Adaptive rational Krylov methods for exponential Runge–Kutta integrators

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Stiff systems of ODEs

We consider **semilinear parabolic PDEs** with the splitting

$$\frac{\partial u(\boldsymbol{x},t)}{\partial t} = F(t,u(\boldsymbol{x},t)) = -\mathcal{A}u(\boldsymbol{x},t) + g(t,u(\boldsymbol{x},t)), \quad u(\boldsymbol{x},t=0) = u_0,$$

with $\mathcal{A}$ linear differential operator (here: $\mathcal{A} = -\Delta$) between appropriate function spaces.

We are interested in *discrete* linear semi-definite differential operators, e.g.,

- finite differences: $\boldsymbol{A} = \frac{1}{h_x^2}(\boldsymbol{T}_{n_x} \otimes \boldsymbol{I} + \boldsymbol{I} \otimes \boldsymbol{T}_{n_x})$, $\Sigma \subseteq \frac{2}{h_x^2}[0,4]$
- discrete graph setting: $\boldsymbol{A} = \boldsymbol{L}$ graph Laplacian, $\Sigma \subseteq [0,n]$

Leads to systems of ODEs

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with $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ and $\boldsymbol{u}\colon [0,T] \mapsto \mathbb{R}^n$.

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Exponential integrators

- Starting point: variation-of-constants formula [Hochbruck, Ostermann, 2010]

$$\boldsymbol{u}(t) = e^{-t\boldsymbol{A}}\boldsymbol{u}_0 + \int_0^t e^{-(t-\tau)\boldsymbol{A}} g(\tau, \boldsymbol{u}(\tau))d\tau$$

- Idea:
  - integrate linear part exactly (solution to homogeneous equation)
  - approximate the rest by exponential quadrature
- We use **explicit exponential Runge–Kutta (RK) methods**:

$$\begin{aligned}
\boldsymbol{U}_{ij} &= \chi_j(-h_i\boldsymbol{A})\boldsymbol{u}_i + h_i \sum_{k=1}^{s} a_{jk}(-h_i\boldsymbol{A})\boldsymbol{G}_{ik}, \\
\boldsymbol{G}_{ik} &= g(t_i + c_k h_i, \boldsymbol{U}_{ik}), \\
\boldsymbol{u}_{i+1} &= \chi(-h_i\boldsymbol{A})\boldsymbol{u}_i + h_i \sum_{j=1}^{s} b_j(-h_i\boldsymbol{A})\boldsymbol{G}_{ij}.
\end{aligned}$$

- Convergence order independent of problem stiffness.

We use

- SW2 (Strehmel & Weiner, stage $s = 2$, order $p = 2$) [Weiner, 2013]
- ETD3RK (Cox & Mathews, stage $s = 3$, order $p = 3$) [Cox, Mathews, 2002]
- `Krogstad4` (Krogstad, stage $s = 4$, order $p = 4$) [Krogstad, 2005]

$$
\begin{aligned}
\boldsymbol{U}_{i1} &= \boldsymbol{u}_i, \quad \boldsymbol{G}_{i1} = g(t_i, \boldsymbol{u}_i),\\
\boldsymbol{U}_{i2} &= \boldsymbol{u}_i + (h_i/2)\varphi_1(-(h_i/2)\boldsymbol{A})(\boldsymbol{G}_{i1} - \boldsymbol{A}\boldsymbol{u}_i), \quad \boldsymbol{G}_{i2} = g\left(t_i + (h_i/2), \boldsymbol{U}_{i2}\right),\\
\boldsymbol{U}_{i3} &= \boldsymbol{u}_i + h_i\left[(1/2)\varphi_1\left(-(h_i/2)\boldsymbol{A}\right)\left(\boldsymbol{G}_{i1} - \boldsymbol{A}\boldsymbol{u}_i\right) - \varphi_2(-(h_i/2)\boldsymbol{A})(\boldsymbol{G}_{i1} - \boldsymbol{A}\boldsymbol{u}_i)\right.\\
&\qquad \left.+\varphi_2(-(h_i/2)\boldsymbol{A})(\boldsymbol{G}_{i2} - \boldsymbol{A}\boldsymbol{u}_i)\right], \quad \boldsymbol{G}_{i3} = g\left(t_i + (h_i/2), \boldsymbol{U}_{i3}\right),\\
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&\qquad \left.+2\varphi_2(-h_i\boldsymbol{A})(\boldsymbol{G}_{i3} - \boldsymbol{A}\boldsymbol{u}_i)\right], \quad \boldsymbol{G}_{i4} = g(t_i + h_i, \boldsymbol{U}_{i4}),\\
\boldsymbol{u}_{i+1} &= \boldsymbol{u}_i + h_i\left[\varphi_1(-h_i\boldsymbol{A})(\boldsymbol{G}_{i1} - \boldsymbol{A}\boldsymbol{u}_i) - 3\varphi_2(-h_i\boldsymbol{A})(\boldsymbol{G}_{i1} - \boldsymbol{A}\boldsymbol{u}_i)\right.\\
&\qquad +4\varphi_3(-h_i\boldsymbol{A})(\boldsymbol{G}_{i1} - \boldsymbol{A}\boldsymbol{u}_i)\\
&\qquad +2\varphi_2(-h_i\boldsymbol{A})(\boldsymbol{G}_{i2} - \boldsymbol{A}\boldsymbol{u}_i) - 4\varphi_3(-h_i\boldsymbol{A})(\boldsymbol{G}_{i2} - \boldsymbol{A}\boldsymbol{u}_i)\\
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- Naively implemented, computation of linear combinations of φ-functions times a vector very expensive

