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Master Thesis

Matrix-free Leja based exponential integrators in Python

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Abstract

1 Introduction

Consider the action of the matrix exponential function

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

It can be difficult or impossible to compute e^A in a first step and then the action $e^A v$ in a seperate 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 feasable 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_n of degree n in A

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

This approach has many advantages. The cost of the computation of $p_n(A)v$ mainly depends on the calculation of $n \in \mathbb{N}$ matrix-vector multiplications with A. Not only can A be sparse, which significantly decreases the costs of the computation, the explicit knowledge of A itself is no longer required. A can be replaced by a linear function, which can be more convenient and saves memory.

2 Experiment 1

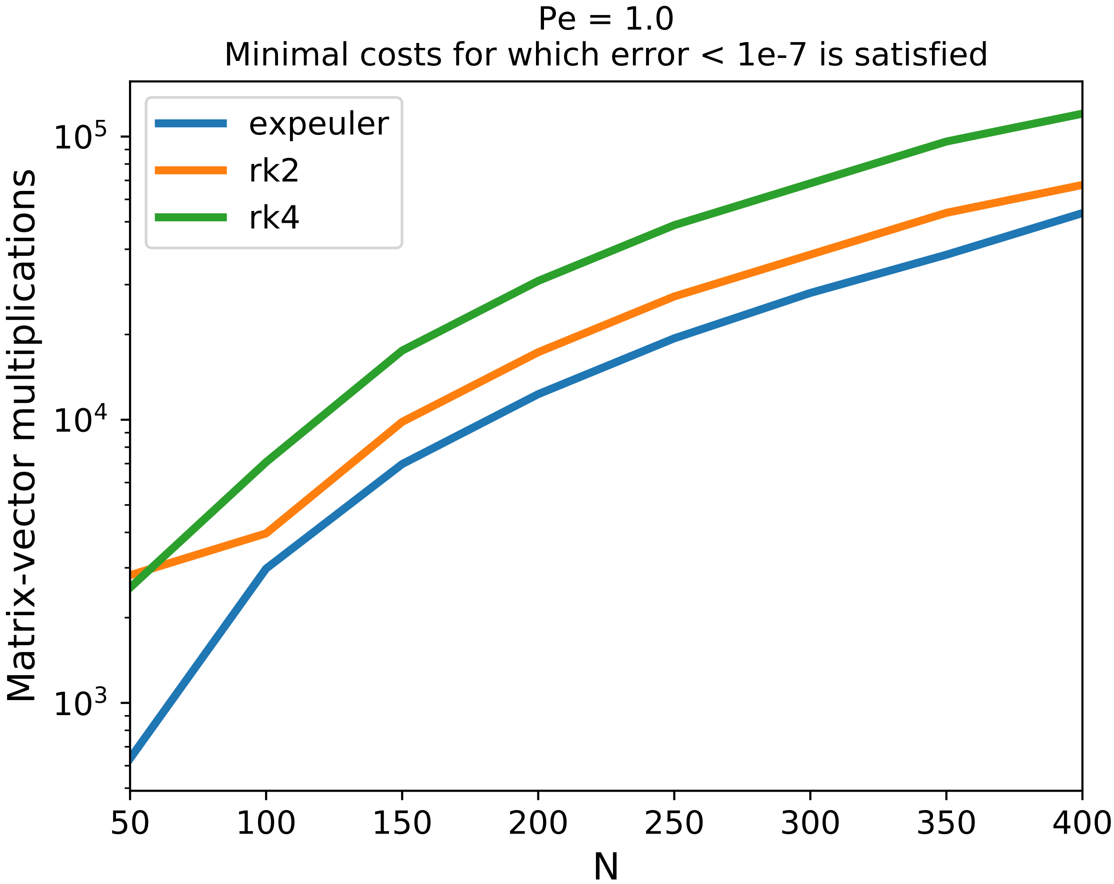
We discretize the one-dimensional advection-diffusion equation

$$\begin{aligned} \partial_t u &= a\partial_{xx}u + b\partial_x u & a, b \in [0,1] \\ u_0(t) &= e^{-80\cdot(t-0,45)^2} & t \in [0, 0.1] \end{aligned}$$

