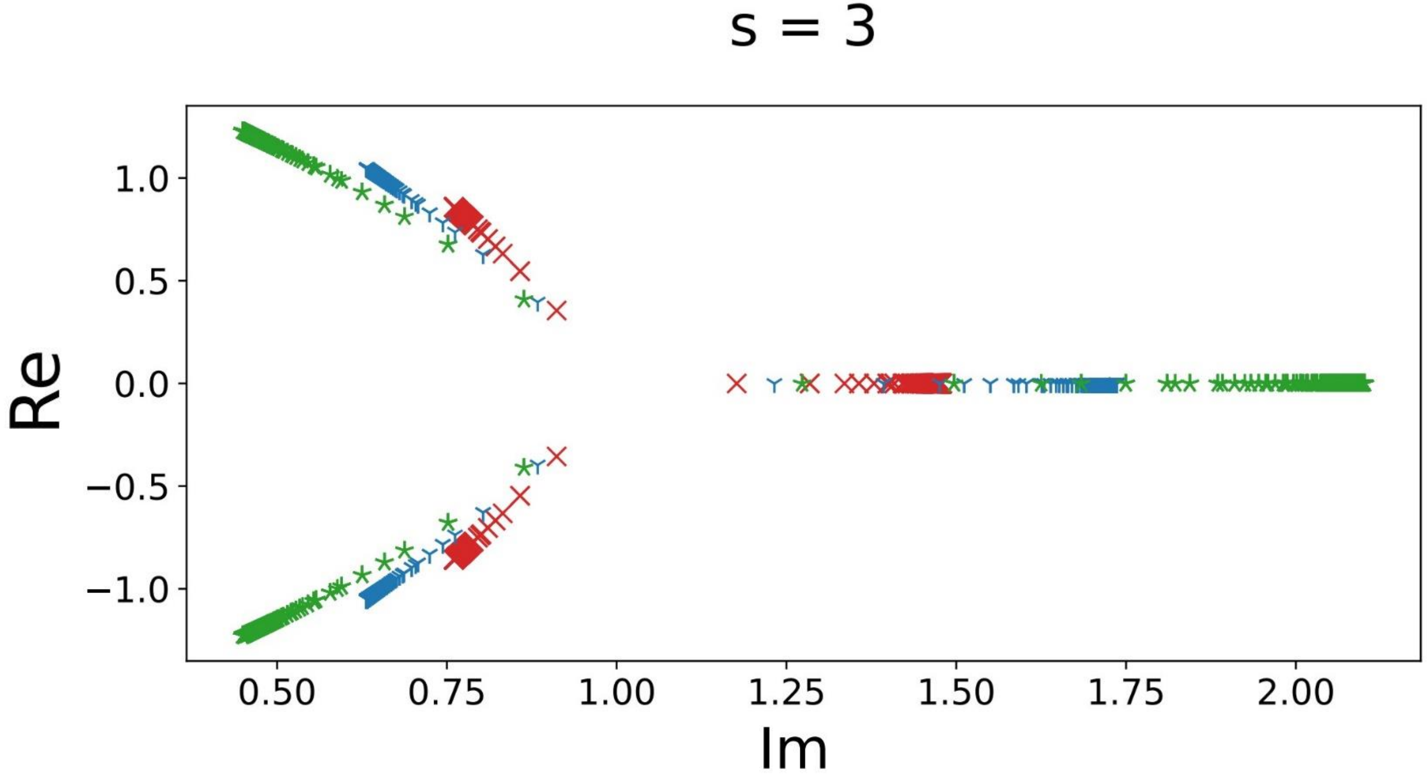

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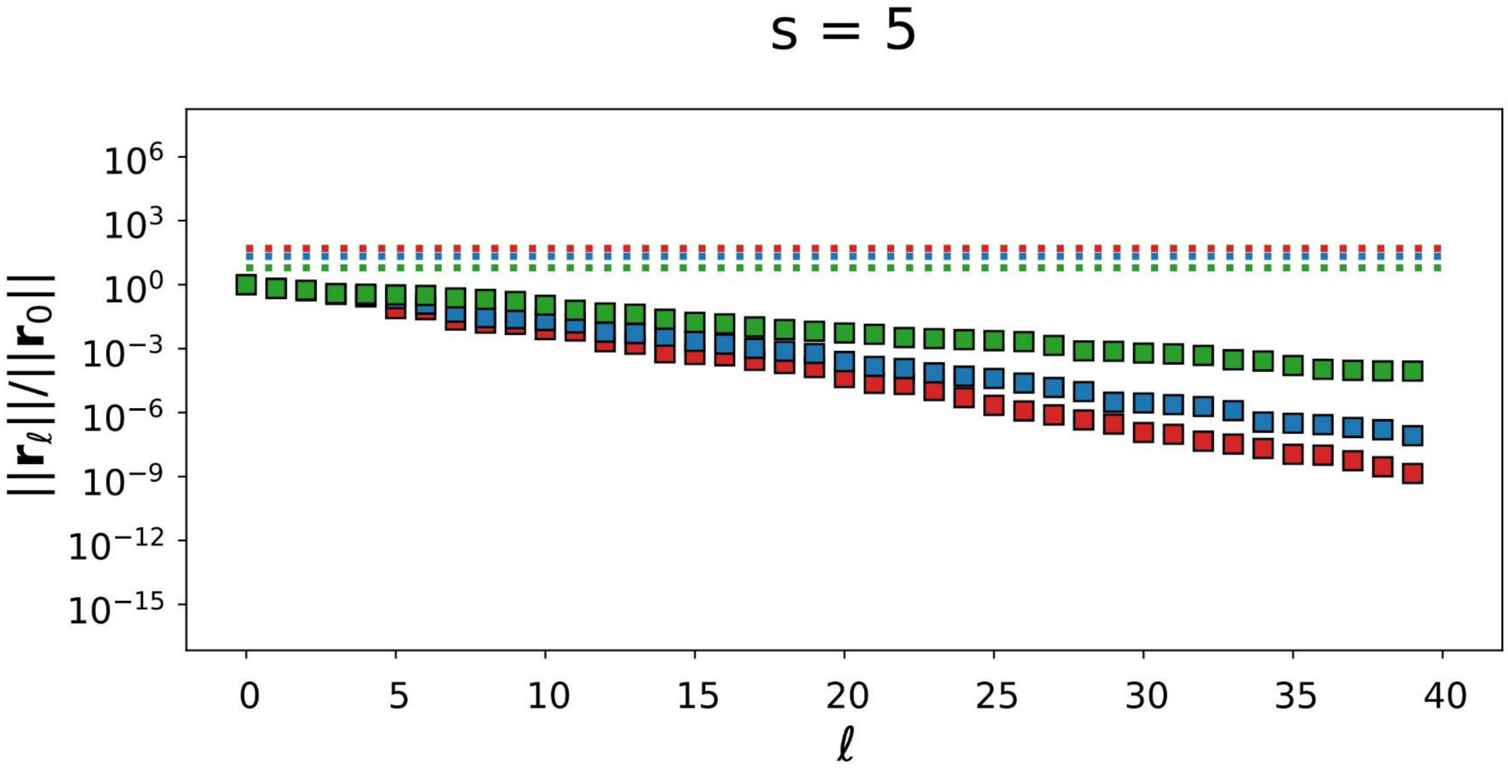

