Master Thesis

Matrix-free Leja based exponential integrators in Python

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February 16, 2020

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Abstract

1 Introduction

Consider the action of the matrix exponential function

$$e^A v, \quad A \in \mathbb{C}^{N\times N}, v \in \mathbb{C}^N.$$

Due to computational constraints it can be difficult or impossible to compute e^A in a first step and then the action $e^A v$ in a separate step. This is especially true in applications where $N > 10000$ is not uncommon. Furthermore the matrix exponential of a sparse matrix is in general no longer sparse. Therefore it is more feasible to compute the action of the matrix exponential in a single step. This can be done by approximating the matrix exponential with a matrix polynomial p_m of degree m in A

$$e^A v \approx p_m(A)v.$$

This approach has many advantages. The cost of the computation of $p_m(A)v$ mainly depends on the calculation of m matrix-vector multiplications with A. Furthermore the explicit knowledge of A itself is no longer required. A can be replaced by a linear operator, which can be more convenient and save memory.

2 The Leja method

This section serves as an introduction to the Leja method for approximating the action of the exponential function. All proofs can be found in a more general form in either [4] or [5].

2.1 Leja interpolation

Let $K \in \mathbb{C}$ be a compact set in the complex plane and $\xi_0 \in K$ be arbitrary. The sequence $(\xi_k)_{k=0}^{\infty}$ recursively defined as

$$\xi_k = \arg\max_{\xi\in K} \prod_{j=0}^{k-1} |\xi - \xi_j|$$

is called a Leja sequence. Due to the maximum principle all elements in the sequence realize their maximum on the border ∂K. Typically ξ_0 is also chosen on ∂K.
For analytical functions $f\colon K \to \mathbb{C}$ the Newton interpolation polynomial p_m with nodes $(\xi_k)_{k=0}^{m}$ has the following beneficial properties.

Convergence properties: The sequence $(p_m)_{m=0}^{\infty}$ converges maximally to f. That is, let $(p_m^*)_{m=0}^{\infty}$ be the best uniform approximation polynomials for f in K. Then

$$\limsup_{m\to\infty} \|f - p_m\|_K^{1/m} = \limsup_{m\to\infty} \|f - p_m^*\|_K^{1/m},$$

where $\|\cdot\|_K$ is the maximum norm on K. Furthermore if f is an entire function, then $(p_m)_{m=0}^{\infty}$ converges superlinearly to f

$$\limsup_{m\to\infty} \|f - p_m\|_{\mathbb{C}}^{1/m} = \limsup_{m\to\infty} \|f - p_m^*\|_{\mathbb{C}}^{1/m} = 0.$$

For entire functions f the corresponding matrix polynomials achieves similar superlinear convergence

$$\limsup_{m\to\infty} \|f(A)v - p_m(A)v\|_2^{1/m} = 0,$$

for $A \in \mathbb{C}^{n\times n}, v \in \mathbb{C}^n$.

Early termination: The Newton interpolation polynomial p_m can be constructed iteratively since the corresponding Leja interpolation points $(\xi_k)_{k=0}^{m}$ are defined recursively. Therefore if the approximation $p_n \approx f$ is accurate enough after $n < m$ steps the interpolation can be stopped early to reduce the cost of the interpolation. Note that this is not possible with Chebyshev nodes.

Leja sequence can be stored: For a given K the Leja interpolation nodes only need to be computed once and for all. These values can be stored a priori and loaded once they are needed for the interpolation. If f is fixed the same is also true for the corresponding divided differences.

In summary the Leja points offer convergence properties similar to Chebyshev nodes for interpolation, while having computational advantages. All results hold true for the corresponding matrix interpolation polynomials.

2.2 Approximating the matrix exponential function:

Inspired by the previous subsection we try to find a low-cost approximation of the action of the matrix exponential $e^A v$ using Leja interpolation polynomials. From now on, we will fix

$$K = [-c, c], \quad f = e^{\cdot} \quad \text{and} \quad \xi_0 = c$$

for $c > 0$. With $L_{m,c}$ we denote the Leja interpolation polynomial on the interval $[-c, c]$ with Leja points $(\xi_j)_{j=0}^{m}$. We use the well-known property of the exponential function

$$e^A v = (e^{s^{-1}A})^s v, \quad \text{with} \quad s \in \mathbb{N}.$$

Now we can approximate the action of the matrix exponential in s substeps

$$v_0 := v, \quad v_{j+1} := L_{m,c}(s^{-1}A)v_j, \quad \text{and} \quad v_s \approx e^A v.$$

m	5	10	15	20	25	30	35
half	6.43e-01	2.12e+00	3.55e+00	5.00e+00	6.37e+00	7.51e+00	8.91e+00
single	9.62e-02	8.33e-01	1.96e+00	3.26e+00	4.69e+00	5.96e+00	7.44e+00
double	1.74e-03	1.14e-01	5.31e-01	1.23e+00	2.16e+00	3.18e+00	4.34e+00

m	40	45	50	55	60	65	70
half	1.00e+01	1.10e+01	1.23e+01	1.35e+01	1.48e+01	1.59e+01	1.71e+01
single	8.71e+00	1.00e+01	1.15e+01	1.27e+01	1.40e+01	1.52e+01	1.64e+01
double	5.48e+00	6.67e+00	7.99e+00	9.24e+00	1.06e+01	1.18e+01	1.32e+01

m	75	80	85	90	95	100
half	1.84e+01	1.94e+01	2.07e+01	2.20e+01	2.30e+01	2.42e+01
single	1.76e+01	1.87e+01	1.99e+01	2.12e+01	2.23e+01	2.35e+01
double	1.46e+01	1.58e+01	1.71e+01	1.86e+01	1.99e+01	2.13e+01

Table 1: Samples of the precomputed values θ_m. The backward error of the Leja interpolation is bounded if $c \leq \theta_m$, where $[-c, c]$ is the interpolation interval and m the interpolation degree. Half, single and double correspond to the tolerances 2^{-10}, 2^{-24} and 2^{-53} respectively [5, Table 1].

So far we placed no restrictions on m, s and c. We choose optimal parameters based on the backward-error analysis done in [5].

Bounding the backward error For a given matrix A we interpret the Leja interpolation polynomial as the exact solution of a perturbed matrix exponential function

$$L_{m,c}(s^{-1}A)^s v =: e^{A+\Delta A} v$$

Our goal is to bound the backward error

$$\frac{\|\Delta A\|}{\|A\|} \leq \text{tol},$$

for a given tolerance tol. Furthermore we want to minimize the cost of the interpolation. A priori it is unclear for which values m, s and c the inequality is satisfied. The authors of [5] conducted a backward error analysis and chose an approach which favors normal matrices. For various tolerances tol they precomputed values θ_m 1 which satisfy

$$\text{If } \|s^{-1}A\| \leq \theta_m \text{ and } 0 < c \leq \theta_m \text{ then } \frac{\|\Delta A\|}{\|A\|} \leq \text{tol}\,.$$

For our purposes it is important to note that the optimal choice for c is given by $c = \rho(s^{-1}A)$, where $\rho(A)$ is the spectral radius of A. However, computing $\rho(A)$ introduces additional costs for the algorithms proposed in [5]. Our matrix-free implementation relies on the computations of the spectral radius, but it does not need to compute the matrix norm $\|A\|$, see section 3.

Choosing cost-minimizing parameters The cost of the Leja interpolation mainly depends on the the number of matrix-vector products

$$C_m = sm.$$

In order to minimize the costs of the interpolation C_m we select the smallest m for any given s such that

$$\|s^{-1}A\| \leq \theta_m$$

is satisfied. This leads to the optimal choice for m and s

$$m_* = \underset{2\leq m\leq m_{\max}}{\arg\min} \left\{ \left\lceil \frac{\|A\|}{\theta_m} \right\rceil m \right\}, \quad s_* = \left\lceil \frac{\|A\|}{\theta_m} \right\rceil.$$

In our algorithm we set $m_{\max} = 100$ in order to avoid over- and underflow errors.

Shifting the matrix The cost of the interpolation can be decreased by employing a shift $\mu \in \mathbb{C}$. Let I be the identity matrix. We replace the matrix A with $A - \mu I$ for all computations. If the shifted matrix $A - \mu I$ satisfies $\|A - \mu I\| < \|A\|$ then the cost C_{m_*} of the interpolation decreases. We compensate for the shift by multiplying with e^{μ} since

$$e^A = e^{\mu} e^{A-\mu I}.$$

A well-chosen shift centers the eigenvalues of $A - \mu I$ around 0. Such a shift can be found by using Gerschgorin's circle theorem. This is, however, not possible in the matrix-free case.