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Exponential integrators

Efficient implementation

- Sequence of results [Saad, 1992] [Sidje, 1998] leading to

Theorem 1 (Al-Mohy, Higham, 2011)

Let $\widetilde{\boldsymbol{A}} = \begin{pmatrix} -\boldsymbol{A} & \boldsymbol{C} \\ \boldsymbol{0} & \boldsymbol{J}_p \end{pmatrix} \in \mathbb{C}^{(n+p)\times(n+p)}$*, where* $\boldsymbol{C} = [\boldsymbol{c}_p, \ldots, \boldsymbol{c}_1] \in \mathbb{C}^{n\times p}$ *and* $\boldsymbol{J}_p \in \mathbb{C}^{p\times p}$ *a Jordan block to the eigenvalue* 0*. Furthermore, we define the matrix exponential* $\boldsymbol{X} = e^{h_i \widetilde{\boldsymbol{A}}}$ *as well as the vector* $\widetilde{\boldsymbol{c}} := \begin{pmatrix} \boldsymbol{c}_0 \\ \boldsymbol{e}_p \end{pmatrix} \in \mathbb{C}^{n+p}$*. Then, we have* $\boldsymbol{X}(1:n, n+p) = \sum_{k=1}^{p} h_i^k \varphi_k(-h_i \boldsymbol{A})\boldsymbol{c}_k$ *and*

$$\boldsymbol{X}\widetilde{\boldsymbol{c}} = e^{h_i \widetilde{\boldsymbol{A}}}\widetilde{\boldsymbol{c}} = \begin{pmatrix} \sum_{k=0}^{p} h_i^k \varphi_k(-h_i \boldsymbol{A})\boldsymbol{c}_k \\ e^{\boldsymbol{J}_p}\boldsymbol{e}_p \end{pmatrix} := \widetilde{\boldsymbol{b}} \in \mathbb{C}^{n+p}.$$

- We are interested in $\widetilde{b}(1:n)$, the rest can be discarded

Remark

The spectrum of $\widetilde{\boldsymbol{A}}$ *is the union of the spectrum of* $-\boldsymbol{A}$ *with the eigenvalue* 0 *with multiplicity* p *independently of the matrix* $\boldsymbol{C}$*.*

Use above results for efficient implementations of exponential integrators!

1. Niesen, Wright use earlier version of Theorem 1 by Sidje for `phipm` [Niesen, Wright, 2012]
2. Gaudreault, Rainwater, Tokman use Theorem 1 for `KIOPS` [Gaudreault, Rainwater, Tokman, 2018]

Common idea:

- Group φ-function terms in exponential integrators and approximate

$$\varphi_0(-h_i\boldsymbol{A})\boldsymbol{c}_0 + h_i\varphi_1(-h_i\boldsymbol{A})\boldsymbol{c}_1 + h_i^2\varphi_2(-h_i\boldsymbol{A})\boldsymbol{c}_2 + \cdots + h_i^p\varphi_p(-h_i\boldsymbol{A})\boldsymbol{c}_p$$

  computing only one matrix exponential via polynomial Krylov methods
- Adaptivity based on error estimate:
  - number of Krylov subspace iterations
  - number of sub-steps in $[t_i, t_{i+1}]$

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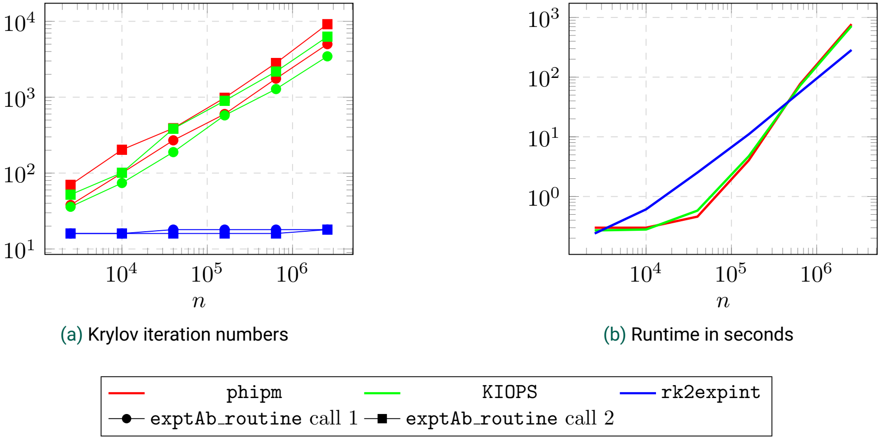
phipm and KIOPS are great! But there is one problem:

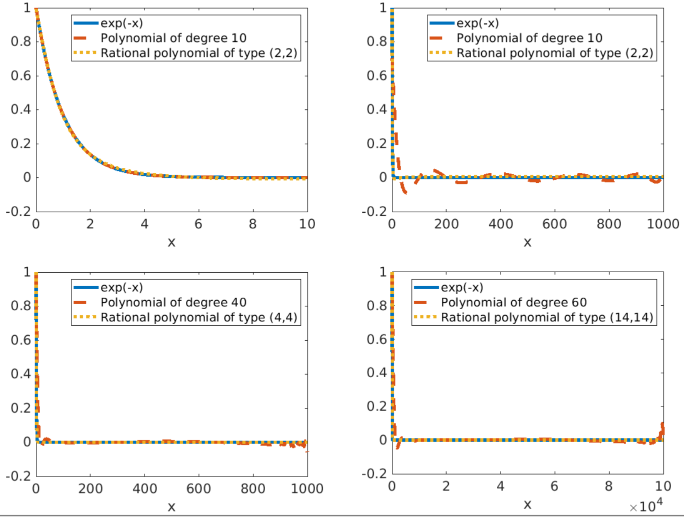


(a) Krylov iteration numbers

(b) Runtime in seconds

Figure: Scaling of 2D Allen–Cahn example

Why this problem? For $\boldsymbol{A} = \boldsymbol{A}^T = \boldsymbol{\Phi}\boldsymbol{\Lambda}\boldsymbol{\Phi}^T \in \mathbb{R}^{n\times n}$, we have $e^{-h_i \boldsymbol{A}} = \boldsymbol{\Phi} e^{-h_i \boldsymbol{\Lambda}} \boldsymbol{\Phi}^T = \sum_{j=1}^{n} e^{-h_i \lambda_j} \phi_j \phi_j^T$.



Rational Krylov subspace methods

- phipm and KIOPS: approximate $f(\widetilde{\boldsymbol{A}})\widetilde{\boldsymbol{c}}$ by projecting the matrix $\widetilde{\boldsymbol{A}}$ onto the polynomial Krylov subspace

$$\mathcal{K}_m(\widetilde{\boldsymbol{A}}, \widetilde{\boldsymbol{c}}) = \text{span}\{\widetilde{\boldsymbol{c}}, \widetilde{\boldsymbol{A}}\widetilde{\boldsymbol{c}}, \ldots, \widetilde{\boldsymbol{A}}^{m-1}\widetilde{\boldsymbol{c}}\}$$

and then use a rational Padé approximation to compute $f(\boldsymbol{H}_m)$.

- Alternative: project $\widetilde{\boldsymbol{A}}$ onto **Rational Krylov (RK) subspace** [Güttel, 2013]

$$\mathcal{Q}_m(\widetilde{\boldsymbol{A}}, \widetilde{\boldsymbol{c}}) = q_{m-1}(\widetilde{\boldsymbol{A}})^{-1}\text{span}\{\widetilde{\boldsymbol{c}}, \widetilde{\boldsymbol{A}}\widetilde{\boldsymbol{c}}, \ldots, \widetilde{\boldsymbol{A}}^{m-1}\widetilde{\boldsymbol{c}}\}$$

with $q_{m-1}(\widetilde{\boldsymbol{A}})$ a matrix polynomial of degree $m-1$, which we assume to be factored as

$$q_{m-1}(z) = \prod_{j=1}^{m-1}(1 - z/\xi_j).$$

  - The $\xi_j \in \mathbb{C} \cup \{\infty\}, j = 1, \ldots, m-1$ are the poles of q_{m-1}
  - We require $0 \neq \xi_j \notin \sigma(\widetilde{\boldsymbol{A}})$ to ensure the invertibility of $q_{m-1}(\widetilde{\boldsymbol{A}})$
  - Special cases:
    - $\xi_1 = \cdots = \xi_{m-1} = \xi$: shift & invert Krylov methods
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- Computation of a basis $\boldsymbol{V}_{m+1}$ of the rational Krylov subspace: Ruhe's rational Arnoldi algorithm [Ruhe, 1994]
  - Set $\boldsymbol{v}_1 = \boldsymbol{b}/\|\boldsymbol{b}\|$
  - Replace $\boldsymbol{x}_{j+1} = \widetilde{\boldsymbol{A}}\boldsymbol{v}_j$
    by $\boldsymbol{x}_{j+1} = (\boldsymbol{I} - \widetilde{\boldsymbol{A}}/\xi_j)^{-1}\widetilde{\boldsymbol{A}}\widetilde{\boldsymbol{v}}_j$
  - Orthonormalize $\boldsymbol{x}_{j+1}$ against $\boldsymbol{v}_1, \ldots, \boldsymbol{v}_j$ to obtain $\boldsymbol{v}_{j+1}$
- More expensive per iteration (linear system solve), but can pay off due to superior approximation quality
- Yields the projection

$$\underline{\boldsymbol{H}_m} = \boldsymbol{V}_{m+1}^T \widetilde{\boldsymbol{A}} \boldsymbol{V}_{m+1} \underline{\boldsymbol{K}_m} \in \mathbb{C}^{(m+1)\times m}$$