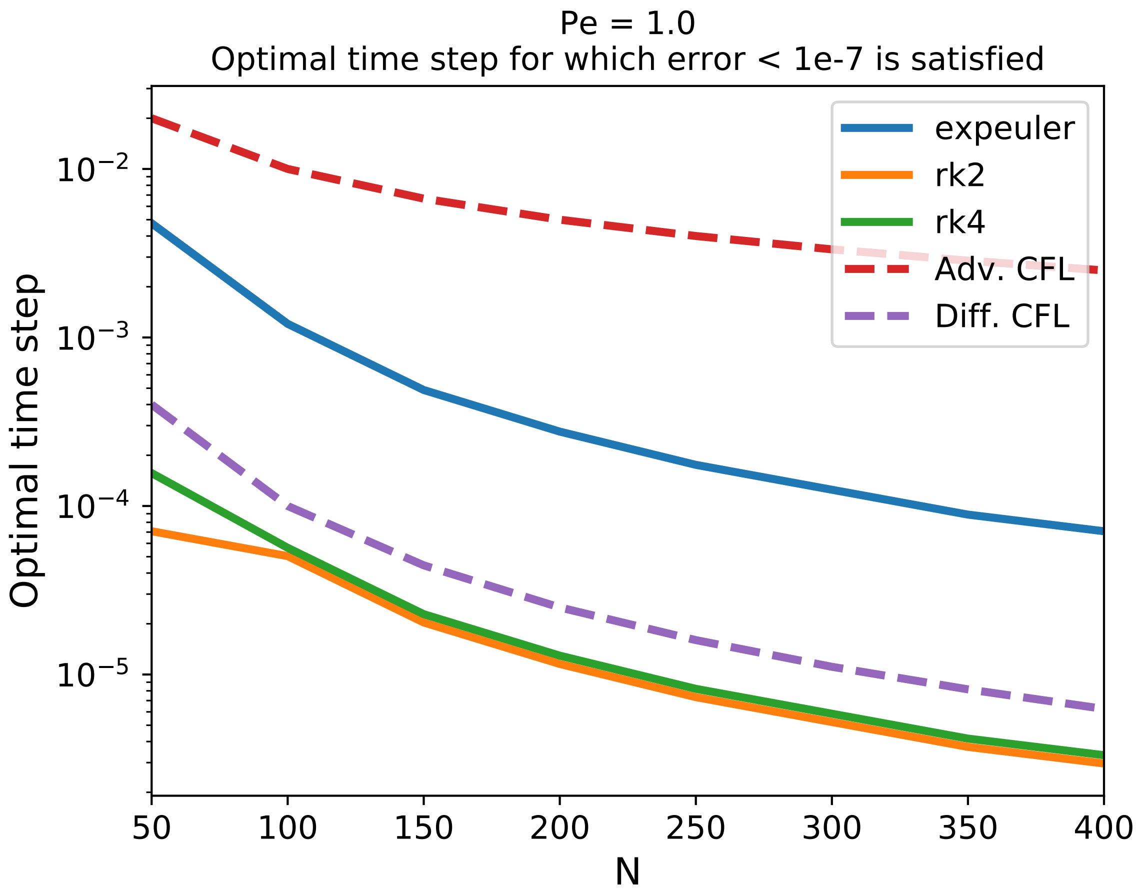
with homogeneous Dirichlet boundary conditions on the domain $\Omega = [0, 1]$.

