Rational approximation to trigonometric matrix operators

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Outline

Matrix exponential operator

assumptions

- A symmetric, positive definite with large $\|A\|$
- $\tau > 0$ step size

Krylov approximation:

$$\exp(-\tau A)v \approx \|v\|\, V_m \exp(-\tau T_m) e_1, \quad \mathcal{R}(V_m) = \mathcal{K}_m(A, v)$$

rational (preconditioned) version:

$$\exp(-\tau A)v \approx \|v\|\, V_m \exp(-\tau \widetilde{T}_m) e_1, \quad \mathcal{R}(V_m) = \mathcal{K}_m((I + \gamma A)^{-1}, v)$$

Moret, Novati; Lopez, Simoncini; van den Eshof, H.

Exponential vs. trigonometric operators

convergence of approximations to matrix exponential $\exp(-\tau A)v$:

	standard	rational
convergence	superlinear	sublinear
steps required	$\geq \|\tau A\|^{1/2}$	independent of $\|\tau A\|$

trigonometric operators: $\cos(\tau A)$, $\sin(\tau A)$, $\exp(i\tau A)$, ...

- no exponential decay
- function oscillatory, largest frequency $\sim \|\tau A\|$
- convergence uniform in $\|\tau A\|$ cannot be expected
- need to take origin of problem into account

Application: wave equation

$$u'' = -Au + g(u), \qquad u(0) = u_0,\ u'(0) = u_0'$$

($g \equiv 0$ for this talk)

exact solution satisfies

$$u(t+\tau) = \cos\tau\sqrt{A}\,u(t) + (\sqrt{A})^{-1}\sin\tau\sqrt{A}\,u'(t)$$

questions

- function spaces?
- existence of solutions?

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general: Gautschi-type exponential integrators

Fundamentals: Hilbert scales

- A selfadjoint, positive operator with bounded resolvent
- then: A has orthonormal set of eigenvectors $e_i \in H$ (Hilbert space), with eigenvalues $\lambda_i \geq 0$, $i = 1, 2, \ldots$
- fractional powers A^α defined on appropriate domains:

$$\mathcal{D}(A^\alpha) := \left\{ x = \sum_{i=1}^{\infty} \mu_i e_i \in H \;\middle|\; \sum_{k=1}^{\infty} |\lambda_i|^{2\alpha} |\mu_i|^2 < \infty \right\}$$
$$= \{x \mid \|A^\alpha x\| < \infty\}$$

- $f(A)x$ for f analytic on $[0, \infty)$ defined via

$$f(A)x := \sum_{i=1}^{\infty} f(\lambda_i)\mu_i e_i, \qquad x = \sum_{i=1}^{\infty} \mu_i e_i \in H$$

$Au = -\Delta u$: $H = L^2(\Omega)$, $\mathcal{D}(\sqrt{A}) = H^1(\Omega)$, $\mathcal{D}(A) = H^2(\Omega)$

Homogeneous wave equations: theory

$$u''(t) = -Au(t), \qquad u(0) = u_0, \quad u'(0) = u'_0$$

	smooth data	nonsmooth data
u_0	$\mathcal{D}(A)$	$V = \mathcal{D}(\sqrt{A})$
u'_0	$V = \mathcal{D}(\sqrt{A})$	H
$u(t)$	$C^2(\mathbb{R}^+, H) \cap C^1(\mathbb{R}^+, V)$	$C^1(\mathbb{R}^+, H) \cap C^0(\mathbb{R}^+, V)$
type	strong solution $u''(t) = -Au(t)$	weak solution $(u''(t), v) = a(u(t), v)$ for all $v \in V$

$$\mathcal{D}(A^\alpha) = \{x \in H \mid \|A^\alpha x\| < \infty\}$$

How to exploit these properties?

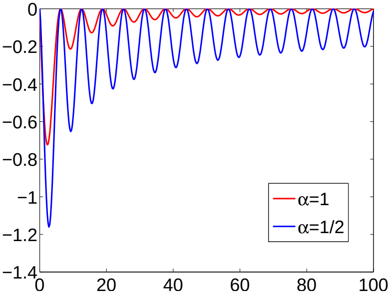
for $\alpha \in (0,1]$ and $v \in \mathcal{D}(A^\alpha)$ write

