Institute of Information and Communication Technologies
Bulgarian Academy of Sciences

Seminar on Scientific Computing and Parallel Algorithms

On 22 October 2019, at 14:00, in the Seminar Room 218 of IICT-BAS, Acad. G. Bonchev Str., Bl. 25A, Dr. Kathryn Lund from Charles University in Prague, Faculty of Mathematics and Physics, Department of Numerical Mathematics, will present a talk on:

Block Krylov methods for functions of matrices

Abstract

A variety of block Krylov subspace methods have been successfully developed for linear systems and matrix equations. The application of block Krylov methods to computing matrix functions is, however, less established, despite the growing prevalence of matrix functions in scientific computing. Of particular importance is the evaluation of a matrix function on not just one but multiple vectors. The main contribution of this work is a class of efficient block Krylov subspace methods tailored precisely to this task. With the full orthogonalization method (FOM) for linear systems forming the backbone of our theory, the resulting methods are referred to as $B(FOM)^2$: block FOM for functions of matrices. Many other important results are obtained in the process of developing these new methods. Matrix-valued inner products are used to construct a general framework for block Krylov subspaces that encompasses already established results in the literature. Convergence bounds for $B(FOM)^2$ are proven for Stieltjes functions applied to a class of matrices which are self-adjoint and positive definite with respect to the matrix-valued inner product. A detailed algorithm for $B(FOM)^2$ with restarts is developed. Its efficiency is based on a recursive expression for the error, which is also used to update the solution. Numerical experiments demonstrate the power and versatility of this new class of methods for a variety of matrix-valued inner products, functions, and matrices.