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where $\boldsymbol{D}_m = \mathrm{diag}(\xi_1^{-1}, \ldots, \xi_m^{-1})$.
- For $\xi_m = \infty$, this leads to

$$f(\widetilde{\boldsymbol{A}})\widetilde{\boldsymbol{c}} \approx \|\widetilde{\boldsymbol{c}}\|_2 \boldsymbol{V}_m f(\boldsymbol{H}_m \boldsymbol{K}_m^{-1}) \boldsymbol{e}_1.$$

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$$(RK)^2\text{EXPINT} = \texttt{KIOPS} - \mathcal{K}_m(\widetilde{\boldsymbol{A}}, \boldsymbol{b}) + \mathcal{Q}_m(\widetilde{\boldsymbol{A}}, \boldsymbol{b})$$

Implementation: rktoolbox [Berljafa, Elsworth, Güttel, 2014]

Questions:

1. What poles to use?
2. How to solve the linear systems efficiently?
3. When to stop?

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Rational Krylov subspace methods

Pole selection

- Rational best approximation to e^{-x} on $[0,\infty)$: [Cody, Meinardus, Varga, 1969], [Carpenter, Ruttan, Varga, 1984], [Gallopoulos, Saad, 1992]
  - Find
$$r_{d,d}(x) = \frac{p_d(x)}{q_d(x)}, \quad p_d, q_d \in \mathbb{P}_d,$$
    that minimizes
$$\sup_{0 \leq x < \infty} \left| r_{d,d}(x) - e^{-x} \right|.$$
  - Coefficients of optimal p_d and q_d tabulated up to $d = 30$ (at least)
  - Take complex conjugated roots of q_d as poles
  - Roots of q_d have positive and negative real and imaginary parts
- Restriction to real poles leads to a single repeated real pole and shift & invert Krylov methods [Moret, Novati, 2004] [Van Den Eshof, Hochbruck, 2006]
- RKFIT poles of q_d for rational polynomials of type $(m+k, m)$ and finite interval $[0, \lambda_{\max}]$ [Berljafa, Güttel, 2015] [Berljafa, Güttel, 2017]
  - Poles can be restricted to one complex half plane
  - Implemented in the rktoolbox [Berljafa, Elsworth, Güttel, 2014]

- Rational best approximation to e^{-x} on $[0, \infty)$: [Cody, Meinardus, Varga, 1969], [Carpenter, Ruttan, Varga, 1984], [Gallopoulos, Saad, 1992]
  - Find
$$r_{d,d}(x) = \frac{p_d(x)}{q_d(x)}, \quad p_d, q_d \in \mathbb{P}_d,$$
    that minimizes
$$\sup_{0 \leq x < \infty} \left| r_{d,d}(x) - e^{-x} \right|.$$
  - Coefficients of optimal p_d and q_d tabulated up to $d = 30$ (at least)
  - Take complex conjugated roots of q_d as poles
  - Roots of q_d have positive and negative real and imaginary parts
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Rational Krylov subspace methods

Linear system solves

- Linear system solves in rational Arnoldi update (for $\boldsymbol{b}_j := \widetilde{\boldsymbol{A}}\widetilde{\boldsymbol{v}}_j$),

$$\boldsymbol{x}_{j+1} = (\boldsymbol{I} - \widetilde{\boldsymbol{A}}/\xi_j)^{-1}\boldsymbol{b}_j \Leftrightarrow (\boldsymbol{I} - \widetilde{\boldsymbol{A}}/\xi_j)\boldsymbol{x}_{j+1} = \boldsymbol{b}_j \Leftrightarrow (\xi_j\boldsymbol{I} - \widetilde{\boldsymbol{A}})\boldsymbol{x}_{j+1} = \xi_j\boldsymbol{b}_j.$$

- By the definition of $\widetilde{\boldsymbol{A}}$,

$$(\xi_j\boldsymbol{I}_{n+p} - \widetilde{\boldsymbol{A}})\boldsymbol{x}_{j+1} = \begin{bmatrix} \xi_j\boldsymbol{I}_n + \boldsymbol{A} & -\boldsymbol{C} \\ \boldsymbol{0} & \xi_j\boldsymbol{I}_p - \boldsymbol{J}_p \end{bmatrix} \begin{bmatrix} [\boldsymbol{x}_{j+1}]_n \\ [\boldsymbol{x}_{j+1}]_p \end{bmatrix} = \xi_j \begin{bmatrix} [\boldsymbol{b}_j]_n \\ [\boldsymbol{b}_j]_p \end{bmatrix},$$