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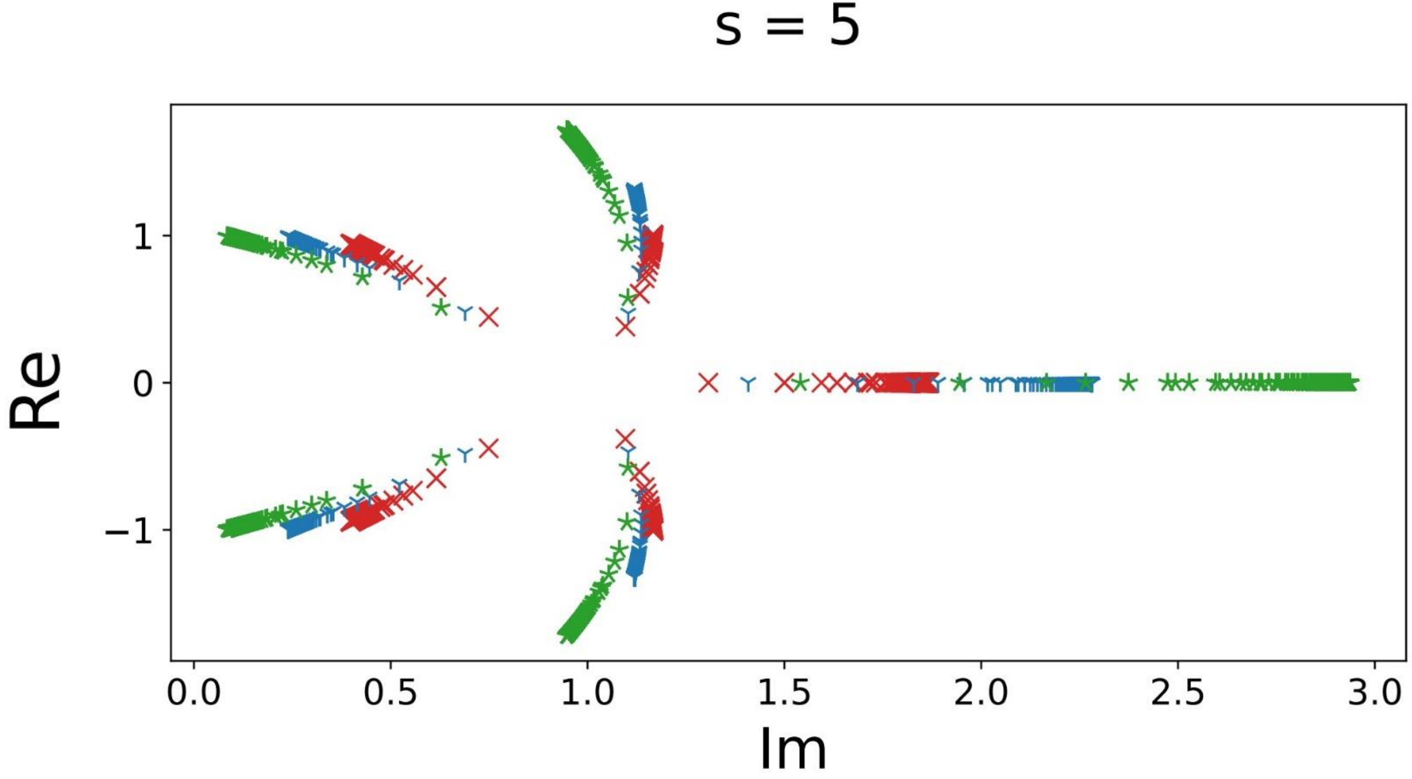

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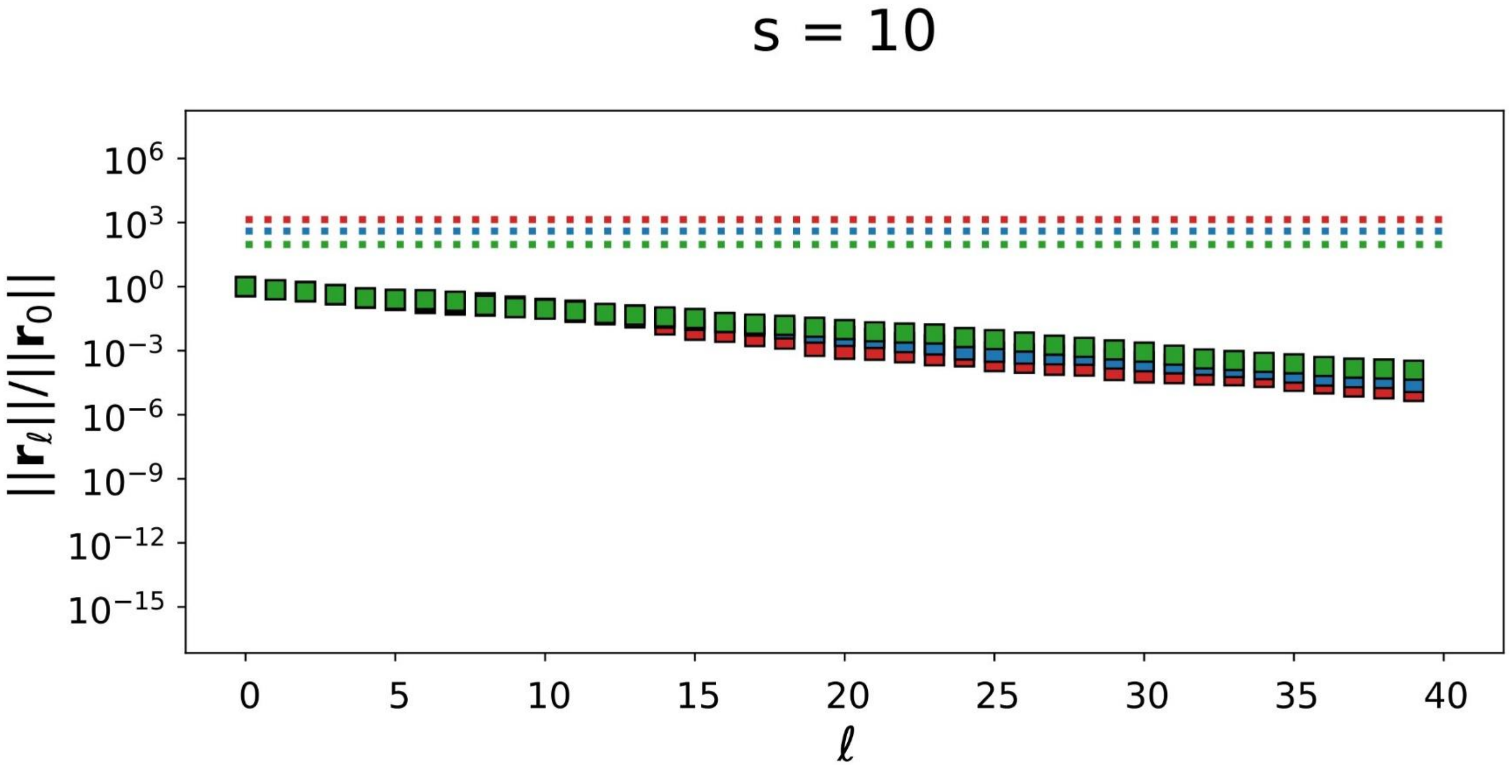

