1-day workshop, TU Eindhoven, April 17, 2012

"Recent developments in the solution of indefinite systems"

Organizers: Wil Schilders (TU Eindhoven), Kees Vuik (TU Delft), Mike Botchev (Univ. Twente)

The numerical approximation of several important scientific and engineering problems leads to block-structured indefinite linear systems in saddle point form. These problems arise in systems of PDEs with conservation laws, in constrained optimization problems, in mixed finite element discretizations, and in generalized least squares problems. Their efficient numerical solution is the subject of much research. The successful design of robust, scalable, and efficient preconditioners is intimately connected with an understanding of the structure of the resulting block matrix system, and relies heavily on exploiting this structure. Effective preconditioners are often based on an approximate block decomposition of the system that derives from a careful consideration of the spectral properties of the component block operators and the Schur complement operators. Through this purely algebraic view of preconditioning, a simplified system of block component equations is developed that encodes a specific "physics based" decomposition. Recent progress based on these ideas has led to the construction of a number of effective preconditioners with optimal or nearly optimal convergence rates for several applications. However, to compute accurate solutions to saddle point problems at a reasonable cost has proved difficult. As a consequence, a significant effort has been devoted to define proper formulations, discretizations, and fast solution methods for discretized saddle point problems and their generalizations.

This workshop brings together experts on the continuous and discrete formulation of saddle point problems from several areas of computational science, both for specific and general problems, and on efficient (parallel) solution techniques for the resulting systems of equations. This workshop will be useful both to researchers dealing with applications that give rise to saddle point problems and to developers of effective solution techniques for the resulting equations.

Invited speakers:

Michele Benzi (Emory State University, Atlanta, USA): "New block preconditioners for saddle point problems"

Andy Wathen (Oxford University, UK): "Combination Preconditioning of saddle-point systems for positive definiteness"

Miroslav Rozloznik (Academy of Sciences, Prague, CZ): "Implementation and numerical stability of saddle point solvers"

Marc Baboulin (University Paris-Sud, Paris, FR): "A parallel tiled solver for dense symmetric indefinite systems on multicore architectures

Luca Bergamaschi (University of Padua, IT): "Relaxed mixed constraint preconditioners for Ill-conditioned symmetric saddle point linear systems"

Participation is free of charge, but registration is mandatory. Please send an e-mail to w.h.a.schilders@tue.nl before April 1, 2012. There is a limited number of time slots available for short (5, 10 or 15 minute) presentations, please include your proposal (title, abstract, duration) in the e-mail.

Michele Benzi: "New block preconditioners for saddle point problems"

In this talk I will describe a class of block preconditioners for linear systems in saddle point form. The main focus is the solution of Stokes and Oseen problems from incompressible fluid dynamics; however, the techniques can be applied to other saddle point problems as well. The main idea is to split the coefficient matrix into the sum of two matrices (three for 3D problems), each of which contains only operators corresponding to components of the solution associated with one space variable. The resulting preconditioner requires the (uncoupled) solution of discretized scalar elliptic PDEs, which can be accomplished using standard algebraic multilevel solvers. The performance of the preconditioner can be improved by means of a relaxation parameter, which can be chosen on the basis of a local Fourier analysis. The robustness of these preconditioners with respect to problem parameters will be discussed, together with the effect of inexact solves. This is joint work with Michael Ng, Qiang Niu and Zhen Wang.

Andy Wathen: "Combination preconditioning of saddle-point systems for positive definiteness"

There are by now several examples of preconditioners for saddle-point systems which destroy symmetry but preserve self-adjointness in non-standard inner products. The method of Bramble and Pasciak was the earliest of these. We will describe how combining examples of this structure allow the construction of preconditioned matrices which are self adjoint and positive definite and allow rapid linear system solution by the Conjugate Gradient method in the appropriate inner product.

Marc Baboulin*:* "A parallel tiled solver for dense symmetric indefinite systems on multicore architectures"

We present an efficient and innovative parallel tiled algorithm for solving symmetric indefinite systems on multicore architectures. This solver avoids the communication overhead due to pivoting by using symmetric randomization. This randomization is computationally inexpensive and requires very little storage. Following randomization, a tiled LDLT factorization is used that reduces synchronization by using static or dynamic scheduling. Performance results are given, together with tests on accuracy.

Implementation and numerical stability of saddle point solvers

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Saddle–point problems arise in many application areas such as computational fluid dynamics, electromagnetism, optimization and nonlinear programming. Particular attention has been paid to their iterative solution. In this contribution we analyze several theoretical issues and practical aspects related to the preconditioning of Krylov subspace methods when applied to saddle point problems. Several structure–dependent schemes have been proposed and analyzed. It is well-known that the application of positive definite block-diagonal preconditioner still leads to the symmetric preconditioned system with a structure similar to the original saddle point system. On the other hand, the application of symmetric indefinite or nonsymmetric block-triangular preconditioner leads to nonsymmetric triangular preconditioned systems and therefore general nonsymmetric iterative solvers should be considered. The experiments however indicate that Krylov subspace methods perform surprisingly well on practical problems even those which should theoretically work only for symmetric systems.