- As $p \ll n$, we efficiently solve for $[\boldsymbol{x}_{j+1}]_p$ and backsubstitute to obtain

$$(\xi_j\boldsymbol{I}_n + \boldsymbol{A})[\boldsymbol{x}_{j+1}]_n = \xi_j[\boldsymbol{b}_j]_n + \boldsymbol{C}[\boldsymbol{x}_{j+1}]_p.$$

- Since $\boldsymbol{A}$ is pos. semi-def., it helps a lot when ξ_j have positive real parts

2 strategies:

- Direct solvers (LU/Cholesky decomposition)
  - Compute decomposition for each $(\xi_j \boldsymbol{I}_n + \boldsymbol{A})$ (and potentially $(\xi_j \boldsymbol{I}_n + c_j h_i \boldsymbol{A})$), depending on the integrator) upfront
  - Cheaply solve linear systems with factors
  - Very efficient for many time steps
  - Problem size limited by memory requirement
  - Use optimized permutations to avoid fill-in
  - Implementation: Pardiso 6.0 [Petra, Schenk, Anitescu, 2014] [Petra, Schenk, Lubin, Gärtner, 2014]
- Preconditioned iterative solvers (MINRES/GMRES)
  - Unpreconditioned, they suffer from the very issue of increasing polynomial Krylov subspace sizes we try to avoid
  - Use preconditioner $\boldsymbol{P} \approx \boldsymbol{A}$ to solve $\boldsymbol{P}^{-1}\boldsymbol{A}\boldsymbol{x} = \boldsymbol{P}^{-1}\boldsymbol{b} \Leftrightarrow \boldsymbol{P}^{-1}(\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}) = 0$
  - Leads to approximately constant iteration numbers and linear scaling w.r.t. the problem size
  - Algebraic Multigrid (AMG) well-suited if Re$(\xi_j) > 0$
  - Implementation: Aggregation-based multigrid package (AGMG) 3.3.5 [Notay, 2010] [Notay, 2012] [Napov, Notay, 2012]

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Rational Krylov subspace methods

A-posteriori error estimate

- Fun fact: initial Theorem by Saad on computing $\varphi_1(\widetilde{\boldsymbol{A}})\widetilde{\boldsymbol{c}}$ had nothing to do with exponential integrators
- Instead:

Theorem 2 (Saad, 1992)

The error produced by the [polynomial] Arnoldi or Lanczos approximation satisfies the following expansion:

$$e^{\widetilde{\boldsymbol{A}}}\widetilde{\boldsymbol{c}} - \boldsymbol{V}_m e^{\boldsymbol{H}_m}\boldsymbol{e}_1 = h_{m+1,m}\sum_{k=1}^{\infty}\boldsymbol{e}_m^T\varphi_k(\boldsymbol{H}_m)\boldsymbol{e}_1\widetilde{\boldsymbol{A}}^{k-1}\boldsymbol{v}_{m+1},$$

where $\|\widetilde{\boldsymbol{c}}\|_2 = 1.$

Truncation of the sum leads to the practical error estimate

$$\|e^{\widetilde{\boldsymbol{A}}}\widetilde{\boldsymbol{c}} - \boldsymbol{V}_m e^{\boldsymbol{H}_m}\boldsymbol{e}_1\|_2 \approx h_{m+1,m}|\boldsymbol{e}_m^T\varphi_1(\boldsymbol{H}_m)\boldsymbol{e}_1|.$$

- Yields stopping criterion in `KIOPS`.

Rational Krylov relation for $\xi_m = \infty$:

$$\widetilde{\boldsymbol{A}}\boldsymbol{V}_m\boldsymbol{K}_m = \boldsymbol{V}_m\boldsymbol{H}_m + h_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^* \in \mathbb{C}^{n\times m}.$$

Theorem 3 (B., Stoll, 2023)

Let $\xi_m = \infty$. Then the approximation error of the rational Krylov approximation $\|\widetilde{\boldsymbol{c}}\|_2\boldsymbol{V}_m e^{h_i\boldsymbol{H}_m\boldsymbol{K}_m^{-1}}\boldsymbol{e}_1$ to $e^{h_i\widetilde{\boldsymbol{A}}}\widetilde{\boldsymbol{c}}$ reads

$$e^{h_i\widetilde{\boldsymbol{A}}}\widetilde{\boldsymbol{c}} - \|\widetilde{\boldsymbol{c}}\|_2\boldsymbol{V}_m e^{h_i\boldsymbol{H}_m\boldsymbol{K}_m^{-1}}\boldsymbol{e}_1$$
$$= h_i\|\widetilde{\boldsymbol{c}}\|_2 h_{m+1,m}\sum_{k=1}^{\infty}\boldsymbol{e}_m^*\boldsymbol{K}_m^{-1}\varphi_k(h_i\boldsymbol{H}_m\boldsymbol{K}_m^{-1})\boldsymbol{e}_1(h_i\widetilde{\boldsymbol{A}})^{k-1}\boldsymbol{v}_{m+1}.$$