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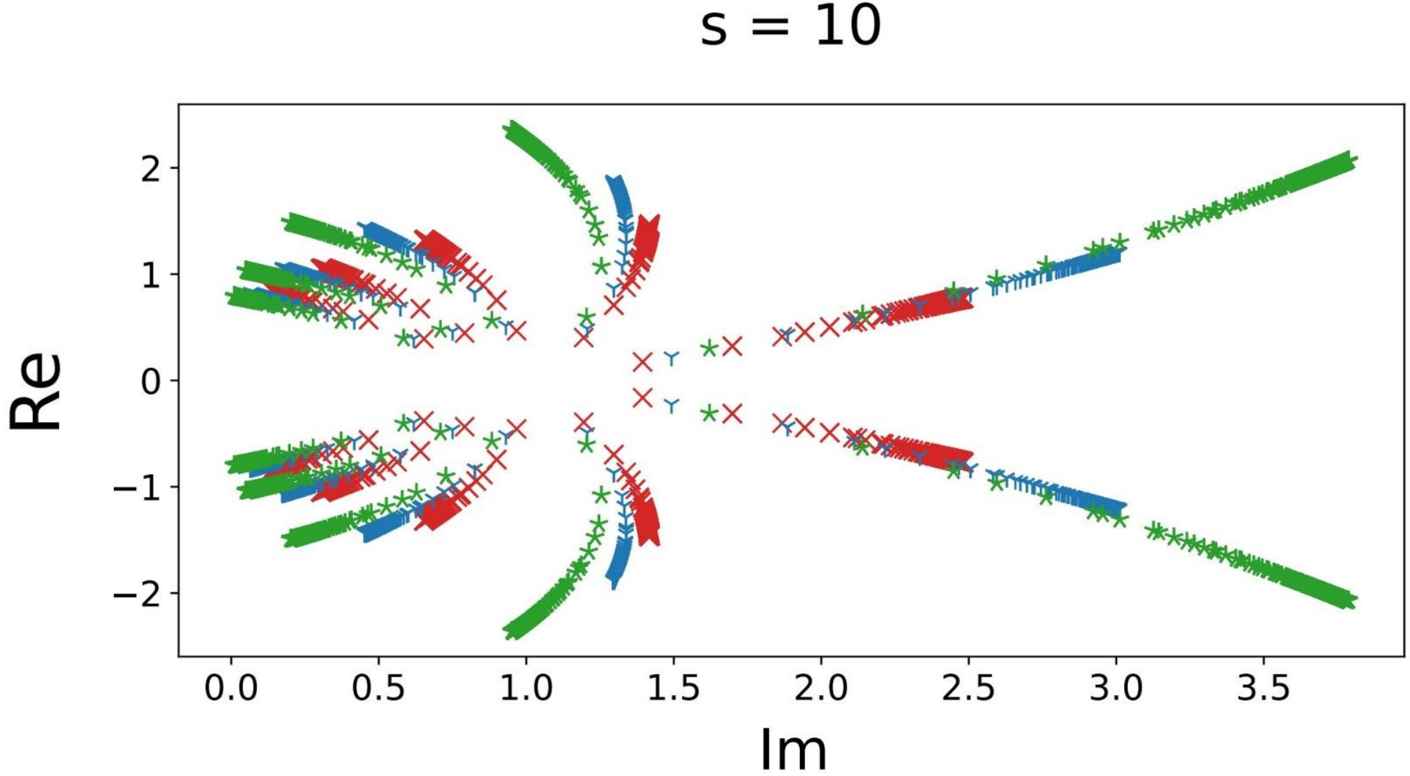

Observations & generalizations

Observations & generalizations

- Staircase-like behavior

Observations & generalizations

- Staircase-like behavior
- Algebraic curves (centered) & GMRES

Observations & generalizations

- Staircase-like behavior
- Algebraic curves (centered) & GMRES
- Other types of preconditioners

Optimization of the method

Optimization of the method

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

- Order of convergence
- Numerical stability

Optimization of the method

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

- Order of convergence
- Numerical stability
- GMRES convergence

Optimization of the method

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

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

Optimization of the method

G. A. Staff, K.-A. Mardal, and T. K. Nilssen. Preconditioning of fully implicit Runge-Kutta schemes for parabolic PDEs. *Modeling, Identification and Control*, 27(2):109–123, 2006.

Optimization of the method

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$$M = I_s \otimes I_n - \frac{\tau}{h^2}(A \otimes L)$$