$$f(x) = \frac{f(x) - f(0)}{x^\alpha} x^\alpha + f(0)$$

then

$$f(A)v = g(A)A^\alpha v + f(0)v, \qquad g(x) = \frac{f(x) - f(0)}{x^\alpha}$$

in this talk:
$f(x) = \cos(\sqrt{x})$
$x \geq 0$
$0 < \alpha \leq 1$



Rational (preconditioned) Krylov methods

$$(I + \gamma A)^{-1} V_m = V_m T_m + \beta_m v_{m+1} e_m^T, \qquad \beta v_1 = A^\alpha v$$

for $t \in (0, 1]$ define

$$g_{\gamma,\alpha}^{\tau}(t) = \frac{\cos\sqrt{\phi_{\tau,\gamma}(t)} - 1}{\left(\phi_{\tau,\gamma}(t)\right)^{\alpha}} \qquad \phi_{\tau,\gamma}(t) = \left(\frac{1}{t} - 1\right)\frac{\tau^2}{\gamma}$$

g s.t.

$$\tau^{2\alpha} g_{\gamma,\alpha}^{\tau}\left((I + \gamma A)^{-1}\right) = \frac{\cos(\tau\sqrt{A}) - 1}{A^\alpha}$$

approximation

$$y(\tau) = \cos(\tau\sqrt{A})v \approx y_m^\alpha(\tau) = \tau^{2\alpha}\beta V_m g_{\gamma,\alpha}^{\tau}(T_m)e_1 + v$$

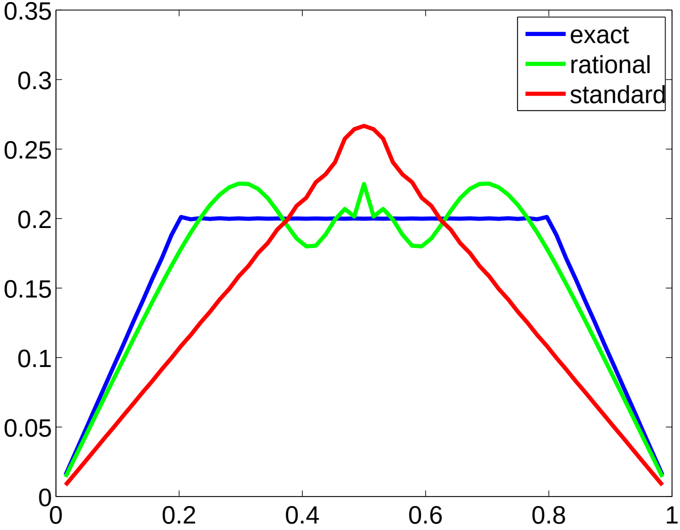
Error bounds

Theorem

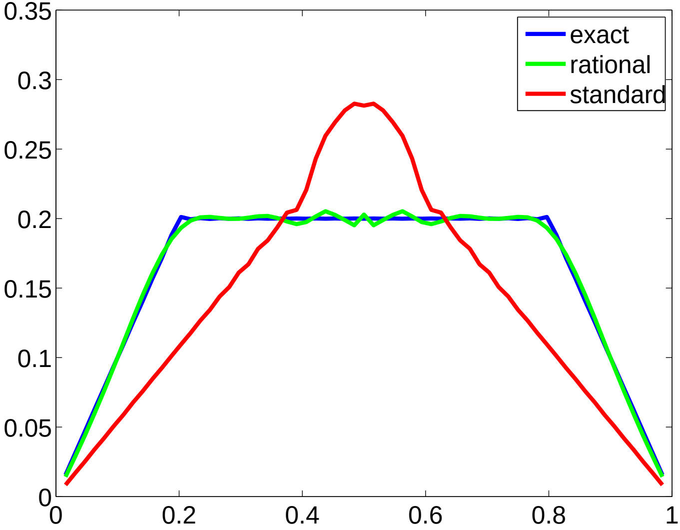
$$\|y_m^{\frac{1}{2}}(\tau) - \cos(\tau\sqrt{A})v\| \leq \frac{C}{m^{1/4}}\tau \, \|\sqrt{A}v\|, \qquad v \in \mathcal{D}(\sqrt{A})$$

$$\|y_m^{1}(\tau) - \cos(\tau\sqrt{A})v\| \leq \frac{C}{m^{1/2}}\tau^2 \, \|Av\|, \qquad v \in \mathcal{D}(A)$$