- Truncation of the sum leads to the practical error estimate

$$\|e^{h_i \widetilde{\boldsymbol{A}}}\widetilde{\boldsymbol{c}} - \|\widetilde{\boldsymbol{c}}\|_2 \boldsymbol{V}_m e^{h_i \boldsymbol{H}_m \boldsymbol{K}_m^{-1}} \boldsymbol{e}_1\|_2 \approx h_i \|\widetilde{\boldsymbol{c}}\|_2 h_{m+1,m} \left| \boldsymbol{e}_m^* \boldsymbol{K}_m^{-1} \varphi_1(h_i \boldsymbol{H}_m \boldsymbol{K}_m^{-1}) \boldsymbol{e}_1 \right|$$

- Being experts on the approximation of φ-functions, we know that for

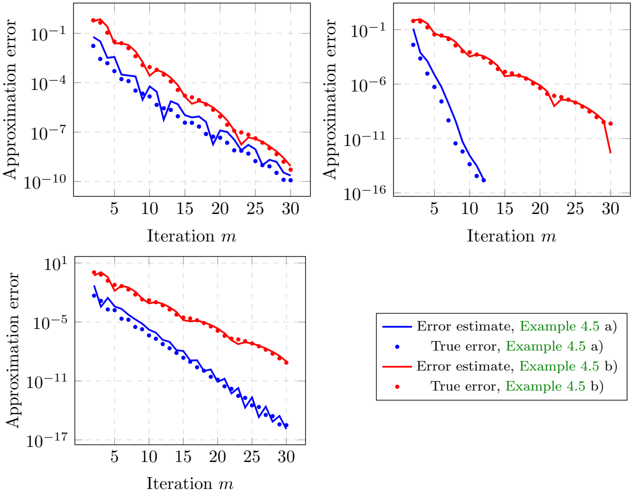
$$\boldsymbol{M}_{m+1} := \begin{bmatrix} \boldsymbol{H}_m \boldsymbol{K}_m^{-1} & \boldsymbol{e}_1 \\ \boldsymbol{0}^T & 0 \end{bmatrix} \in \mathbb{C}^{(m+1)\times(m+1)},$$

we get

$$e^{h_i \boldsymbol{M}_{m+1}} = \begin{bmatrix} e^{h_i \boldsymbol{H}_m \boldsymbol{K}_m^{-1}} & h_i \varphi_1(h_i \boldsymbol{H}_m \boldsymbol{K}_m^{-1}) \boldsymbol{e}_1 \\ \boldsymbol{0}^T & 1 \end{bmatrix}.$$

- Yields stopping criterion for $(RK)^2$EXPINT.

And it works:


Approximation error
10^{-1}
10^{-4}
10^{-7}
10^{-10}
5 10 15 20 25 30
Iteration m
Approximation error
10^{-1}
10^{-6}
10^{-11}
10^{-16}
5 10 15 20 25 30
Iteration m
Approximation error
10^{1}
10^{-5}
10^{-11}
10^{-17}
5 10 15 20 25 30
Iteration m
Error estimate, Example 4.5 a)
True error, Example 4.5 a)
Error estimate, Example 4.5 b)
True error, Example 4.5 b)

Algorithm

Algorithm

Input: $\boldsymbol{A} \in \mathbb{R}^{n\times n}$, Discrete linear differential operator.
$g : [0,T] \times \mathbb{R}^n \to \mathbb{R}^n$, Semi-linear function.
$\boldsymbol{u_0} \in \mathbb{R}^n$, Initial conditions.
$[0,T] \subset \mathbb{R}_{\geq 0}$, Time interval.

Parameters: $h_i \in \mathbb{R}_{>0}$; tol$\in \mathbb{R}_{>0}$; m_min, m_max $\in \mathbb{N}$; $\xi_j \in \mathbb{C}, j = 1, \ldots,$m_max

Subroutines: exp_rk_int, exptAb_routine, linear_system_solver

1: **if** linear_system_solver == *direct* **then**
2: Compute decompositions of $(\xi_j \boldsymbol{I}_n + \boldsymbol{A})$ for $j = 1, \ldots,$m_max
3: **end if**
4: **function** exp_rk_int *% solve* (2.1)
5: **for** every time step **do**
6: **for** each linear combination of φ-functions **do**
7: Assemble $\widetilde{\boldsymbol{A}}$ and $\widetilde{\boldsymbol{c}}$