3 Matrix-free implementation

For matrix-free linear operators it can be expensive to compute the matrix norm $\|A\|$. We will circumvent this problem by replacing $\|A\|$ with the spectral radius $\rho(A)$.

The backward error analysis in [5] holds true for every matrix norm. We use a well-known result from the matrix analysis literature [11, Lemma 5.6.10.]. For every A and for every $\varepsilon > 0$ exists an induced matrix norm $\|\cdot\|_{A,\varepsilon}$ such that

$$\rho(A) \leq \|A\|_{A,\varepsilon} \leq \rho(A) + \varepsilon.$$

The first inequality holds true for every matrix norm. We choose ε small enough, such that

$$\|s^{-1}A\|_{A,\varepsilon} \leq \min_{\rho(s^{-1}A)<\theta_m} \theta_m.$$

For this choice of $\|\cdot\|_{A,\varepsilon}$ the cost-minimizing parameters are given by

$$m_* = \underset{2\leq m\leq m_{\max}}{\arg\min} \left\{ \left\lceil \frac{\rho(A)}{\theta_m} \right\rceil m \right\}, \quad s_* = \left\lceil \frac{\rho(A)}{\theta_m} \right\rceil.$$

The explicit knowledge of $\|\cdot\|_{A,\varepsilon}$ is no longer required. Additionally we can choose $c = \rho(A)$ without introducing additional costs, since we have to compute $\rho(A)$ to determine m_* and s_*. For positive and negative semi-definite operators A we can choose the shift $\mu = -\rho(A)/2$ and $\mu = \rho(A)/2$ respectively. This shift works particularly well if the absolutely smallest eigenvalue of A is close to 0.
This approach has some drawbacks though. While we are able to bound the backward error

$$\frac{\|\Delta A\|_{A,\varepsilon}}{\|A\|_{A,\varepsilon}} \leq \text{tol}$$

we can no longer specify in which norm this error has to be bound. Furthermore, it is hard to find a good shift μ for non-semi-definite operators.
The spectral radius $\rho(A)$ can be cheaply approximated using the power iteration algorithm. However, this procedure underestimates the largest eigenvalue. Therefore we have to compensate for that by multiplying the estimate with a safety factor.

From now on we denote the Leja method for the matrix exponential function as `expleja`. Depending on the chosen tolerance 1 we will refer to the algorithm as half, single or double precision `expleja` respectively.

4 Linear advection-diffusion equation

Consider the one-dimensional advection-diffusion equation

$$\begin{aligned} \partial_t u &= a\partial_{xx} u + b\partial_x u \quad \text{with} \quad a, b \geq 0 \quad \text{and} \\ u_0(t) &= e^{-80\cdot(t-0{,}45)^2} \quad \text{with} \quad t \in [0, 0.1] \end{aligned}$$

on the domain $\Omega = [0, 1]$. For a fixed $N \in \mathbb{N}$ we approximate the diffusive part of the differential equation with second-order central differences on an equidistant grid with grid size $h = \frac{1}{N-1}$ and grid points $x_k = kh$, $k = 0 \ldots, N-1$

$$\partial_{xx} u(x_k) = \frac{u(x_{k+1}) - 2u(x_k) + u(x_{k-1})}{h^2} + \mathcal{O}(h^2).$$

In order to avoid numerical instabilities we discretize the advective part with forward differences, similar to the upwind scheme

$$\partial_x u(x_k) = \frac{u(x_{k+1}) - u(x_k)}{h} + \mathcal{O}(h).$$

The resulting system of ordinary differential equation is given by

$$\partial_t u = Au.$$

In order to measure the stiffness of the differential equation we employ the Péclet number $\text{Pe} = \frac{b}{a}$. The Péclet number is a dimensionless quantities representing the ratio of the advective velocity b to the diffusive velocity a.
The solution of the differential equation is given by $e^{0.1A}u_0$, which can be approximated using the Leja method 1. For the matrix-free case we need to compute the spectral radius of A, which can be done using the power method.

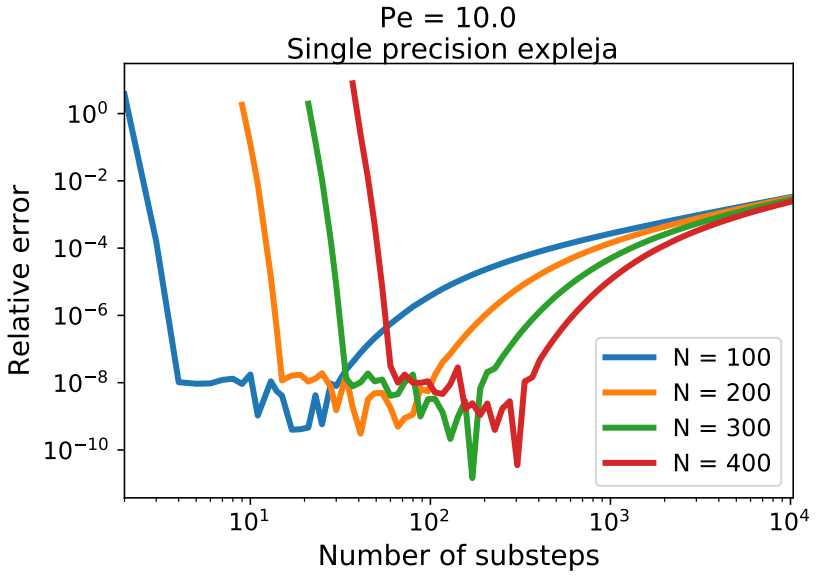


Figure 1: Approximation of $e^{0.1A}u_0$ using single precision `expleja` for a fixed interpolation degree $m = 100$ and varying number of substeps s. The relative error is measured in the Eucledian norm. The reference solution was computed using the double precision `expleja` algorithm.

4.1 Power iteration analysis

In this section we investigate the rate of convergence of the power method to the absolutely largest eigenvalue λ_{max} of A. For our analysis we assume periodic boundary conditions

$$A = \frac{a}{h^2}\begin{bmatrix} -2 & 1 & 0 & \cdots & 0 & 1 \\ 1 & -2 & 1 & & & 0 \\ 0 & 1 & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & 1 & 0 \\ 0 & & & 1 & -2 & 1 \\ 1 & 0 & \cdots & 0 & 1 & -2 \end{bmatrix} + \frac{b}{h}\begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 1 \\ 0 & -1 & 1 & & & 0 \\ \vdots & 0 & \ddots & \ddots & & \vdots \\ \vdots & & \ddots & \ddots & 1 & 0 \\ 0 & & & 0 & -1 & 1 \\ 1 & 0 & \cdots & \cdots & 0 & -1 \end{bmatrix}.$$

Consider the discrete Fourier basis

$$v_j = \frac{1}{\sqrt{N}}\begin{bmatrix} e^{i\frac{2\pi}{N}j0} \\ e^{i\frac{2\pi}{N}j1} \\ \vdots \\ e^{i\frac{2\pi}{N}j(N-1)} \end{bmatrix}, \quad j \in 0 \ldots N-1.$$

Each v_j is an eigenvector of A

$$Av_j = \lambda_j v_j,$$

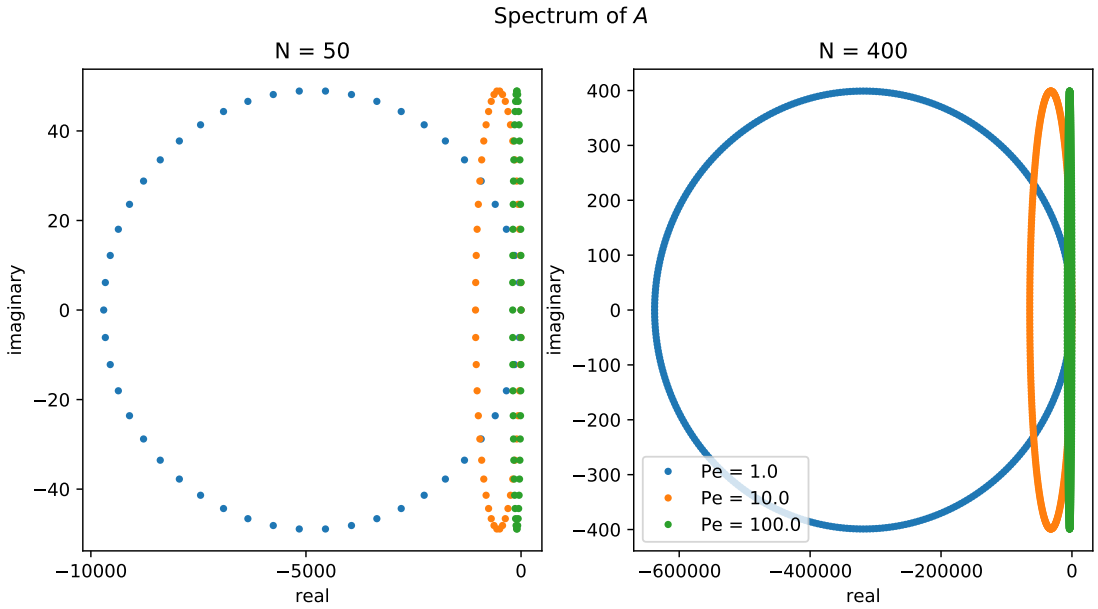


Figure 2: The spectrum of A. We assume periodic boundary conditions.