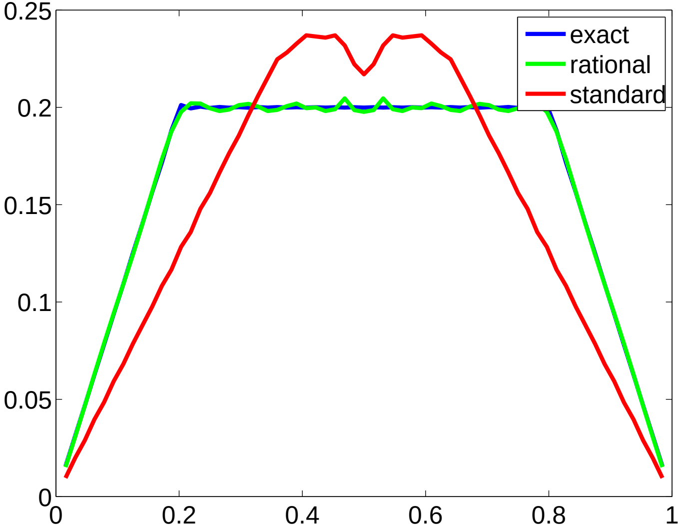
5 steps, $u_0 \in \mathcal{D}(\sqrt{A})$, $\tau = 0.3$, $N = 63$



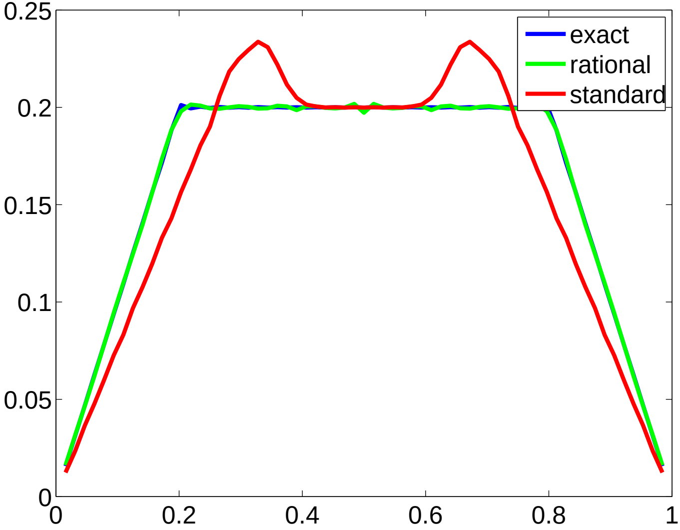
10 steps, $u_0 \in \mathcal{D}(\sqrt{A})$, $\tau = 0.3$, $N = 63$



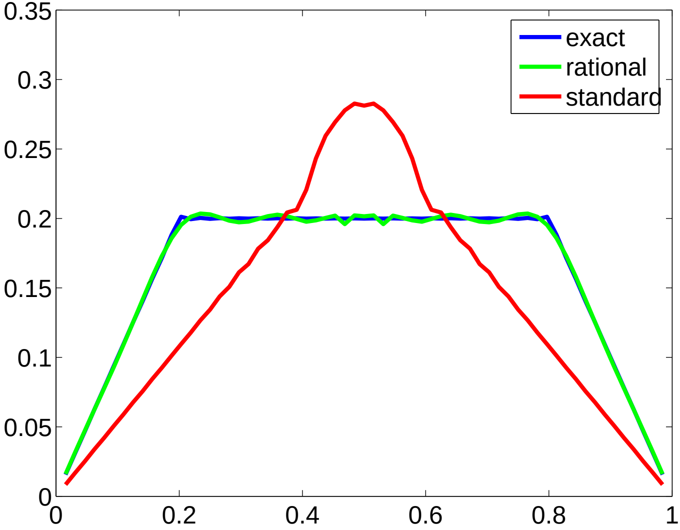
15 steps, $u_0 \in \mathcal{D}(\sqrt{A})$, $\tau = 0.3$, $N = 63$



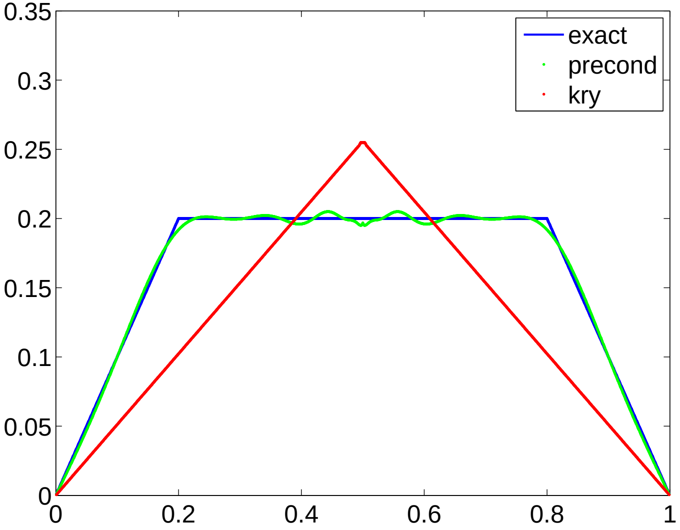
20 steps, $u_0 \in \mathcal{D}(\sqrt{A})$, $\tau = 0.3$, $N = 63$