$$P^{\text{diag}} = I_s \otimes I_n - \frac{\tau}{h^2} D\tilde{A} \otimes L$$

Optimization of the method

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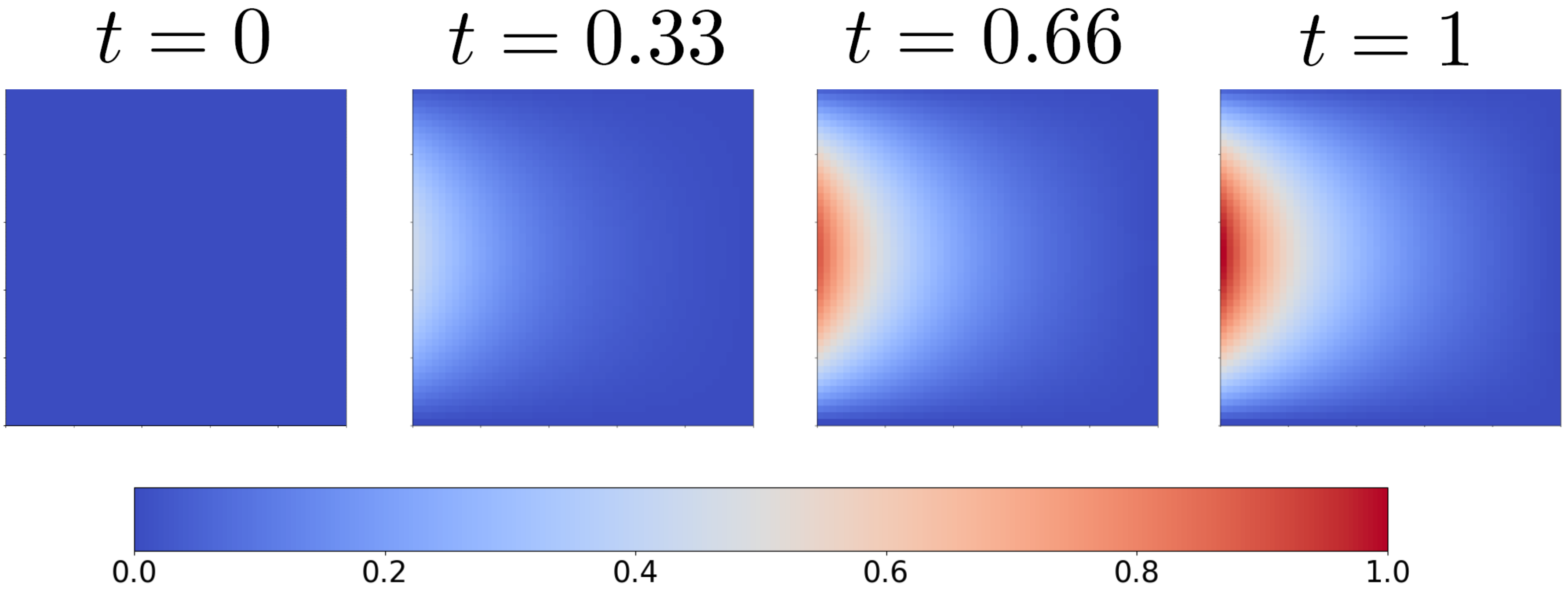
Optimization of the method

Optimization of the method

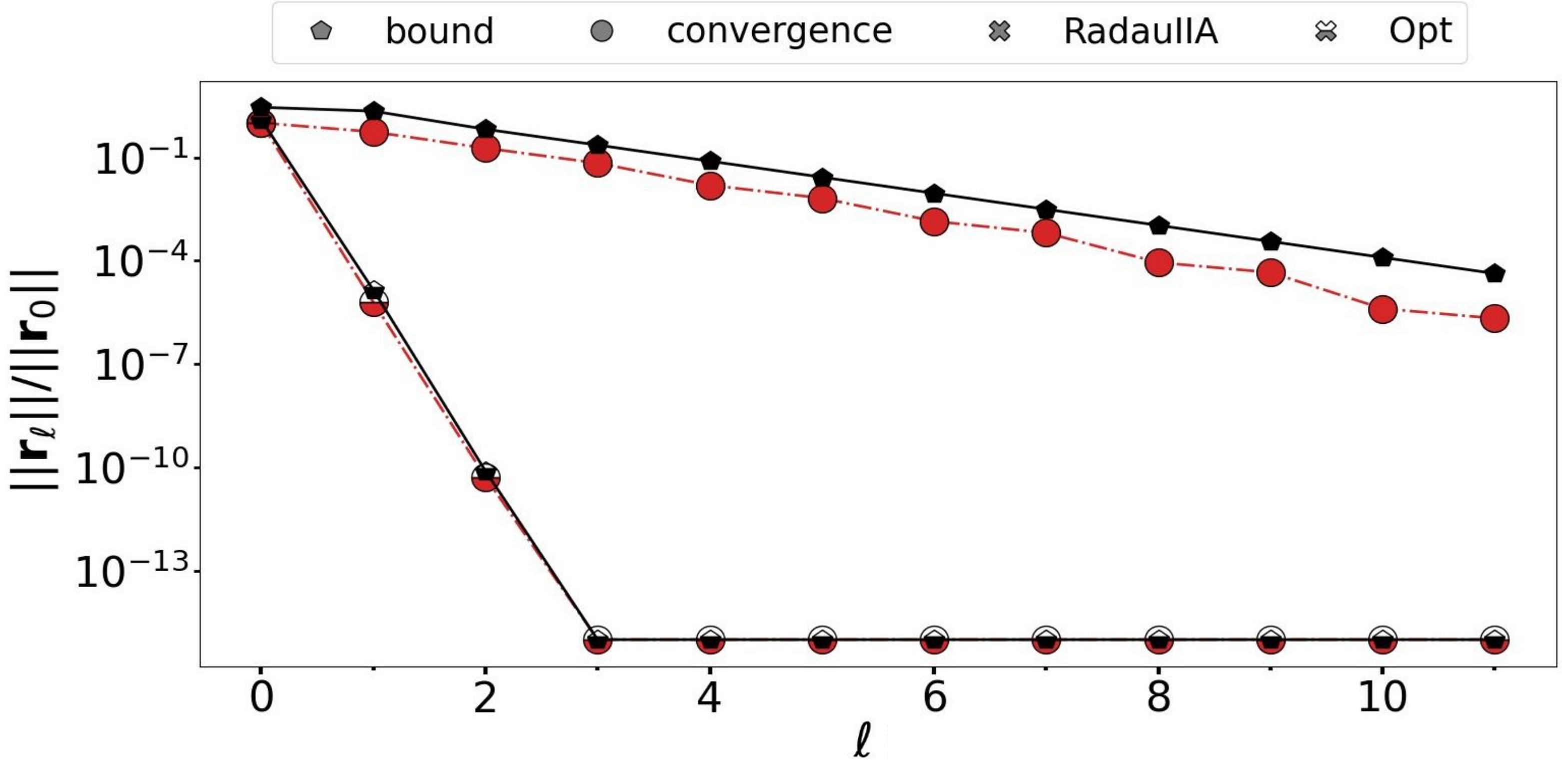
How much can we understand and predict ?

