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Ivan Lirkov
Svetozar Margenov
Jerzy Waśniewski
Plamen Yalamov (Eds.)

Large-Sale Scientific Computing

4th International Conference, LSSC 2003
Sozopol, Bulgaria, June 2003
Revised Papers



Springer

Ivan Lirkov Svetozar Margenov
Jerzy Waśniewski Plamen Yalamov

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Editors

Ivan Lirkov
Svetozar Margenov
Central Laboratory for Parallel Processing
Bulgarian Academy of Sciences
Acad. G.Bonchev Str., Bl. 25A, 1113 Sofia, Bulgaria
E-mail: {ivan,margenov}@parallel.bas.bg

Jerzy Waśniewski
Technical University of Denmark
Department of Informatics and Mathematical Modelling, IMM, DTU
Bldg. 305, 2800 Lyngby, Denmark
E-mail: jw@imm.dtu.dk

Plamen Yalamov
University of Rousse
Center of Applied Mathematics and Informatics
Studentska 8, 7017 Rousse, Bulgaria
E-mail: plamen.yalamov@allianz.bg

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Preface

The papers in this volume were presented at the 4th International Conference on Large-Scale Scientific Computations ICLSSC 2003. It was held in Sozopol, Bulgaria, June 4–8, 2003. The conference was organized and sponsored by the Central Laboratory for Parallel Processing at the Bulgarian Academy of Sciences. Support was also provided from the Center of Excellence “BIS 21” (funded by the European Commission), SIAM and GAMM. A co-organizer of this traditional scientific meeting was the Division of Numerical Analysis and Statistics of the University of Rousse.

The success of the conference and the present volume in particular are the outcome of the joint efforts of many colleagues from various institutions and organizations. First thanks to all the members of the Scientific Committee for their valuable contribution to forming the scientific face of the conference, as well as for their help in reviewing contributed papers. We would like to specially thank the organizers of the special sessions: R. Blaheta, N. Dimitrova, A. Ebel, K. Georgiev, O. Iliev, A. Karaivanova, H. Kosina, M. Krastanov, U. Langer, P. Minev, M. Neytcheva, M. Schäfer, V. Veliov, and Z. Zlatev. We are also grateful to the staff involved in the local organization.

Special Events:

- The conference was devoted to the 60th anniversary of Raytcho Lazarov.
- During the conference, the nomination for the World Level of the Hall of Fame for Engineering, Science and Technology, HOFEST, was officially awarded to Owe Axelsson.

Traditionally, the purpose of the conference is to bring together scientists working with large-scale computational models of environmental and industrial problems, and specialists in the field of numerical methods and algorithms for modern high-speed computers. The key lectures reviewed some of the advanced achievements in the field of numerical methods and their efficient applications. The ICLSSC 2003 talks were presented by university researchers and practical industry engineers, including applied mathematicians, numerical analysts and computer experts. The general theme for ICLSSC 2003 was Large-Scale Scientific Computing, focusing on:

- Recent achievements in preconditioning techniques;
- Monte Carlo and quasi-Monte Carlo methods;
- set-valued numerics and reliable computing;
- environmental modelling;
- large-scale computations for engineering problems.

More than 90 participants from all over the world attended the conference, representing some of the strongest research groups in the field of advanced large-

scale scientific computing. This volume contains 55 papers submitted by authors from over 20 countries, out of which 5 were invited and 50 were contributed.

The 5th International Conference LSSC 2005 is planned for June 2005.

November 2003

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Part I

Invited Papers

Eigenvalue Estimates for Preconditioned Saddle Point Matrices

Owe Axelsson

University of Nijmegen, Nijmegen, The Netherlands
axelsson@math.kun.nl

Abstract. Eigenvalue bounds for saddle point matrices on symmetric or, more generally, nonsymmetric form are derived and applied for preconditioned versions of the matrices. The preconditioners enable efficient iterative solution of the corresponding linear systems.

1 Introduction

Matrices on saddle point form arise in constrained problems which in various forms occur in applications such as in constrained optimization, flow problems for incompressible materials, and domain decomposition methods, to name a few. For large scale such problems iterative methods must be used and require then efficient preconditioners.

We derive first bounds on the eigenvalues of symmetric forms of saddle point matrices, showing how they depend on the top matrix block and the Schur complement matrix. The bounds are then improved using a congruence transformation of the matrix, which makes the off-diagonal matrices small. The transformation is followed by a block-diagonal preconditioner. It is seen that the off-diagonal blocks have only a second order influence on the resulting eigenvalue bounds, and the eigenvalues depend mainly only on the preconditioned top matrix and negative Schur complement matrix, which, by assumption, both have positive eigenvalues. The eigenvalues of the resulting preconditioned matrix are real and cluster around -1 and $+1$.

A corresponding form of transformation can be applied for nonsymmetric matrices. One source of nonsymmetry can be due to a shift of sign of the constrained equations and we show in this case how the eigenvalues of the preconditioned matrix cluster around the unit number in the complex plane.

The preconditioned matrix problems can be solved using a generalized minimal residual form of the conjugate gradient method. For intervals symmetrically located around the origin, the effective condition number equals the square of the condition number for each of the two intervals, showing the importance of having preconditioned the matrices to have intervals with sufficiently small condition numbers.

For problems where the matrix defining the constraint is (nearly) rank deficient or, equally, the corresponding term in the Schur complement matrix has a zero or small eigenvalues, one can apply a regularization technique to stabilize the smallest eigenvalue. Such methods have been used in [1, 3], for instance.