where

$$\begin{aligned}\lambda_j &= \frac{a}{h^2}\left(e^{i\frac{2\pi}{N}j} - 2 + e^{-i\frac{2\pi}{N}j}\right) - \frac{b}{h}\left(e^{i\frac{2\pi}{N}j} - 1\right) \\ &= -\left(\frac{4a}{h^2} - \frac{2b}{h}\right)\sin^2\left(\frac{\pi j}{N}\right) + i\frac{b}{h}\sin\left(\frac{2\pi j}{N}\right).\end{aligned}$$

From now on we study the behaviour of $v = \sum_{j=0}^{N-1} v_j$, the sum of all normalized eigenvectors. Let $n \in \mathbb{N}$ be the number of power iterations. We begin our analysis with the following auxiliary calculation.

$$\begin{aligned}\frac{h^{4n}}{N}\|A^n v\|_2^2 = \frac{h^{4n}}{N}\sum_{j=0}^{N-1}|\lambda_j|^{2n} &= \frac{1}{N}\sum_{j=0}^{N-1}|h^2\lambda_j|^{2n} \\ &= \frac{1}{N}\sum_{j=0}^{N-1}\left((4a-2bh)^2\sin^4\left(\frac{\pi j}{N}\right) + bh\sin^2\left(\frac{2\pi j}{N-1}\right)\right)^n \\ &\xrightarrow{N\to\infty} (4a)^{2n}\int_0^1 \sin^{4n}(\pi x)dx \\ &= (4a)^{2n}\frac{2}{\pi}\int_0^{\frac{\pi}{2}}\sin^{4n}(x)dx \\ &= (4a)^{2n}\frac{1}{\pi}\,\mathrm{B}(2n+0.5, 0.5),\end{aligned}$$

where B is the beta function. The first equality holds since all eigenvectors are orthogonal. When the limit is taken all terms depending on h vanish. The remaining sum is a left Riemann sum of the integrable function $x \to (4a)^{2n} \sin^{4n}(\pi x)$. In the limit we underestimate the absolutely largest eigenvalue λ_{max} after $n \geq 2$ power iterations by a factor of

$$\begin{aligned}
\lim_{N\to\infty} \frac{\|A^{n-1}v\|_2}{\|A^n v\|_2}|\lambda_{max}| &= \lim_{N\to\infty} \frac{\frac{h^{2n-2}}{\sqrt{N}}\|A^{n-1}v\|_2}{\frac{h^{2n}}{\sqrt{N}}\|A^n v\|_2}|h^2\lambda_N| \\
&= \sqrt{\frac{(4a)^{2n-2}\,\mathrm{B}(2n-1.5,0.5)}{(4a)^{2n}\,\mathrm{B}(2n+0.5,0.5)}}4a \\
&= \sqrt{\frac{\mathrm{B}(2n-1.5,0.5)}{\mathrm{B}(2n+0.5,0.5)}}
\end{aligned}$$

We have

$$\begin{aligned}
\frac{\mathrm{B}(2n-1.5,0.5)}{\mathrm{B}(2n+0.5,0.5)} &= \frac{\Gamma(2n+1)\Gamma(2n-1.5)}{\Gamma(2n-1)\Gamma(2n+0.5)} \\
&= \frac{(2n)!}{(2n-2)!}\frac{\Gamma(2n-1.5)}{\Gamma(2n+0.5)}\frac{\Gamma(2n)}{\Gamma(2n)}\frac{\Gamma(2n-2)}{\Gamma(2n-2)} \\
&= 2n(2n-1)\frac{2^{5-4n}\sqrt{\pi}}{2^{1-4n}\sqrt{\pi}}\frac{\Gamma(4n-4)}{\Gamma(4n)}\frac{\Gamma(2n)}{\Gamma(2n-2)} \\
&= 32n(2n-1)\frac{(4n-5)!}{(4n-1)!}\frac{(2n-2)!}{(2n-4)!} \\
&= \frac{32n(2n-1)(2n-2)(2n-3)}{(4n-1)(4n-2)(4n-3)(4n-4)} \\
&= \frac{4n(4n-6)}{(4n-1)(4n-3)} \\
&= \left(1+\frac{1}{4n-1}\right)\left(1-\frac{3}{4n-3}\right)
\end{aligned}$$

For the third equality we applied the duplication formula for the gamma function. All in all we underestimate the absolutely largest eigenvalue λ_{max} by a factor of

$$\lim_{N\to\infty} \frac{\|A^{n-1}v\|}{\|A^n v\|}|\lambda_{max}| = \sqrt{\left(1+\frac{1}{4n-1}\right)\left(1-\frac{3}{4n-3}\right)}$$

at the limit $N \to \infty$.

n	2	3	4	5	6
formula	0.6761	0.7273	0.9058	0.9310	0.9457

5 Matrix-free Leja based exponential integrators

Exponential integrators are a class of numerical integrators which excel at solving stiff differential equations. Unlike most numerical ordinary differential equation (ODE) solvers their construction is based on the variation-of-constants formula. Consider the semilinear initial value problem

$$\begin{aligned} \partial_t u &= F(u) = Au + g(u) \\ u(0) &= u_0 \end{aligned} \tag{1}$$

where $A = \partial_u F$ and $g(u) = F(u) - Au$ is the linear and nonlinear part of F respectively. The solution of the ODE is given by the variation-of-constants formula

$$u(t) = e^{At}u_0 + \int_0^t e^{(t-\tau)A} g(u(\tau))d\tau.$$

Similar to Runge-Kutta methods we replace the integrand with a polynomial approximation. Unlike Runge-Kutta methods we leave the matrix exponential untouched and only replace g. The most well-known Rosenbrock-type exponential integrator, the exponential Rosenbrock-Euler method, can be obtained by using the left hand rule. By replacing g with $g(u_0)$ we get

$$u(t) \approx e^{At}u_0 + \int_0^t e^{(t-\tau)A} g(u_0)d\tau = e^{At}u_0 + \varphi_1(tA)g(u_0),$$

where $\varphi_1(z) = \frac{e^z - 1}{z}$. The exponential Rosenbrock-Euler method is of order 2 and is exact for fully linear problems. We will refer to it as `exprb2` in section 7.

5.1 Higher order Rosenbrock methods

Exponential Rosenbrock methods are a special class of exponential integrators which efficiently solve semi-linear problems (1). For a given time step size τ the numerical solution u_1 is given by

$$\begin{aligned} U_i &= e^{c_i \tau A}u_0 + \tau \sum_{j=1}^{i-1} a_{ij}(\tau A) g(U_j), \\ u_1 &= e^{\tau A}u_0 + \tau \sum_{i=1}^{s} b_i(\tau A) g(U_i), \end{aligned} \tag{2}$$

where $s \in \mathbb{N}$ and a_{ij}, b_i are matrix functions. The numerical scheme can be represented as a Butcher tableau

$$\begin{array}{c|cccc} c_1 & & & & \\ c_2 & a_{21}(\tau A) & & & \\ \vdots & & \ddots & & \\ c_s & a_{s1}(\tau A) & \dots & a_{s,s-1}(\tau A) & \\ \hline & b_1(\tau A) & \dots & b_{s-1}(\tau A) & b_s(\tau A) \end{array}.$$

The functions a_{ij} and b_i are typically given as linear combinations of the φ_k-functions, which in turn are recursively defined as

$$\varphi_{k+1}(z) = \frac{\varphi_k(z) - 1}{z}, \quad \varphi_0(z) = e^z, \quad k \in \mathbb{N}.$$

For example consider the embedded method

0			
$\frac{1}{2}$	$\frac{1}{2}\varphi_1(\frac{1}{2}\cdot)$		
1	0	φ_1	
`exprb3`	$\varphi_1 - 14\varphi_3$	$16\varphi_3$	$-2\varphi_3$
`exprb4`	$\varphi_1 - 14\varphi_3 + 36\varphi_4$	$16\varphi_3 - 48\varphi_4$	$-2\varphi_3 + 12\varphi_4$

.