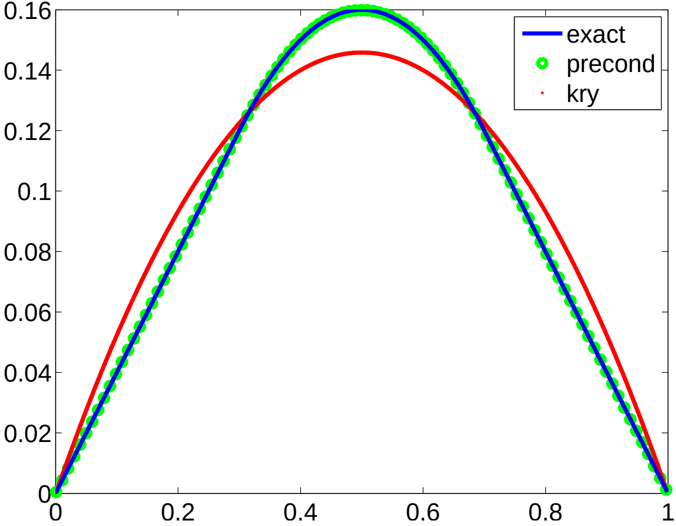
25 steps, $u_0 \in \mathcal{D}(\sqrt{A})$, $\tau = 0.3$, $N = 63$



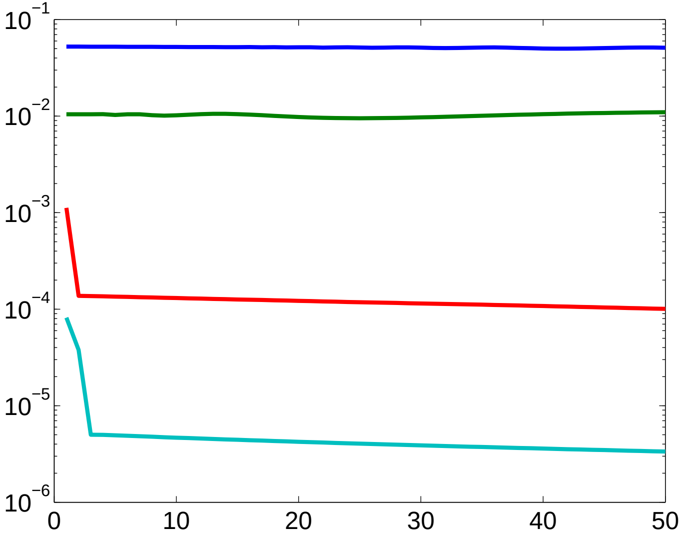
10 steps, $u_0 \in \mathcal{D}(\sqrt{A})$, $\tau = 0.3$, $N = 1023$



10 steps, $u_0 \in \mathcal{D}(A)$, $\tau = 0.3$, $N = 1023$

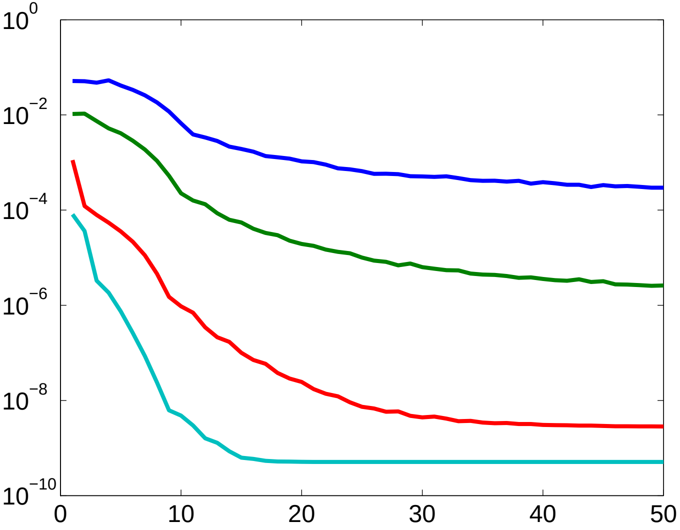


Convergence vs. smoothness of u_0, standard Krylov



$u_0 \in \mathcal{D}(A^{1/2})$, $\mathcal{D}(A)$, $\mathcal{D}(A^2)$, $\mathcal{D}(A^4)$

