Adaptive rational Krylov methods for exponential Runge–Kutta integrators

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We consider the solution of large stiff systems of ordinary differential equations with explicit exponential Runge–Kutta integrators. These problems arise from semi-discretized semi-linear parabolic partial differential equations on continuous domains or on inherently discrete graph domains. A series of results reduces the requirement of computing linear combinations of φ-functions in exponential integrators to the approximation of the action of a smaller number of matrix exponentials on certain vectors. State-of-the-art computational methods use polynomial Krylov subspaces of adaptive size for this task. They have the drawback that the required Krylov subspace iteration numbers to obtain a desired tolerance increase drastically with the spectral radius of the discrete linear differential operator, e.g., the problem size. We present an approach that leverages rational Krylov subspace methods promising superior approximation qualities. We prove a novel a-posteriori error estimate of rational Krylov approximations to the action of the matrix exponential on vectors for single time points, which allows for an adaptive approach similar to existing polynomial Krylov techniques. We discuss pole selection and the efficient solution of the arising sequences of shifted linear systems by direct and preconditioned iterative solvers. Numerical experiments show that our method outperforms the state of the art for sufficiently large spectral radii of the discrete linear differential operators. The key to this are approximately constant rational Krylov iteration numbers, which enable a near-linear scaling of the runtime with respect to the problem size.

Primary author: BERGERMANN, Kai (TU Chemnitz)

Co-author: Prof. STOLL, Martin (TU Chemnitz)

Presenters: BERGERMANN, Kai (TU Chemnitz);   Prof. STOLL, Martin (TU Chemnitz)

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