This scheme is known as `exprb43` [6, Example 2.24]. It uses `exprb3` as a third-order estimator for its fourth-order method `exprb4`. Both integrators are well suited for numerical computations since all internal stages can be cheaply computed using the exponential Euler method.
Under the simplifying assumptions

$$\sum_{j=1}^{s} b_j = \varphi_1, \quad \sum_{j=1}^{s} a_{ij} = c_i \varphi_1(c_i \cdot)$$

for $1 \leq i \leq s$ the scheme (2) can be expressed as

$$\begin{aligned} U_i &= u_0 + c_i \tau \varphi_1(c_i \tau A) F(u_0) + \tau \sum_{j=2}^{i-1} a_{ij}(\tau A) D_j, \\ D_j &= g(U_j) - g(u_0), \quad 2 \leq j \leq s, \\ u_1 &= u_0 + \tau \varphi_1(\tau A) F(u_0) + \tau \sum_{i=2}^{s} b_i(\tau A) D_i. \end{aligned} \tag{3}$$

The main advantage of this reformulation lies in the fact that the norm of all D_j is expected to be small. This can be exploited by the Leja method by allowing an early termination of the Newton interpolation.
For an efficient implementation of exponential Rosenbrock integrators it is crucial to compute only a single action of a matrix function per stage U_i and for solution u_1. Since the most frequently employed methods depend on linear combinations of φ_k-functions this can be done using the matrix exponential function.

5.2 Computing the action of the φ-functions

Exponential integrators rely on the efficient computation of φ_k-functions. In the matrix case $A \in \mathbb{C}^{N \times N}$ this can be done by slightly expanding A, see [2, Theorem 2.1].
Let $V = [V_p \dots V_2, V_1] \in \mathbb{C}^{N \times p}$, $u \in \mathbb{C}^{N \times 1}$, $\tau \in \mathbb{C}$ and

$$\tilde{A} = \begin{bmatrix} A & V \\ 0 & J \end{bmatrix}, \quad J = \begin{bmatrix} 0 & I_{p-1} \\ 0 & 0 \end{bmatrix},$$

where I_n is the $n \times n$ identity matrix. Let e_n denote the n-th $p \times 1$ unity vector. Then

$$\begin{bmatrix} I_N & 0 \end{bmatrix} e^{\tau \tilde{A}} \begin{bmatrix} u \\ e_j \end{bmatrix} = e^{\tau A} u + \sum_{k=1}^{j} \tau^k \varphi_k(\tau A) V_{p-j+k}, \quad j \in \{1, \ldots, p\}.$$

In particular for $j = p$ we have

$$\begin{bmatrix} I_N & 0 \end{bmatrix} e^{\tau \tilde{A}} \begin{bmatrix} u \\ e_p \end{bmatrix} = e^{\tau A} u + \sum_{k=1}^{p} \tau^k \varphi_k(\tau A) V_k$$

This formulation can be directly applied to each stage in (3) assuming a_{ij} and b_j are linear combinations of φ_k-functions. Therefore for each stage only a single action of an expanded matrix exponential has to be evaluated. In total this has to be done s times for an exponential Rosenbrock method with s stages.
For a matrix-free implementation of $\tilde{A}$ given an operator A we can simply compute the action of $\tilde{A}$ as follows

$$\tilde{A} \begin{bmatrix} v \\ w \end{bmatrix} = \begin{bmatrix} Av \\ 0 \end{bmatrix} + \begin{bmatrix} Uw \\ Jw \end{bmatrix}, \quad v \in \mathbb{C}^{N \times 1}, w \in \mathbb{C}^{p \times 1}.$$

The Leja method only relies on matrix-vector multiplications with $\tilde{A}$ and therefore the explicit knowledge of A is not required. To summarize, an efficient matrix-free implementation of exponential Rosenbrock-methods can be achieved using the Leja method. In particular `exprb3` and `exprb4` can be evaluated by computing three actions of matrix exponentials.

6 Nonlinear Advection-Diffusion-Reaction Equation

Consider the one-dimensional advection-diffusion-reaction equation

$$\begin{aligned} \partial_t u &= \alpha \partial_x((u + \partial_x u)) + \beta \partial_x(u^2) + u(u - 0.5) \quad \alpha, \beta, \geq 0 \\ u_0(t) &= e^{-80 \cdot (t - 0{,}45)^2} \quad t \in [0, 0.1] \end{aligned}$$

on the domain $\Omega = [0, 1]$.

7 Numerical experiments

For the first experiments we will discretize multiple one-dimensional advection-diffusion-reaction equations with hybrid difference schemes.[1] We will always choose an equidistant

[1] Need a source, https://en.wikipedia.org/wiki/Hybrid_difference_scheme

grid with grid size $h = \frac{1}{N}$, $N \in \mathbb{N}$ and grid points $x_i = ih$ for $i = 0 \ldots, N$ on the domain $\Omega = [0, 1]$. The resulting ordinary differential equations (ODEs) will be solved with four different integrators. Our goal is to investigate the respective computational costs of these methods while achieving a prescribed relative tolerance `tol`.

Crank-Nicolson method: We refer to the Crank-Nicolson method of order 2 as `cn2`. In our implementation of `cn2`, we used the SciPy[10] package `scipy.sparse.linalg.gmres` to solve linear equations. We set the relative tolerance to $\texttt{tol}/s$, where s is the total number of substeps taken for solving the ODE. This choice guarantees that the sum of errors made by `gmres` is always lower than our specified tolerance `tol`, since we have to solve exactly one linear equation per substep. No preconditioner was used for `gmres`. The Crank-Nicolson method is unconditionally stable and therefore does not have to satisfy the Courant-Friedrichs-Lewy (CFL) conditions imposed by the advective and diffusive part of the differential equations.

Exponential Rosenbrock-Euler method: We refer to the Exponential Rosenbrock-Euler method of order 2 as `exprb2`. The approximate the action of the matrix exponential with the Leja method. No hump reduction is used. The maximal interpolation degree is set to 100. Note that the total number of matrix-vector multiplication per time step can still exeed 100 since we have to compute a single matrix norm. This typically happens for $s = 1$.

Explicit midpoint method: We refer to the explicit midpoint method of order 2 as `rk2`.

Classical Runge-Kutta method: We refer to the classical Runge-Kutta method of order 4 as `rk4`.

For our experiments we will often fix one of two different Péclet numbers

$$\texttt{Pe} = \frac{b}{a}, \quad \texttt{pe} = \frac{hb}{2a},$$

The Péclet numbers are dimensionless quantities representing the ratio of the advective velocity b to the diffusive velocity a. While `Pe` characterizes the original partial differential equation, the grid Péclet number `pe` is the dimensionless quantity for the resulting ODE after discretization. Note that by fixing `pe` for varying grid sizes, we have to change the original partial differential equantion. Unless otherwise noted we accomplish that by replacing b with $2b$ and a with ah.

7.1 Experiment 1: Linear advection diffusion equation

Consider the one-dimensional advection-diffusion equation

$$\begin{aligned} \partial_t u &= a\partial_{xx} u + b\partial_x u \quad a, b \geq 0 \\ u_0(t) &= e^{-80\cdot(t-0{,}45)^2} \quad t \in [0, 0.1] \end{aligned}$$

with homogeneous Dirichlet boundary conditions on the domain $\Omega = [0, 1]$. For a fixed $N \in \mathbb{N}$ we approximate the diffusive part with second-order central differences on an equidistant grid with grid size $h = \frac{1}{N}$ and grid points $x_i = ih$, $i = 0 \dots, N$.

$$\partial_{xx} u(x_i) = \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2} + \mathcal{O}(h^2)$$

In order to limit numerical instabilities we discretize the advective part with forward differences, similar to the upwind scheme.[2]

$$\partial_x u(x_i) = \frac{u(x_{i+1}) - u(x_i)}{h} + \mathcal{O}(h)$$

The resulting system of ordinary differential equation is given by

$$\partial_t u = Au.$$

Some eigenvalues of A can have an extremely large negative real part. Therefore, since no explicit Runge-Kutta method is A-stable, this imposes very stingend conditions on the time step size τ for rk2 and rk4.[3] We will refer to the Courant-Friedrich-Lewy (CFL) conditions imposed by the advective and diffusive part of A respectively by C_{adv} and C_{dif}.

$$C_{adv} = \frac{b\tau}{h} \leq 1, \quad C_{dif} = \frac{a\tau}{h^2} \leq \frac{1}{2}$$

In our case the problem is fully linear and therefore `exprb2` simplifies to the computation of the action of the matrix exponential function with the Leja method. We write `expleja` for the single precision Leja method approximation. Note that reference solution was computed with double precision and therefore uses different nodes.