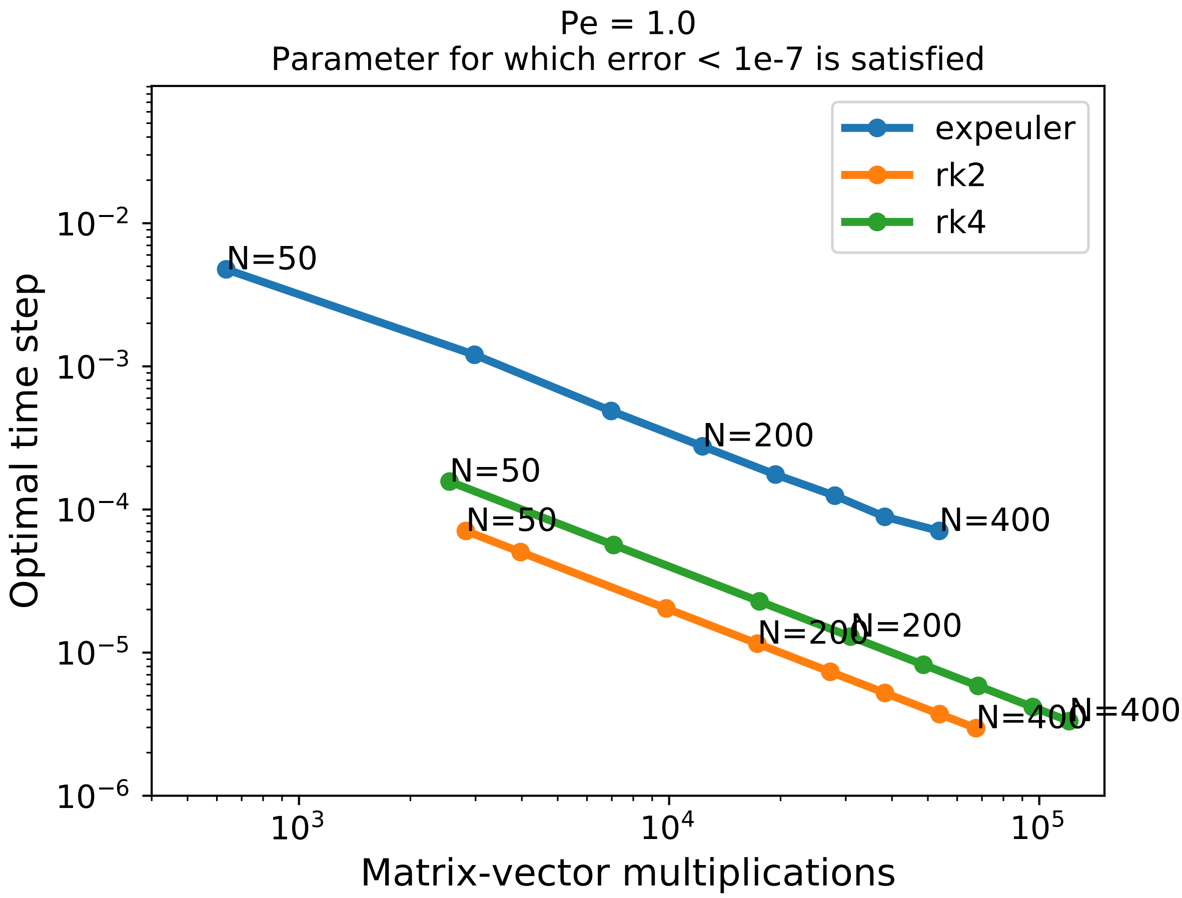
$$\mathrm{Pe} = \frac{\Delta x}{|c|}$$

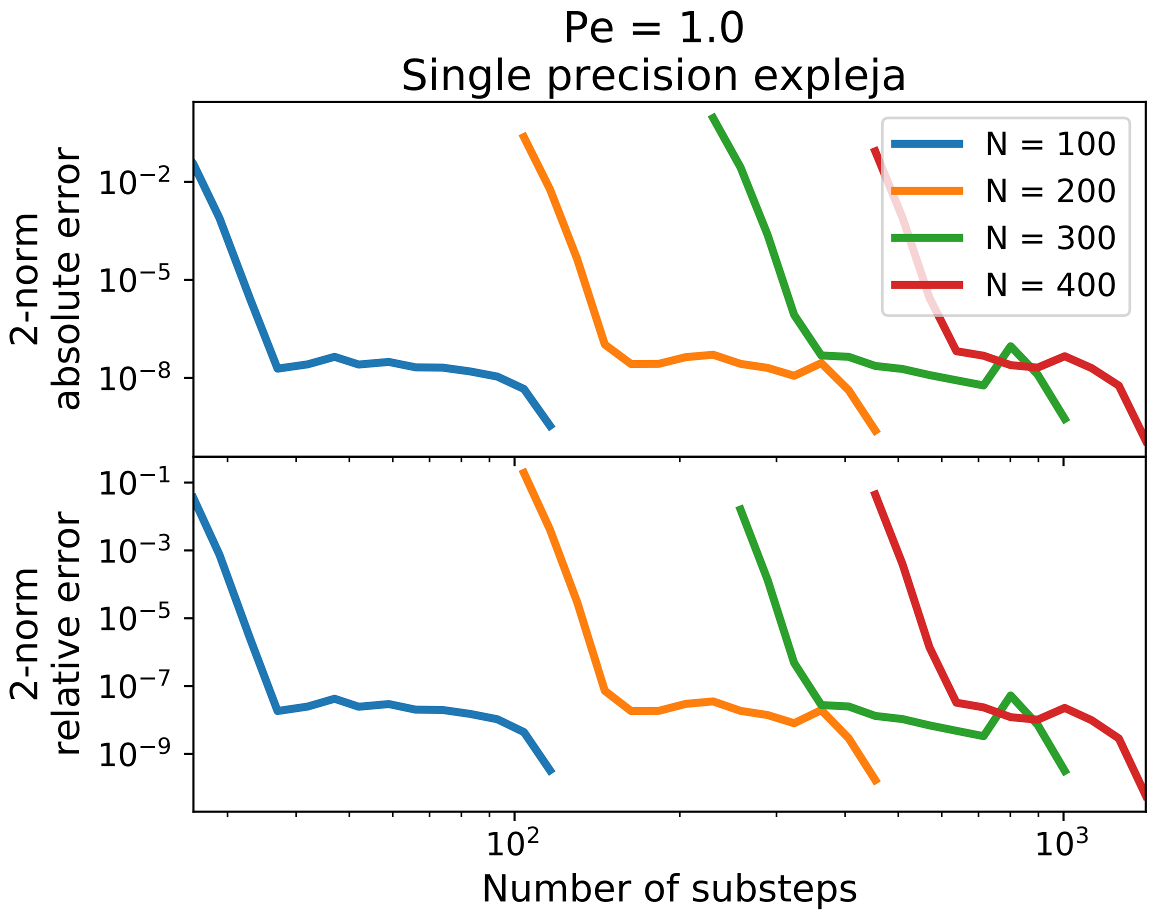
we denote the grid Péclet number. In the following experiments we will denote the advection-diffusion ratio, scaled by grid size $\Delta x = (N + 1)^{-1}$



Pe = 1.0
Minimal costs for which error < 1e-7 is satisfied
expeuler
rk2
rk4
Matrix-vector multiplications
10^5
10^4
10^3
50
100
150
200
250
300
350
400
N


Pe = 1.0
Optimal time step for which error < 1e-7 is satisfied
Optimal time step
N
expeuler
rk2
rk4
Adv. CFL
Diff. CFL
10^{-2}
10^{-3}
10^{-4}
10^{-5}
50
100
150
200
250
300
350
400


Pe = 1.0
Parameter for which error < 1e-7 is satisfied
expeuler
rk2
rk4
N=50
N=200
N=400
N=50
N=50
N=200
N=200
N=400
N=400
Optimal time step
10^{-2}
10^{-3}
10^{-4}
10^{-5}
10^{-6}
10^{3}
10^{4}
10^{5}
Matrix-vector multiplications



Question: Do we only care about the relative error? If yes, in which norm? Argument for 2

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