$$s = 2$$

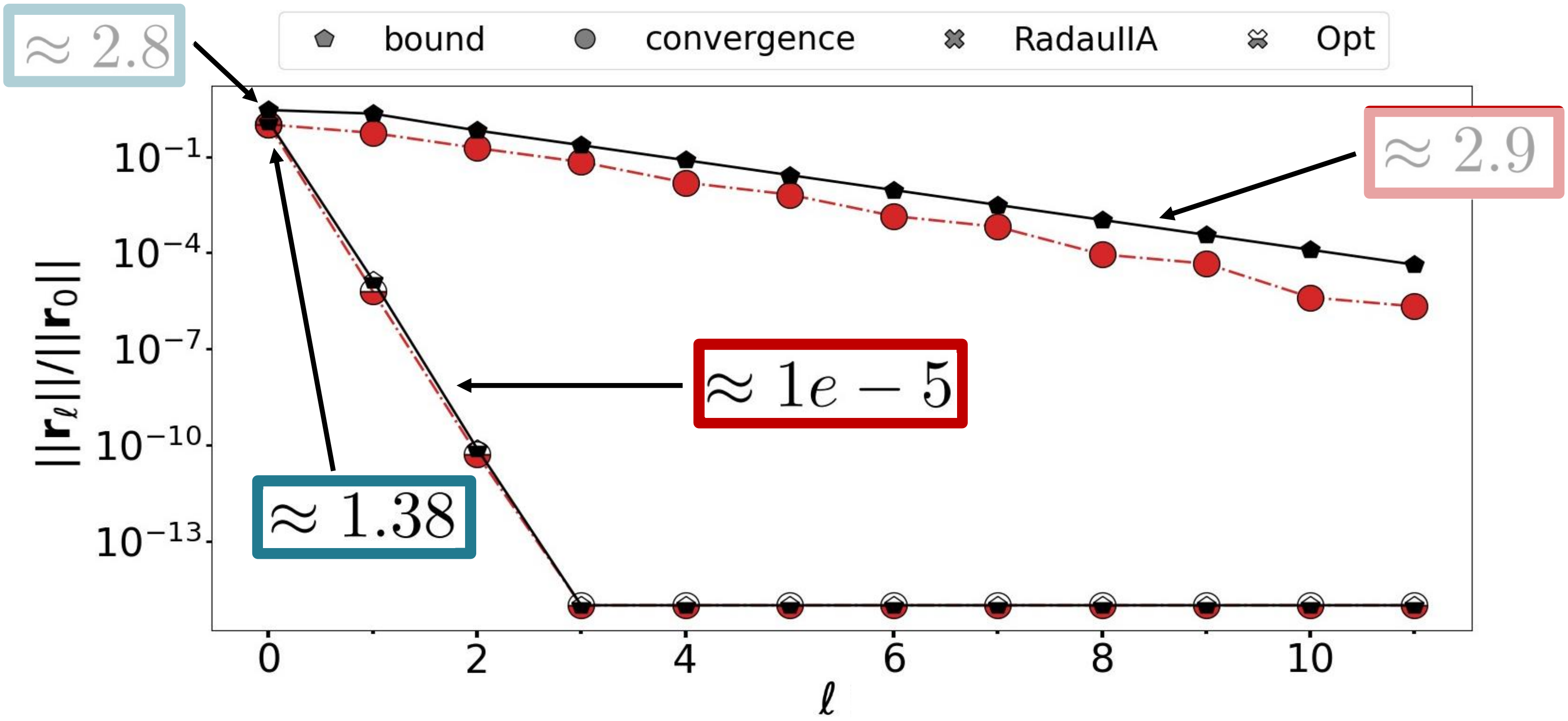
Optimization of the method



Optimization of the method



Optimization of the method



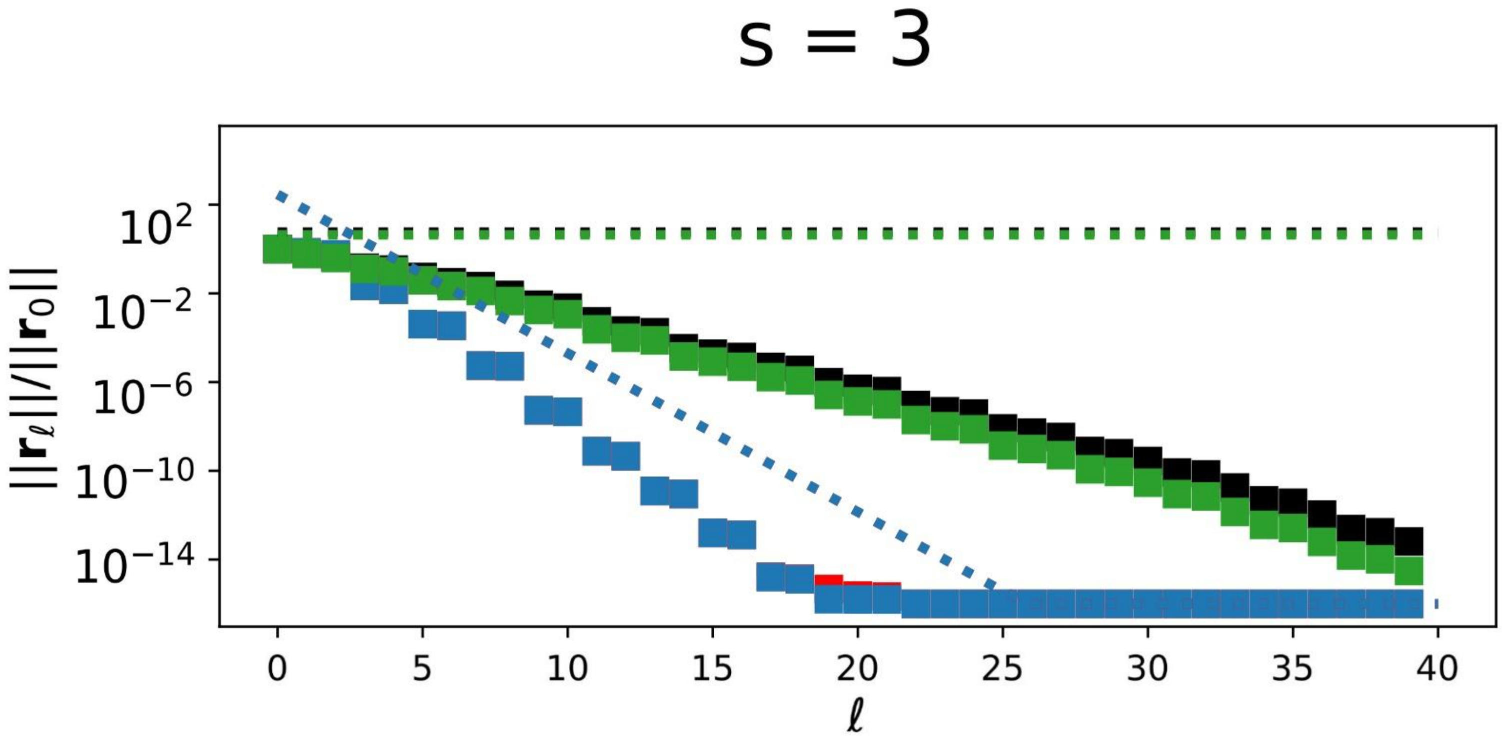
Optimization of the method

How about