Convergence vs. smoothness of u_0, rational Krylov



$u_0 \in \mathcal{D}(A^{1/2})$, $\mathcal{D}(A)$, $\mathcal{D}(A^2)$, $\mathcal{D}(A^4)$

Galerkin approximation / implementation

finite element discretization

$$My'' + Ay = 0, \qquad y(0) = y_0, \qquad y'(0) = y_0',$$

mass matrix $M = M_h$, stiffness matrix $A = A_h$

transformation $z = M^{\frac{1}{2}} y$ leads to

$$z'' + \widetilde{A}z = 0, \qquad z(0) = M^{\frac{1}{2}} y_0, \qquad z'(0) = M^{\frac{1}{2}} y_0'$$

with $\widetilde{A} = M^{-\frac{1}{2}} A M^{-\frac{1}{2}}$

standard vs. rational approximation

standard Lanczos:

$$AV_m = MV_m T_m + \beta_m v_{m+1} e_m^T, \qquad V_m^T M V_m = I_m,$$

per step:

- one decomposition / solve with M
- one matrix-vector multiplication with A

rational Lanczos:

$$(M + \gamma A)^{-1} M V_m = V_m T_m + \beta_m z_{m+1} e_m^T, \qquad V_m^T M V_m = I_m,$$

per step:

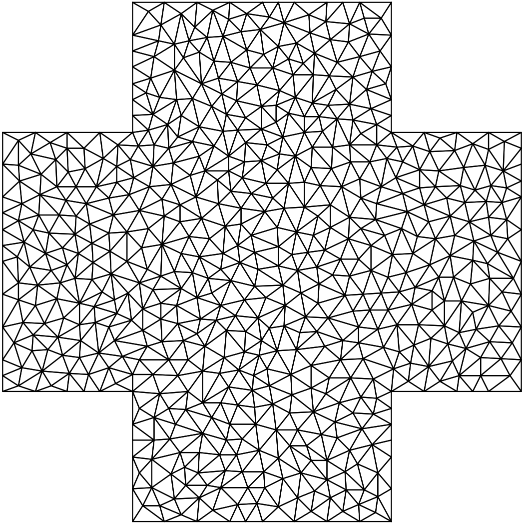
- one decomposition / solve with $M + \gamma A$

Rational Lanczos method

to compute a basis of $K_m(I + \gamma\widetilde{A})^{-1}, Ay_0)$

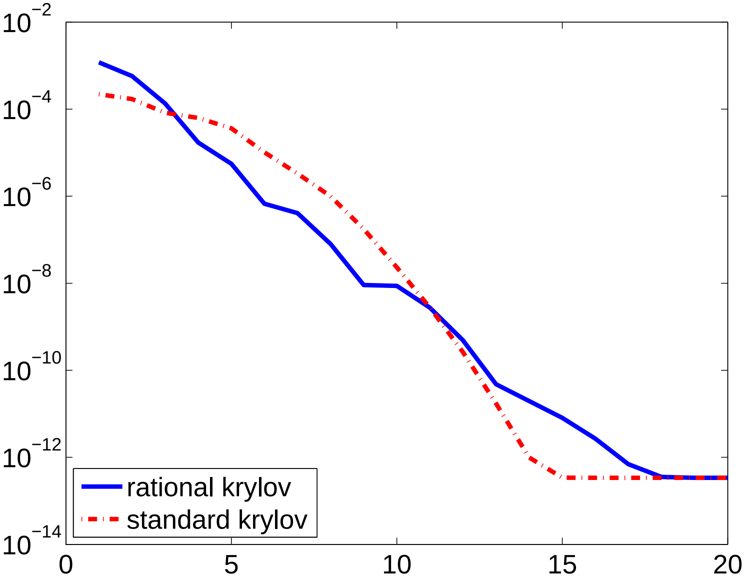
$$
\begin{aligned}
& v = M^{-1}Ay_0,\ \ w = Mv,\ \ \beta = \sqrt{v^H w} > 0; \\
& v_1 = v/\beta,\ \ w_1 = w/\beta \\
& \textbf{for } m = 1, 2, \ldots \textbf{ do} \\
& \quad t_{m-1,m} = \overline{t_{m,m-1}} \\
& \quad z_m = (M + \gamma\tau^2 A)^{-1} w_m \\
& \quad t_{m,m} = w_m^H z_m \\
& \quad \tilde{v}_{m+1} = z_m - t_{m,m} v_m - t_{m-1,m} v_{m-1} \\
& \quad \tilde{w}_{m+1} = M\tilde{v}_{m+1} \\
& \quad t_{m+1,m} = \sqrt{\tilde{v}_{m+1}^H \tilde{w}_{m+1}} \\
& \quad v_{m+1} = \tilde{v}_{m+1}/t_{m+1,m},\ \ w_{m+1} = \tilde{w}_{m+1}/t_{m+1,m} \\
& \textbf{end for}
\end{aligned}
$$