In order to keep the solution from vanishing, we fix $b = 1$ and only consider coefficients $a \in [0, 1]$. The advection-diffusion ratio scaled by the grid size h is represented by the grid Péclet number

7.2 Experiment 2: 1D Nonlinear advection diffusion equation

$$\partial_t u = \alpha \partial_x((u + 1)\partial_x u) + \partial_x(u^2) + u(u - 0.5)$$

We discretize, solve again with rk2, rk4, cn2 and exprb2.

8 Appendix

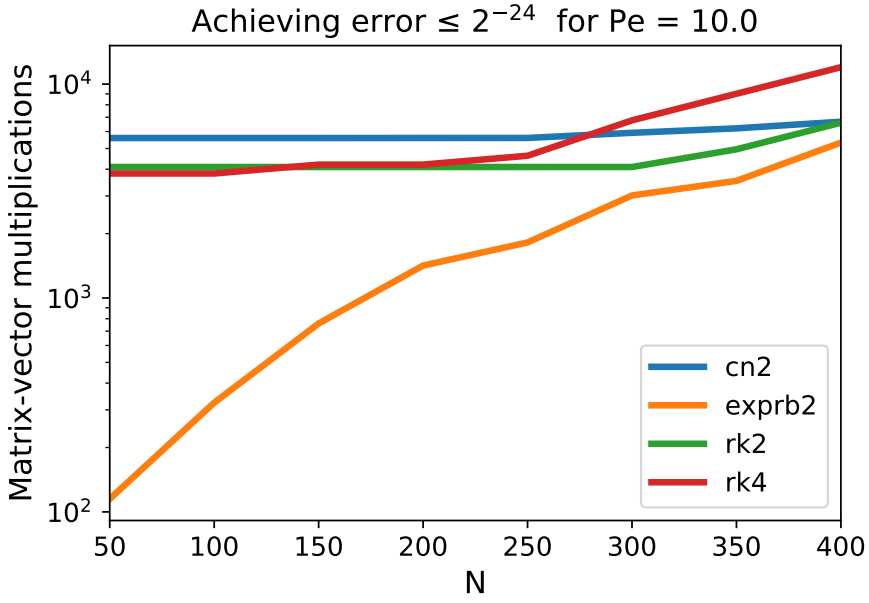
Matrix analysis, Horn and Johnson, Lemma 5.6.10

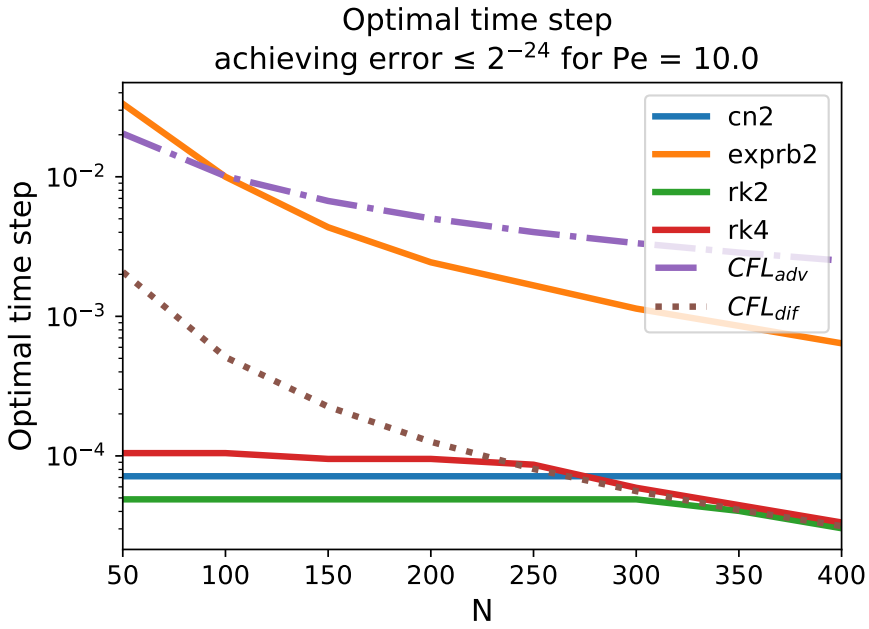
$$\rho(A) = \inf\{\|A\| : \|\cdot\| \text{ is an induced matrix norm}\}$$

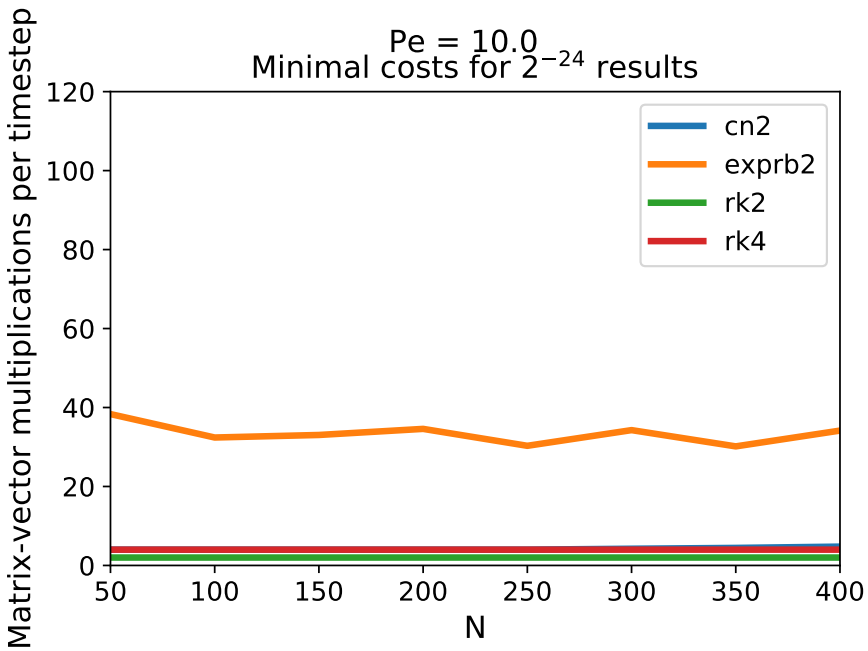
[2] Maybe create a seperate section on hybrid difference schemes? There we can also analyze the resulting matrix A itself and plot the eigenvalues. I need sources for that though.