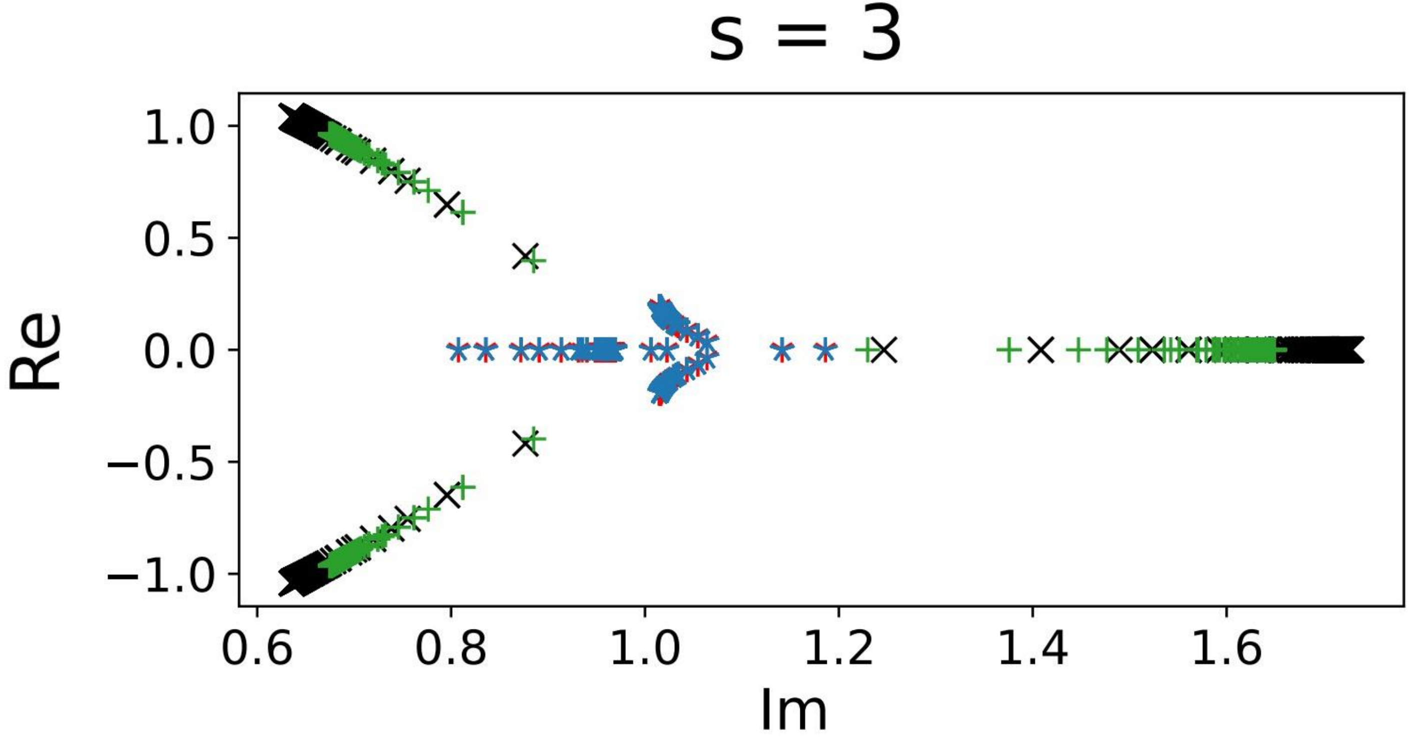
$$s \geq 2$$

■ RadauIIA ■ optimized ■ A-stable optimized ■ L-stable optimized

Optimization of the method

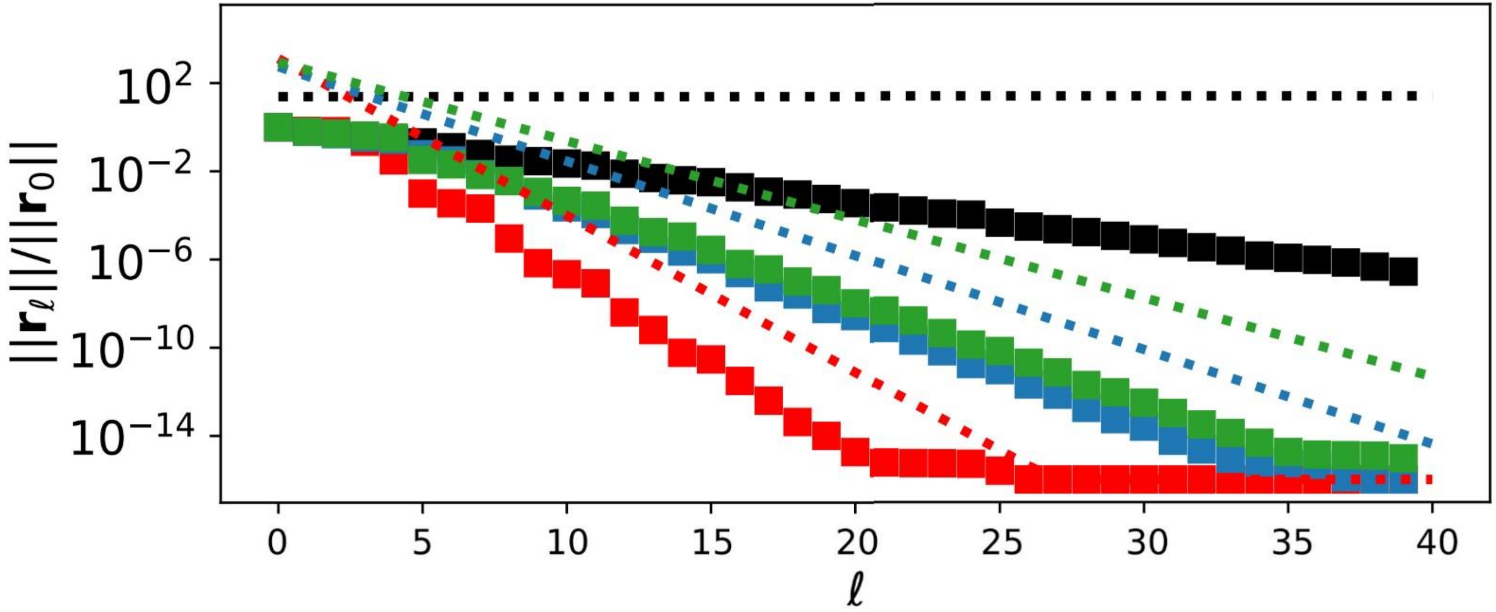


Optimization of the method

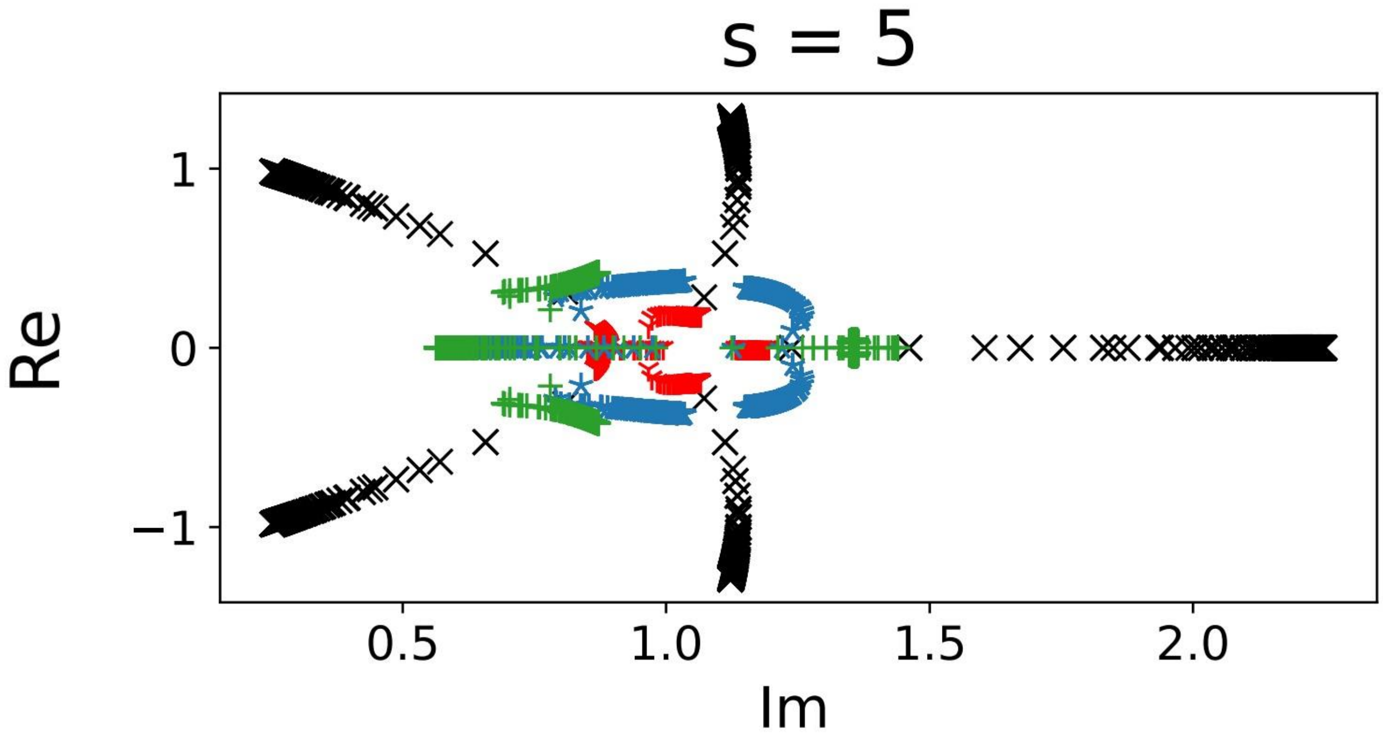


