A Restarting Method for Matrix Function Operation with Sequential Processing of Multiple Right Hand Sides

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Abstract

Multistage exponential integrators require approximation of matrix function operations $z^{(i)} = f(A)b^{(i)}$ at each time step. The vectors $b^{(i)}$ are not known in advance. They appear sequentially during the course of approximation. For large sparse matrices the Krylov subspace approximation is the method of choice. Typically, an s-stage exponential integrator requires generation of s Krylov subspaces at each time step. This renders naive implementations computationally inefficient.

We use wavelet Galerkin semi-discretization of parabolic problems to obtain the matrix A. Since vectors $b^{(i)}$ are close to each other and the condition number of A remains bounded, it is reasonable to expect the solution vectors $z^{(i)}$ to be close to each other as well. We propose a restarting method for sequential processing of multiple right hand sides that uses $z^{(i-1)}$ as an initial guess to obtain an approximation for $z^{(i)}$. If more information is required to be passed from one system to another, the method is also capable of incorporating Ritz vectors. The target matrices here are symmetric and the block Lanczos algorithm is used to obtain the projection matrices. Since the Lanczos vectors/blocks are known to lose orthogonality with growing dimensions of the underlying Krylov subspace, the proposed method takes appropriate measures to prevent orthogonality loss. A method for efficient detection of loss of orthogonality is generalized to the current setting. The method uses Ritz vectors while restarting. The selection of Ritz vectors is based on fundamental error analysis of Paige, originating in eigenvalue problems. A result shows that the selection criteria delivers vectors that are usable with Cauchy integral formula. Finally some a-posteriori error estimates, intended to be used in an under-construction object oriented framework for the implementation of exponential integrators, are presented.