

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 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_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

$$\begin{aligned} \partial_t u &= \partial_{xx} u + \frac{1}{\text{Pe}} \partial_x u \quad t \in [0, 0.1] \\ u_0(t) &= e^{-80 \cdot (t-0.45)^2} \end{aligned}$$

with homogeneous Dirichlet boundary conditions on the domain $\Omega = [0, 1]$. With $\text{Pe} > 0$ we denote the grid Péclet number.

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