Optimization of the method

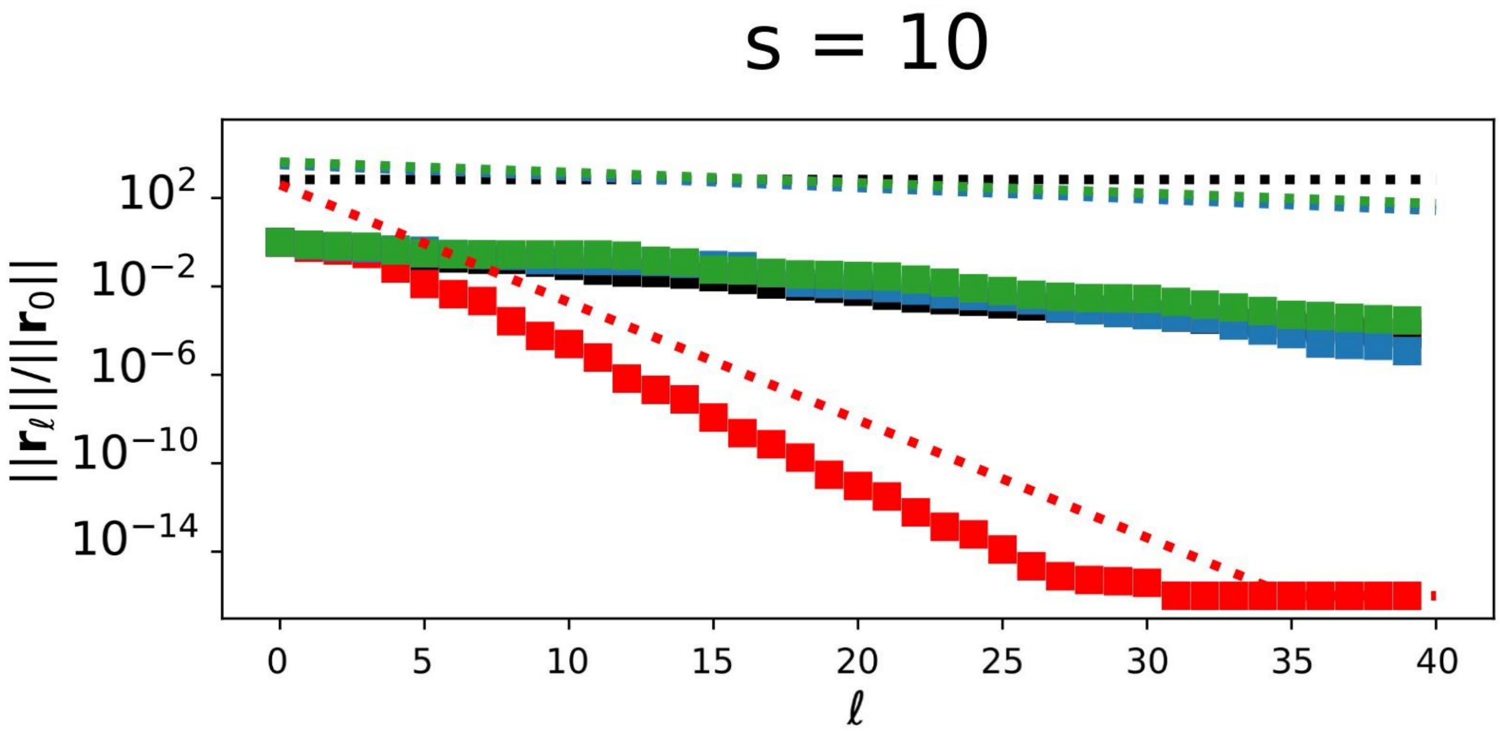
$s = 5$



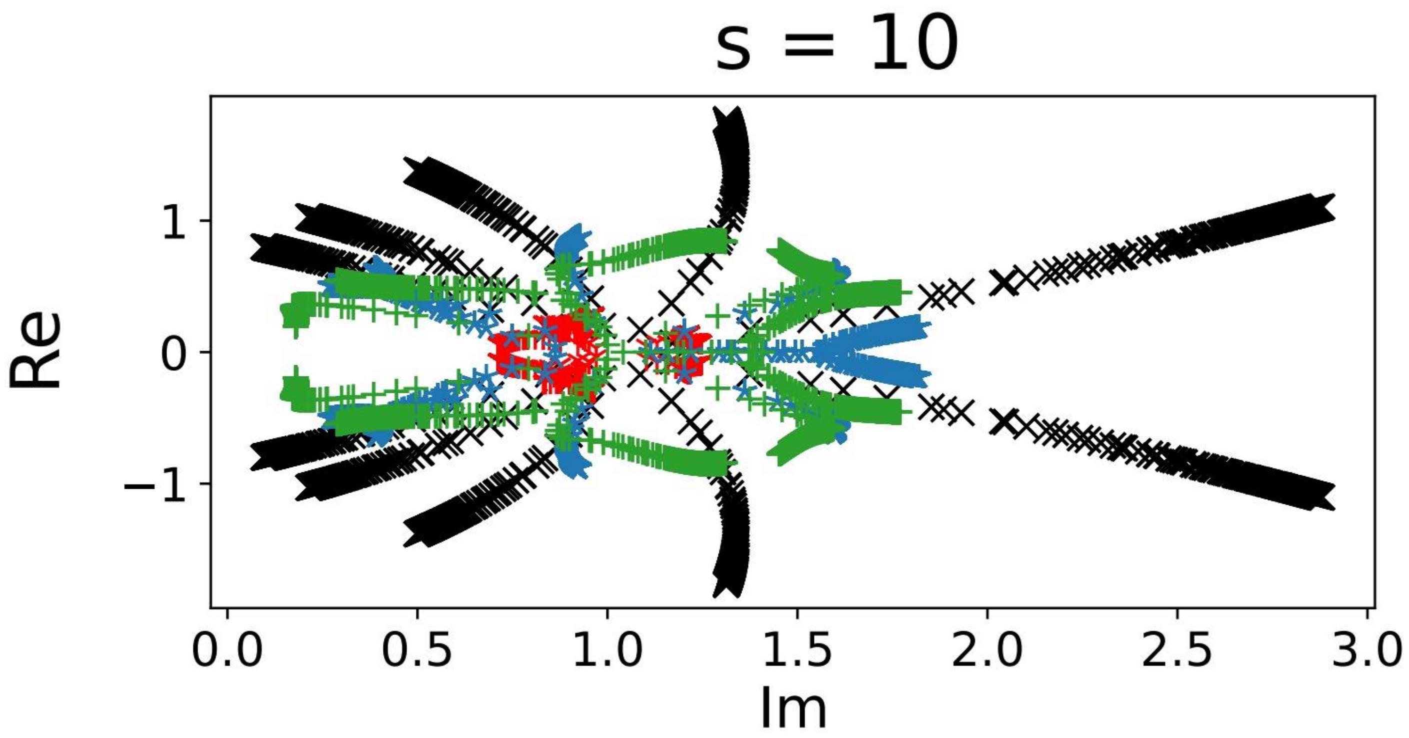
Optimization of the method



Optimization of the method



Optimization of the method



Observations & generalizations