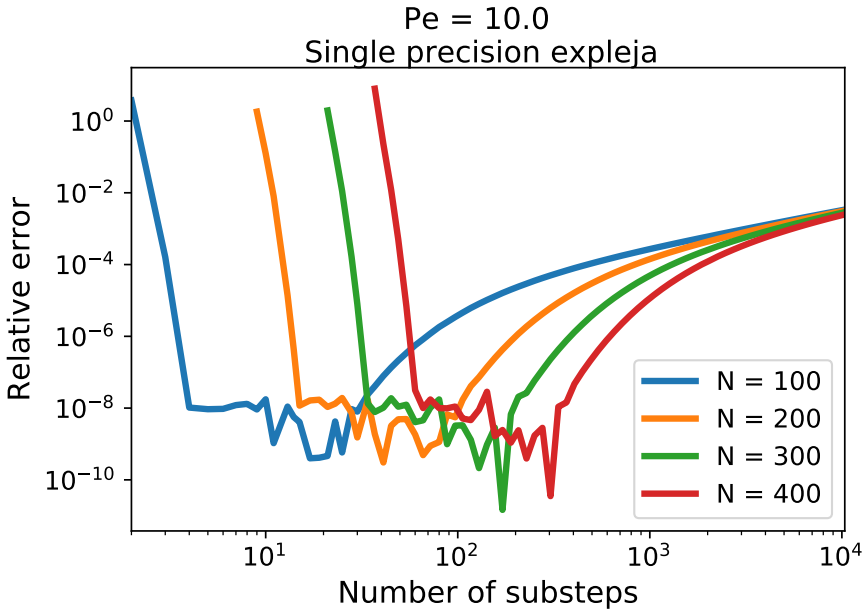
[3] See section **??**

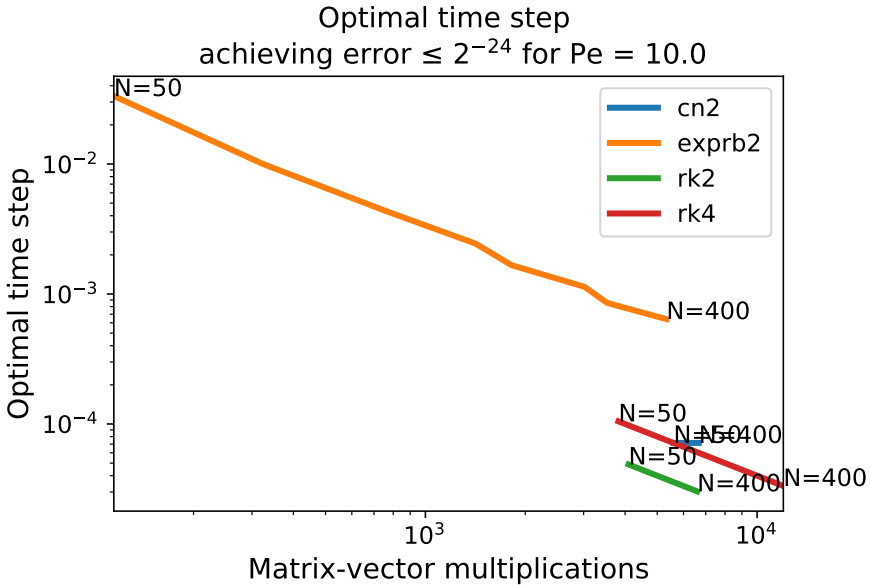
8.1 Experiment Linear






Pe = 10.0
Minimal costs for 2^{-24} results
Matrix-vector multiplications per timestep
N
cn2
exprb2
rk2
rk4
0
20
40
60
80
100
120
50
100
150
200
250
300
350
400


Pe = 10.0
Single precision expleja
Relative error
Number of substeps
N = 100
N = 200
N = 300
N = 400
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
10^{-10}
10^{1}
10^{2}
10^{3}
10^{4}



8.2 Experiment Linear: Power iterations

In the matrix-free case the linear operator A is not explicitly given. In order to compute the matrix norm $\|A\|_2$ we use power iterations to estimate the absolutely largest eigenvalue of A. A priory it is not clear how many power iterations it are necessary for a good approximation.

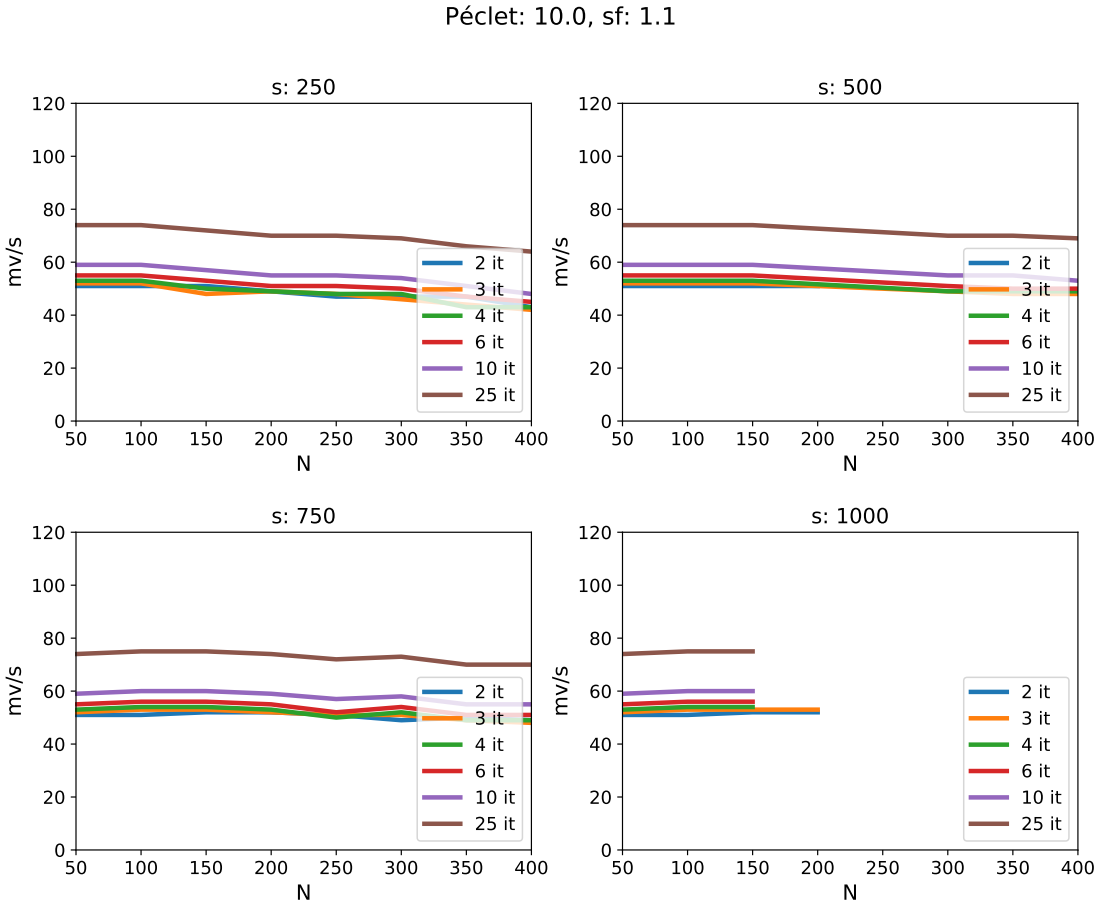
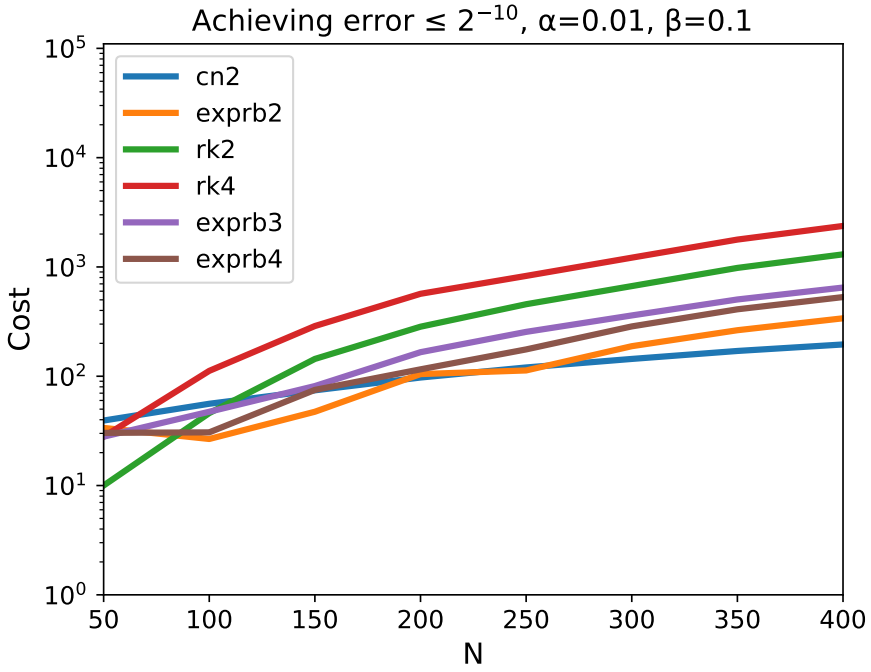
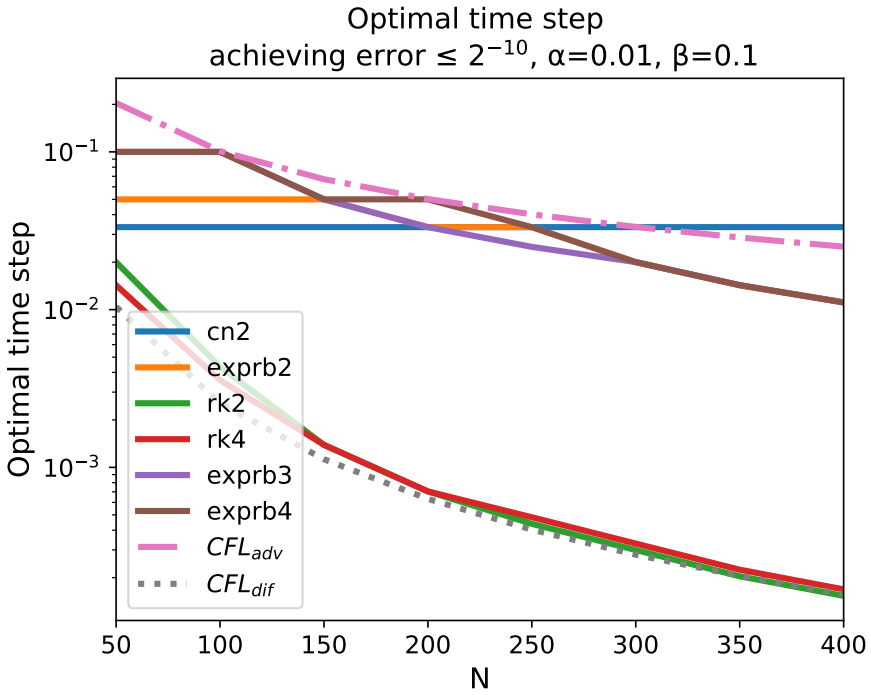