Example: wave equation

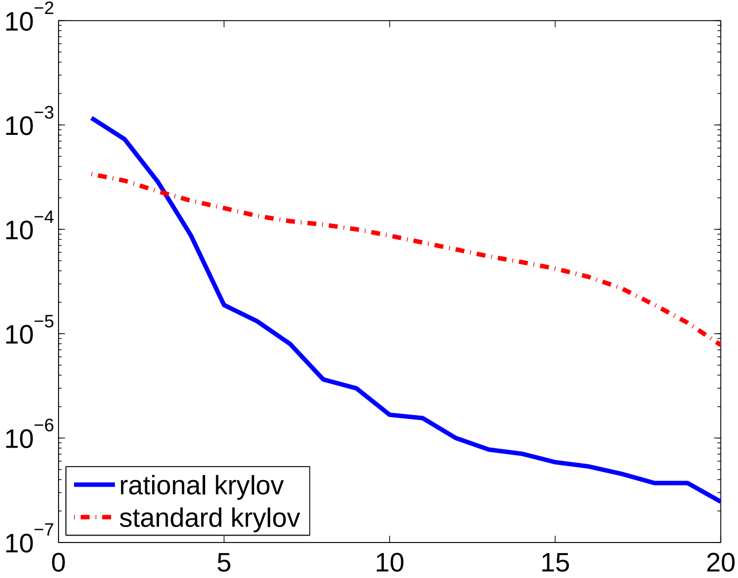


refined twice,
dimension $\sim 5 \cdot 10^5$

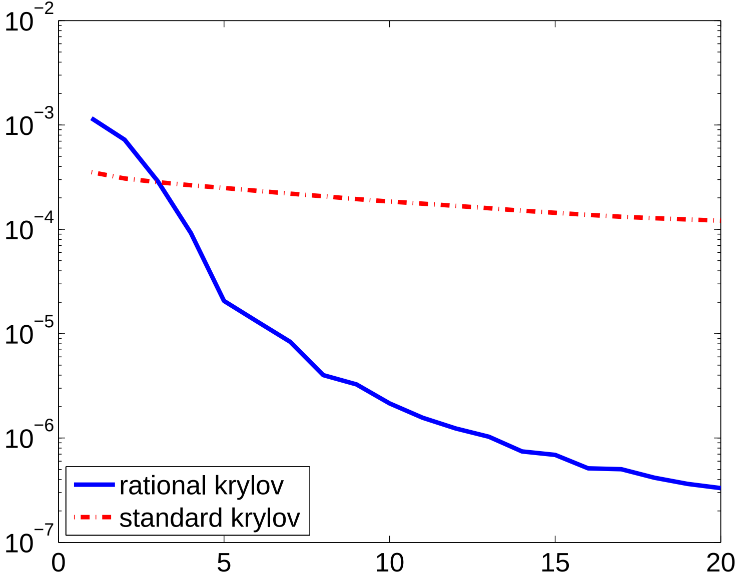
Errors, $\tau = 0.3$, coarse grid, 43 nodes



Errors, $\tau = 0.3$, coarse grid, 546 nodes



Errors, $\tau = 0.3$, coarse grid, 5.723 nodes



Summary

- grid independent approximation to trigonometric operators like $\cos(\tau\sqrt{A})v$ under reasonable assumptions on v
- applies to finite element discretizations on arbitrary (e.g. locally refined) grids
- general domains
- application: exponential integrators for Schrödinger and wave equations (time integration error independent of spatial discretization), removes CFL condition

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Reference: Grimm, H., submitted to BIT, avaible on
`www.am.uni-duesseldorf.de`