We illustrate our theory mainly on the constraint (null-space projection) preconditioner, but several results hold and can be extended for other classes of systems and preconditioners. The research in case of the indefinite constraint preconditioner has focused on the use of the conjugate gradient method (PCG). The convergence of PCG for a typical choice of right-hand side has been analyzed and it was shown that solving the preconditioned system by means of PCG is mathematically equivalent to using the CG method applied to the projected system onto the kernel of the constraint operator. Consequently, the primary variables in the PCG approximate solution always converge to the exact solution, while the dual variables may not converge or they can even diverge. The (non)convergence of the dual variables is then reflected onto the (non)convergence of the total residual vector. It can be often observed in practical problems that even simple scaling of the leading diagonal block by diagonal entries may easily recover the convergence of dual iterates. An alternative strategy consists in changing the conjugate gradient direction vector when computing the dual iterates into a minimum residual direction vector. The necessity of scaling the system is even more profound if the method is applied in finite precision arithmetic. It can be shown that rounding errors may considerably influence the numerical behavior of the scheme. More precisely, bad scaling, and thus nonconvergence of dual iterates, affects significantly the maximum attainable accuracy of the computed primary iterates. Therefore, applying a safeguard or pre–scaling technique, not only ensures the convergence of the method, but it also leads to a high maximum attainable accuracy of (all) computed iterates.

For large–scale saddle point problems, the exact application of preconditioners may be computationally expensive. In practical situations, only approximations to the inverses of the diagonal block or the related cross-product matrices are considered, giving rise to inexact versions of various solvers. Therefore, the approximation effects must be carefully studied. Two main representatives of the segregated solution approach are analyzed: the Schur complement reduction method, based on an (iterative) elimination of primary variables and the null-space projection method which relies on a basis for the null-space for the constraints. In particular, for several mathematically equivalent implementations we study the influence of inexact solving the inner systems and estimate their maximum attainable accuracies. We can show that some implementations lead ultimately to residuals on the level of the roundoff, independently of the fact that the inner systems were solved inexactly on a much higher level than their level of limiting accuracy. Indeed, our results confirm that some implementations can deliver approximate solutions which satisfy either the second or the first block equation to working accuracy. We give a theoretical explanation for some behavior which has been observed, or is tacitly known. The implementations that we point out as optimal are seen to be those which are widely used and often suggested in applications.

Relaxed Mixed Constraint Preconditioners for Ill-conditioned Symmetric Saddle Point Linear Systems

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The aim of this communication is to describe efficient preconditioners for the iterative solution of the generalized saddle point linear system of the form $\mathcal{A}\boldsymbol{x} = \boldsymbol{b}$, where $\mathcal{A} = \begin{bmatrix} A & B^\top \\ B & -C \end{bmatrix}$. The matrix block A is SPD, C is symmetric semi-positive definite (possibly the zero matrix) and B is a full-rank rectangular matrix. The MCP (Mixed Constraint Preconditioner) [2] is based on two preconditioners for A (P_A and $\widetilde{P_A}$) and a preconditioner (P_S) for the Schur complement matrix $S = B\widetilde{P_A}^{-1}B^\top + C$. It is defined as $\mathcal{M}^{-1}$ where $\mathcal{M}^{-1}\mathcal{A}$ where

$$\mathcal{M} = \begin{bmatrix} I & 0 \\ BP_A^{-1} & I \end{bmatrix} \begin{bmatrix} P_A & 0 \\ 0 & -P_S \end{bmatrix} \begin{bmatrix} I & P_A^{-1}B^\top \\ 0 & I \end{bmatrix}.$$

We analyze the spectral properties of $\mathcal{M}^{-1}\mathcal{A}$ providing very tight bounds [1] especially for extremal real eigenvalues.

A further evolution of MCP is the family of Relaxed Mixed Constraint Preconditioners (RMCP), based on a relaxation parameter ω, which we denote by $\mathcal{M}^{-1}(\omega)$ where

$$\mathcal{M}(\omega) = \begin{bmatrix} I & 0 \\ BP_A^{-1} & I \end{bmatrix} \begin{bmatrix} P_A & 0 \\ 0 & -\omega P_S \end{bmatrix} \begin{bmatrix} I & P_A^{-1}B^\top \\ 0 & I \end{bmatrix}.$$

Eigenanalysis of $\mathcal{M}^{-1}(\omega)\mathcal{A}$ shows that the optimal ω is related to the spectral radius of $P_A^{-1}A(\rho_A)$and $P_S^{-1}S(\rho_S)$. The values of ρ_A and ρ_S can be cheaply approximated by a few iterations of e.g. the Lanczos method.

We will present a set of numerical results onto large linear systems arising from realistic coupled consolidation models in geomechanics as well as from Mixed Finite Element discretization of Darcy's law in porous media. These results [3] show that proper choice of ω driven by approximate knowledge of ρ_A and ρ_S leads to a CPU time reduction up to a factor three in the most ill-conditioned test case with respect to MCP.

References

[1] L. Bergamaschi, *Eigenvalue distribution of constraint-preconditioned symmetric saddle point matrices*, Numer. Lin. Alg. Appl., (2012). Published online on October 18, 2011.

[2] L. Bergamaschi, M. Ferronato, and G. Gambolati, *Mixed constraint preconditioners for the solution to FE coupled consolidation equations*, J. Comp. Phys., 227 (2008), pp. 9885–9897.

[3] L. Bergamaschi and A. Martínez, *RMCP: Relaxed mixed constraint preconditioners for saddle point linear systems arising in geomechanics*, Comp. Methods App. Mech. Engrg., (2012). Submitted.