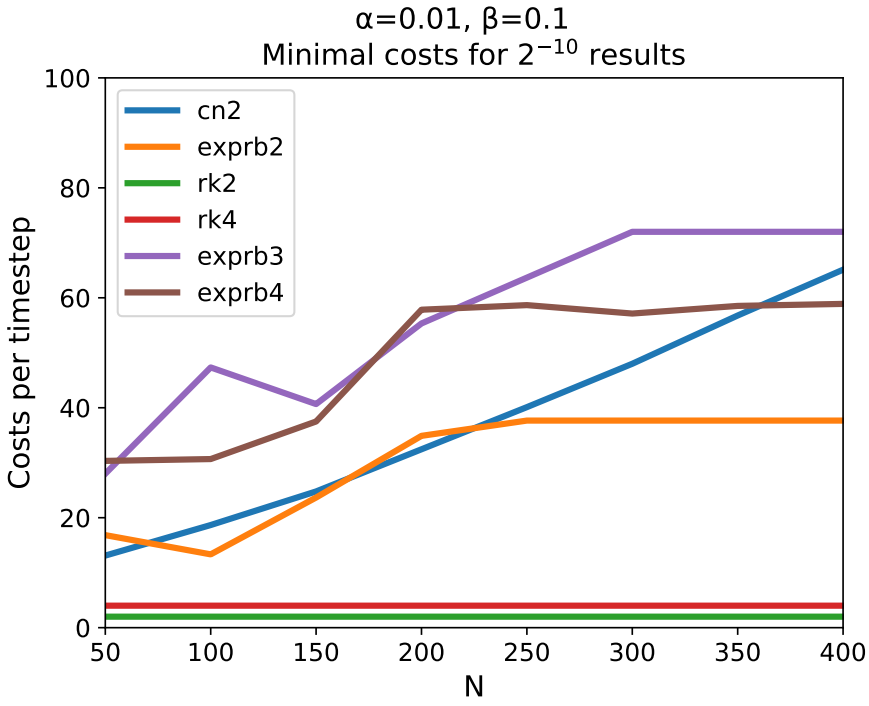
Figure 3: Space dimension N vs costs `mv` per timestep `s` for the exponential Rosenbrock method `exprb2`. Results are only shown if they achieve single precision.

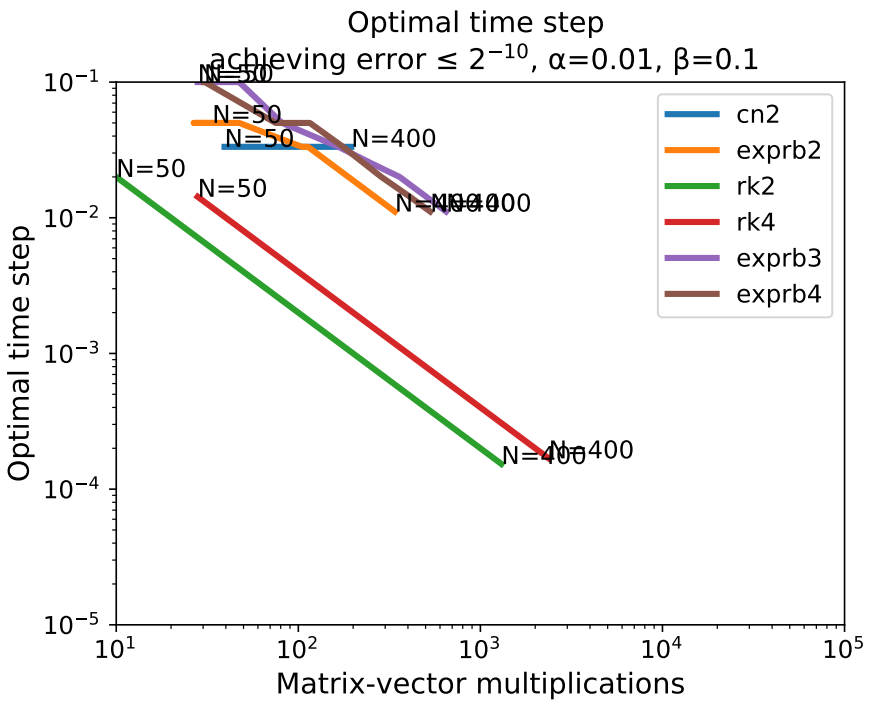
8.3 Experiment Nonlinear 1D

1, half, =0.01, =0.1


Achieving error ≤ 2^{-10}, α=0.01, β=0.1
Cost
N
cn2
exprb2
rk2
rk4
exprb3
exprb4
10^0
10^1
10^2
10^3
10^4
10^5
50
100
150
200
250
300
350
400

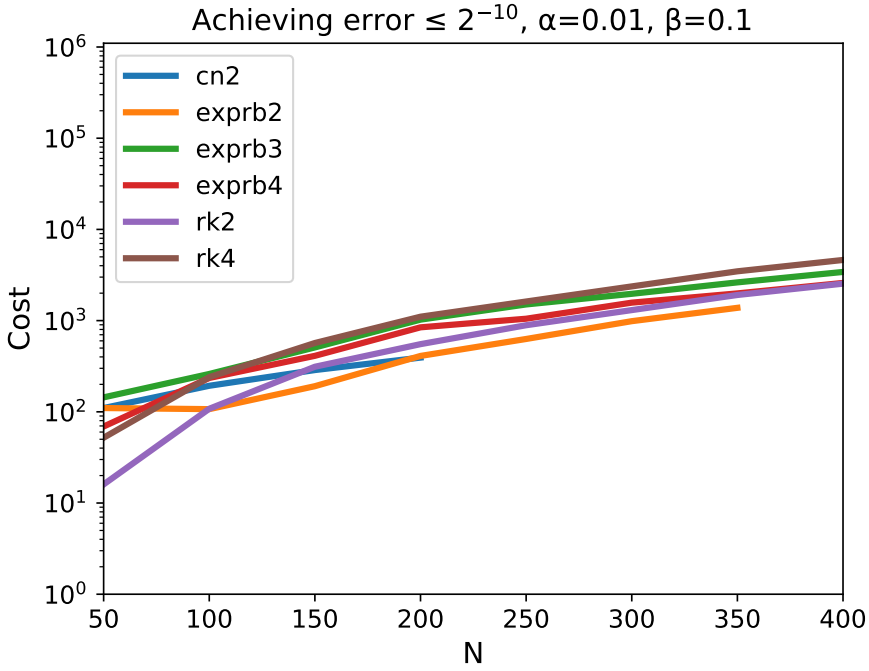

Optimal time step
achieving error ≤ 2^{-10}, α=0.01, β=0.1
Optimal time step
N
cn2
exprb2
rk2
rk4
exprb3
exprb4
CFL_{adv}
CFL_{dif}
10^{-1}
10^{-2}
10^{-3}
50
100
150
200
250
300
350
400