Algorithm

function `exptAb_routine` *% approximate* $e^{h_i \widetilde{\boldsymbol{A}}} \widetilde{\boldsymbol{c}}$
  while (4.12) $<$ `tol` **do**
    Compute continuation vector $\widetilde{\boldsymbol{v}}_j$ ($\widetilde{\boldsymbol{v}}_j = \boldsymbol{v}_j$ if not `rk2expint`)
    Compute $\boldsymbol{b}_j = \widetilde{\boldsymbol{A}} \widetilde{\boldsymbol{v}}_j$
    if `exptAb_routine` $==$ `rk2expint` $\&\&$ $j <$ `m_max` **then**
      if `linear_system_solver` $==$ *direct* **then**
        Solve (4.4) with back-subst. and the decomposition of $(\xi_j \boldsymbol{I}_n + \boldsymbol{A})$
      else if `linear_system_solver` $==$ *iterative* **then**
        Setup AGMG hierarchy for $(\xi_j \boldsymbol{I}_n + \boldsymbol{A})$
        Solve (4.4) with back-subst. and iterative AGMG solver
      end if
    end if
    Extend Krylov decomposition, i.e, $\boldsymbol{V}_m$, $\boldsymbol{H}_m$ (and $\boldsymbol{K}_m$ if `rk2expint`)
    Compute $\|\widetilde{\boldsymbol{c}}\|_2 \boldsymbol{V}_m e^{h_i \boldsymbol{H}_m \boldsymbol{K}_m^{-1}} \boldsymbol{e}_1$
  end while
end `exptAb_routine`
end for
Update solution $\boldsymbol{u}$ for current time step according to (3.2)–(3.4)
end for
end `exp_rk_int`

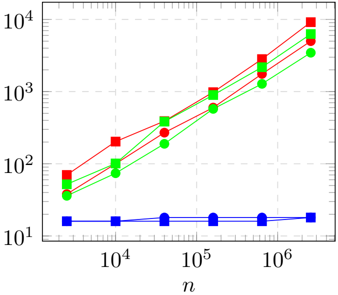
Output: $\boldsymbol{u} \in \mathbb{R}^{n \times n_t}$ Trajectory of the solution of (2.1) along the n_t time steps.

Numerical experiments

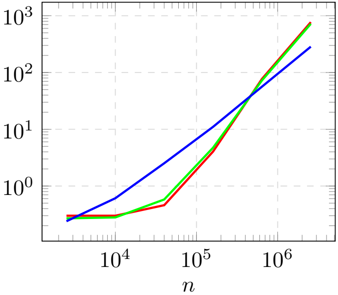
Numerical experiments

2D Allen–Cahn

$$\frac{\partial u}{\partial t} = \epsilon^2 \Delta u + u - u^3, \quad \epsilon \in \mathbb{R}.$$



(a) Krylov iteration numbers



(b) Runtime in seconds

phipm KIOPS rk2expint
exptAb_routine call 1 exptAb_routine call 2

Figure: Scaling of 2D Allen–Cahn example.

Numerical experiments

2D Gierer–Meinhardt

Gierer–Meinhardt equations

$$\frac{\partial a}{\partial t} = D_a \Delta a + p\frac{a^2}{h} - \mu a,$$
$$\frac{\partial h}{\partial t} = D_h \Delta h + p' a^2 - \nu h, \qquad D_a, D_h, p, p', \mu, \nu \in \mathbb{R}.$$

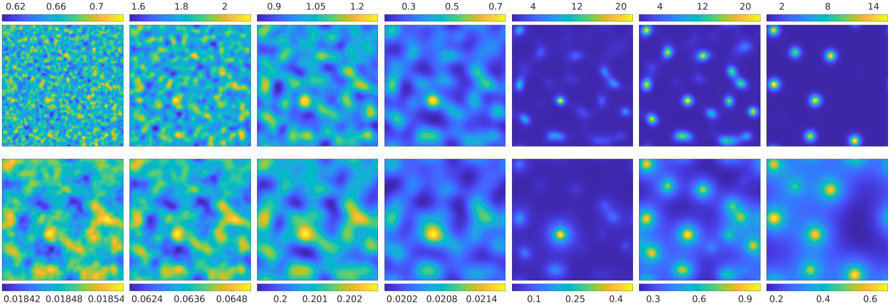
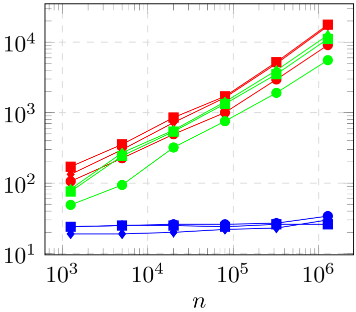
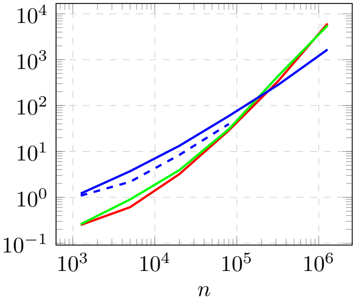


Figure: Example solution in 2D.



(a) Krylov iteration numbers



(b) Runtime in seconds

phipm KIOPS rk2expint iterative rk2expint direct
exptAb_r. call 1 exptAb_r. call 2 exptAb_r. call 3

Figure: Scaling of 2D Gierer–Meinhardt example.

