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Numerical Solution of PDE Eigenvalue Problems

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Abstract. This workshop brought together researchers from many different areas of numerical analysis, scientific computing and application areas, ranging from quantum mechanics, acoustic field computation to material science, working on eigenvalue problems for partial differential equations. Major challenges and new research directions were identified and the interdisciplinary cooperation was strengthened through a very lively workshop with many discussions.

Mathematics Subject Classification (2010): 35P30, 45C05, 65L15.

Introduction by the Organisers

The numerical solution of eigenvalue problems for partial differential equations (PDEs) is an important task in many application areas such as:

- dynamics of electromagnetic fields;
- electronic structure calculations;
- band structure calculations in photonic crystals;
- vibration analysis of heterogeneous material structures;
- particle accelerator simulations;
- vibrations and buckling in mechanics, structural dynamics;
- neutron flow simulations in nuclear reactors; and many more.

The topic involves theoretical research in several different areas of mathematics ranging from operator theory and matrix computation to modern numerical treatment of partial differential equations. It is also related to computer science, since the novel mathematical ideas, related to efficient computation of eigenvalues and invariant subspaces, need to be efficiently implemented in modern high performance software. This must be highly parallel, taking advantage of availability of thousands of multi-core computer processors, which adds significant constraints on possible algorithms and brings new practical and theoretical challenges.

In recent years major research developments in the area of PDE eigenvalue problems have taken place including the following:

- meshless and generalized finite element method approximation methods;
- adaptive finite element methods;
- methods for polynomial and other nonlinear eigenvalue problems
- a priori and a posteriori eigenvalue and eigenvector error estimation;
- convergence theory for preconditioned and inexact eigensolvers;
- multigrid, domain decomposition and incomplete factorization based preconditioning for eigenproblems;
- public software implementing efficient eigensolvers for parallel computers.

Novel research directions have appeared for non-linear, non-selfadjoint, and parameter-dependent problems. New homotopy approaches are combined with PDE eigensolvers in order to deal with optimization problems, where the PDE eigenvalue problem appears in the inner loop. Very recently, a new perturbation/error analysis has evolved that applies directly to nonlinear eigenvalue problems.

Nevertheless, many difficult questions remain open even for linear eigenvalue problems including the design of good error estimators, the solution effective recycling of computed information in homotopy or optimization methods, and the treatment of multiple eigenvalues and other ill-conditioned problems. As computers continue getting more powerful, the size of matrices involved in eigenvalue and singular value computations keeps growing. Numerical solution of billion-size problems is now typical in quantum mechanics as well as in many engineering applications. The issues of numerical stability and round-off error analysis thus attract renewed attention.

These topics were addressed during the workshop, successfully taking advantage of the interdisciplinary interaction between researchers representing many different scientific fields related to eigenvalue problems and PDEs. Major challenges and further research directions were discussed and the road for further research cooperation was paved.

Workshop: Numerical Solution of PDE Eigenvalue Problems

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