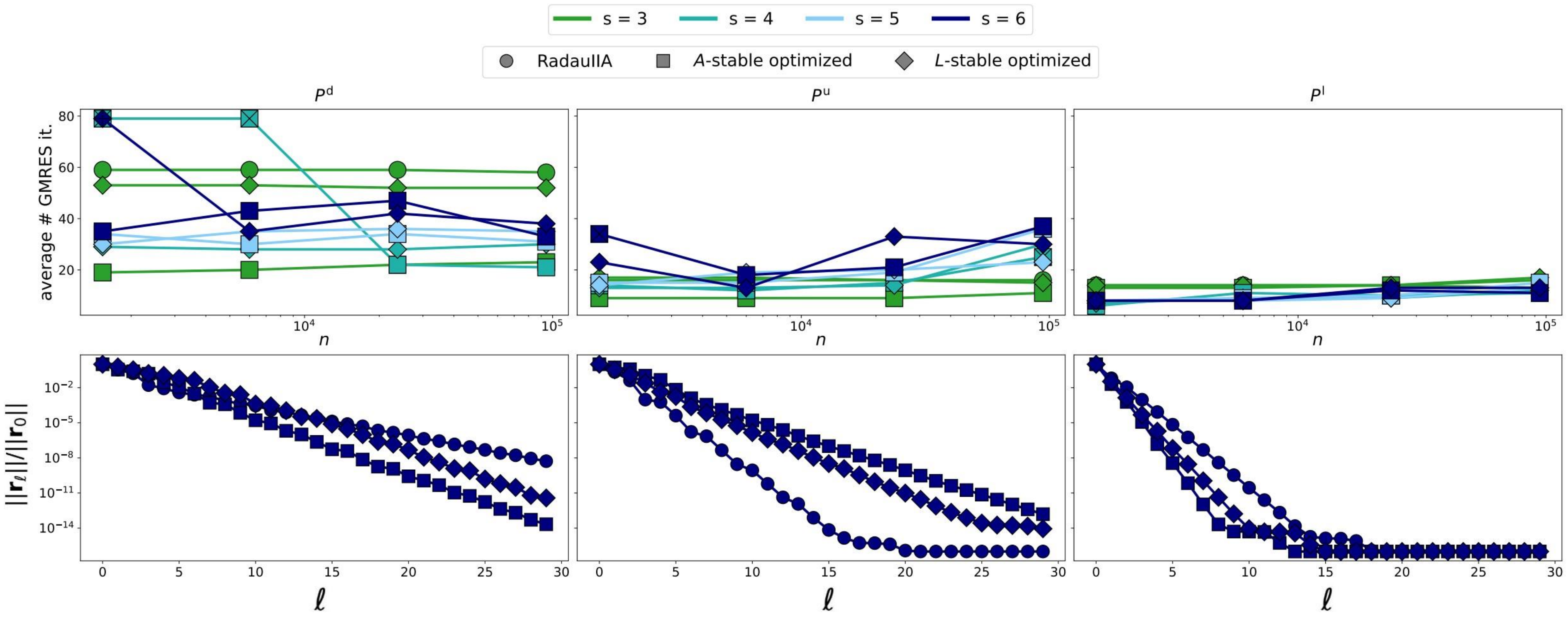
Observations & generalizations

- Algebraic curves (centered) & GMRES
- Other types of preconditioners

Numerical examples

The average GMRES performance

Numerical examples



Numerical examples