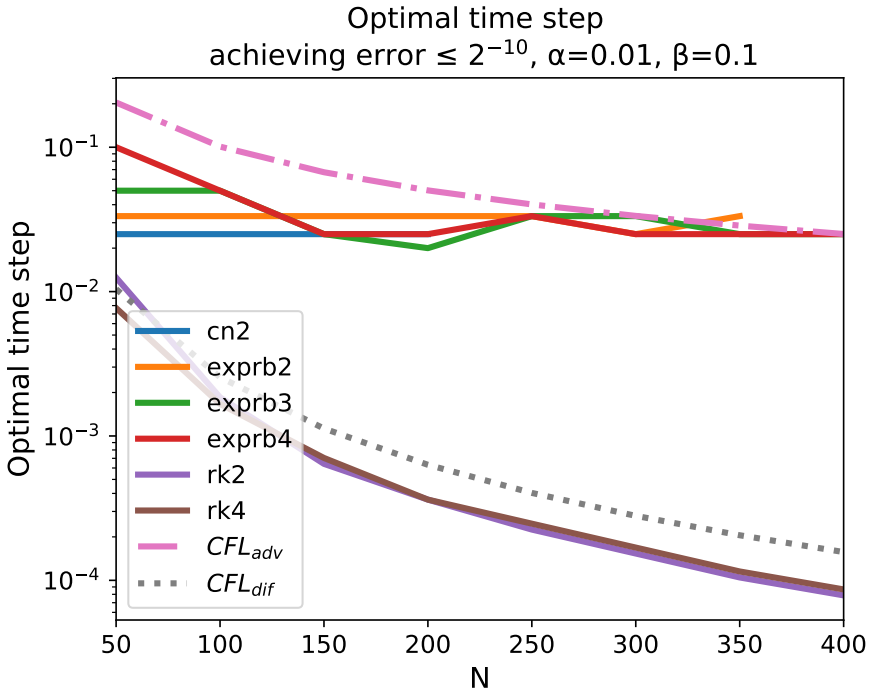

α=0.01, β=0.1
Minimal costs for 2^{-10} results
Costs per timestep
N
cn2
exprb2
rk2
rk4
exprb3
exprb4
0
20
40
60
80
100
50
100
150
200
250
300
350
400

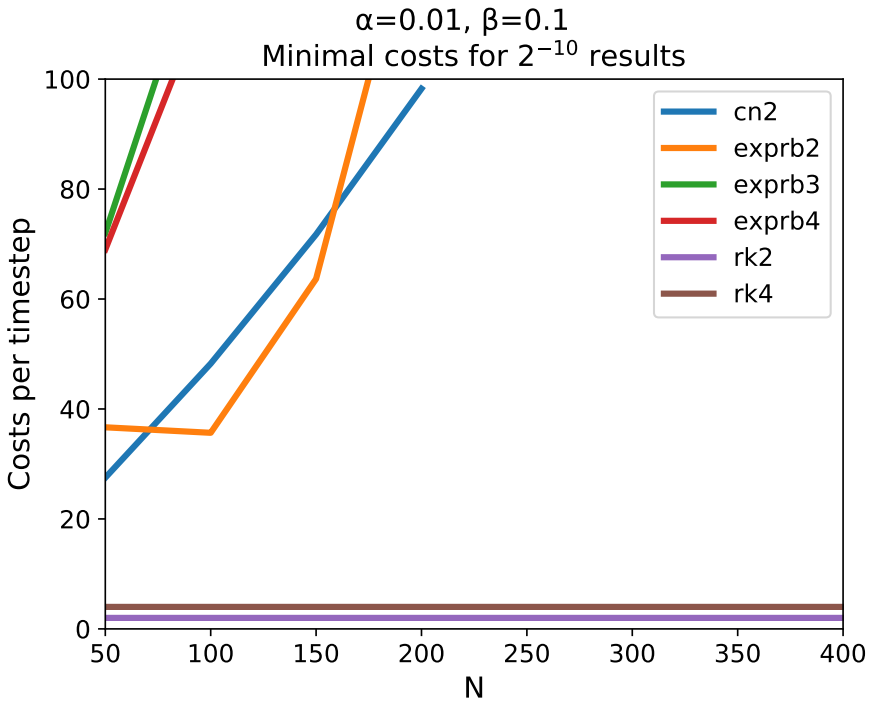

Optimal time step
achieving error ≤ 2^{-10}, α=0.01, β=0.1
Optimal time step
Matrix-vector multiplications
cn2
exprb2
rk2
rk4
exprb3
exprb4
N=50
N=400
10^{-1}
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}

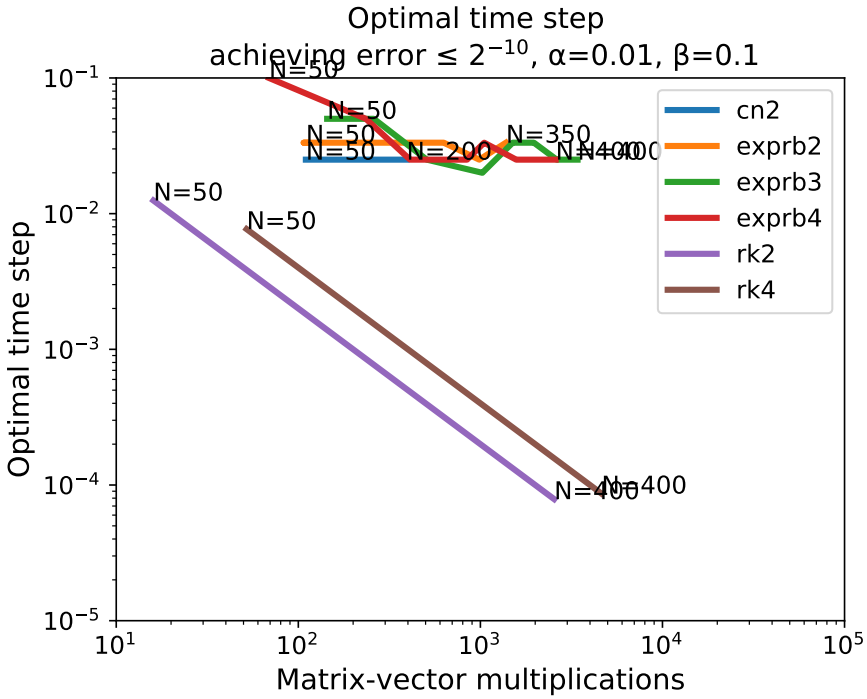
8.4 Experiment Nonlinear 2D

1, half, =0.01, =0.1




Optimal time step
achieving error ≤ 2^{-10}, α=0.01, β=0.1
Optimal time step
10^{-1}
10^{-2}
10^{-3}
10^{-4}
cn2
exprb2
exprb3
exprb4
rk2
rk4
CFL_{adv}
CFL_{dif}
50
100
150
200
250
300
350
400
N


α=0.01, β=0.1
Minimal costs for 2^{-10} results
Costs per timestep
100
80
60
40
20
0
cn2
exprb2
exprb3
exprb4
rk2
rk4
50
100
150
200
250
300
350
400
N


Optimal time step
achieving error ≤ 2^{-10}, α=0.01, β=0.1
Optimal time step
Matrix-vector multiplications
cn2
exprb2
exprb3
exprb4
rk2
rk4
N=50
N=50
N=50
N=50
N=200
N=350
N=50
N=400
N=400

References

[1] M. Caliari, A. Ostermann. Implementation of exponential Rosenbrock-type integrators, Applied Numerical Mathematics 59 (2009), 568-581.

[2] A. Al-Mohy, N. Higham. Computing the action of the matrix exponential, with an application to exponential integrators, SIAM Journal on Scientific Computing 33 (2011), 488-511.

[3] L. Reichel. Newton interpolation at Leja points, BIT Numerical Mathematics 30 (1990), 332-346.

[4] M. Caliari, M. Vianello, L. Bergamaschi. Interpolating discrete advection-diffusion propagators at Leja sequences, Journal of Computational and Applied Mathematics 172 (2004), 79-99.

[5] M. Caliari, P. Kandolf, A. Ostermann, S. Rainer. The Leja method revisited: backward error analysis for the matrix exponential, SIAM Journal on Scientific Computation, Accepted for publication (2016). arXiv:1506.08665.

[6] M. Hochbruck, A. Ostermann. Exponential integrators, Acta Numerica 19 (2010), 209-286

[7] Python Software Foundation. Python Language Reference, version 2.7. Available at http://www.python.org. Manual at https://docs.python.org/2/. [Online; accessed 2015-12-14]

[8] P. Novati, Polynomial methods for the computation of functions of large unsymmetric matrices, Ph.D. Thesis in Computational Mathematics, University of Trieste, advisor I. Moret, 2000.

[9] L. Reichel, Newton interpolation at Leja points, BIT 30 (2) (1990) 332–346.

[10] E. Jones, E. Oliphant, P. Peterson, SciPy: Open Source Scientific Tools for Python, Available at http://www.scipy.org/. [Online; accessed 2015-12-14]

[11] R. Horn, C. Johnson, Matrix Analysis, Cambridge University Press (2012).