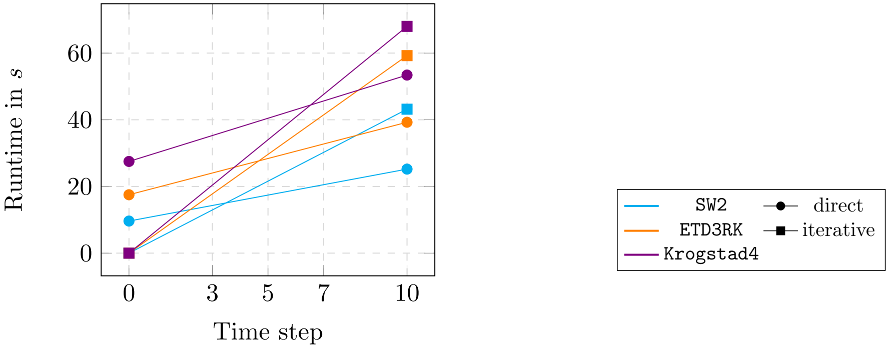


Figure: Comparison of direct and preconditioned iterative solvers.

Numerical experiments

Allen–Cahn on networks

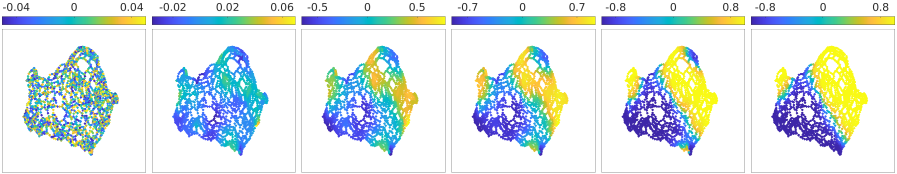


Figure: Example solution on *minnesota* network.

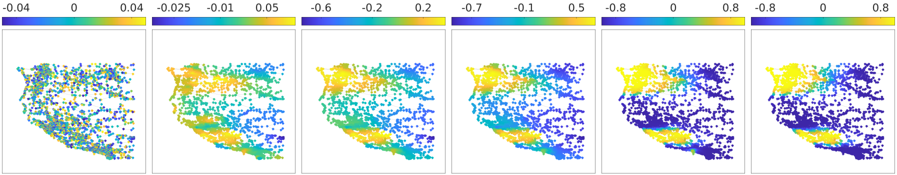
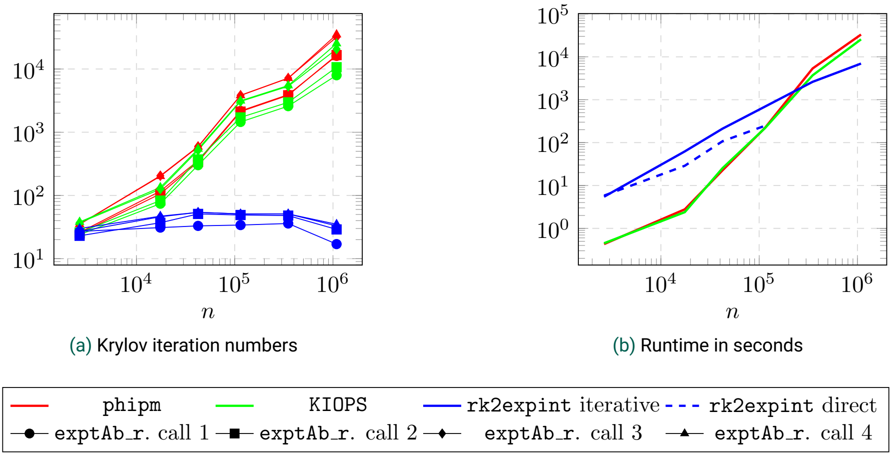


Figure: Example solution on *US roads (subset)* network.



(a) Krylov iteration numbers

(b) Runtime in seconds

Figure: Scaling of Allen–Cahn on networks.

Conclusion

- We applied adaptive rational Krylov subspace methods to the efficient evaluation of exponential Runge–Kutta integrators.
- This required
  - Optimal pole selection
  - Efficient solution of the sequences of shifted linear systems
  - An a-posteriori error estimate to rational Krylov approximations of $e^{h_i \widetilde{A}} \widetilde{c}$
- It enables
  - constant rat. Krylov iteration numbers w.r.t. the problem size (spectral radius of the discrete linear differential operator A)
  - a near-linear scaling of the runtime
  - runtime gains for sufficiently large spectral radii of A
- Left for later:
  - (Sensible) Application to multilayer networks
  - Nonsymmetric problems, e.g., including advection
  - General right-hand sides (exp. Rosenbrock/EPIRK methods)

K. B., M. Stoll (2023). **Adaptive rational Krylov methods for exponential Runge–Kutta integrators**. *arXiv Preprint*. arXiv:2303.09482

Thanks for your attention!

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