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

"Recent developments in the solution of indefinite systems"

Location: "De Zwarte Doos" (TU/e campus)

:10.25-10.30: Opening and word of welcome
10.30-11.15: Michele Benzi: "New block preconditioners for saddle point problems"
11.15-11.30: Coffee break
11.30-12.15: Andy Wathen: "Combination Preconditioning of saddle-point systems for positive definiteness"
12.15-12.30: Jos Maubach: ""Micro- and macro-block factorizations for regularized saddle point systems"
12.30-12.45: Karl Meerbergen: "A shifted preconditioner for the damped Helmholtz equation"
12.45-13.45: Lunch
13.45-14.30: Miroslav Rozloznik: "Implementation and numerical stability of saddle point solvers"
14.30-14.45: Fred Wubs: "Structure preserving preconditioner for the incompressible Navier-Stokes equations"
14.45-15.00: Christiaan Klaij: The use of SIMPLE-type preconditioners in maritime CFD applications"
15.00-15.30: Coffee/tea
15.30-16.15: Marc Baboulin: "A parallel tiled solver for dense symmetric indefinite systems on multicore architectures
16.15-17.00: Luca Bergamaschi: "Relaxed mixed constraint preconditioners for Ill-conditioned symmetric saddle point linear systems"
17.00-17.15: Pawan Kumar: "A Purely algebraic domain decomposition method for the incompressible Navier-Stokes equation"
17.15-17.30: Sebastiaan Breedveld: "Optimization in cancer treatment: indefinitely a problem?"
17.30: Closing
18.00: Dinner for invited speakers

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.

3TU.AMI

MATHEMATICS FOR INNOVATION

NDNS+

CASA

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.

Jos Maubach: “Micro- and macro-block factorizations for regularized saddle point systems”

We present a unique micro-/macro-block Crout-based factorization for matrices from regularized saddle-point problems, and prove that this factorization exists for semi-positive definite regularization blocks. For the classical case of saddle-point problems we show that the induced macro-block factorizations strongly resembles the Schilders' factorization. The presented factorization can be used as a direct solution algorithm for regularized saddle-point problems as well as for the construction of preconditioners.

Christiaan Klaij: “The use of SIMPLE-type preconditioners in maritime CFD applications”

CFD applications in maritime industry typically require the solution of the incompressible, Reynolds-averaged Navier-Stokes equations at high Reynolds numbers. At the Maritime Research Institute Netherlands (MARIN), we use a finite volume method for cell centered, collocated variables on unstructured grids. The system of equations, linearized with Picard, is solved by using SIMPLE-type methods either as solver or as preconditioner. In this presentation, we discuss both approaches and compare their performance for the flow around ship hulls with Reynolds number up to 1e9 and cell aspect ratio up to 1e6.

Karl Meerbergen: “A shifted preconditioner for the damped Helmholtz equation”

Ref. K. Meerbergen and J.-P. Coyette, Connection and comparison between frequency shift time integration and a spectral transformation preconditioner , Numerical Linear Algebra and Applications, 16:1-17, 2009.

Fred Wubs: "Structure preserving preconditioner for the incompressible Navier-Stokes equations"

In the talk a new preconditoner for the coupled incompressible Navier-Stokes equation will be discussed for matrices arising from a marker and cell finite volume discretization. This preconditioner shows optimal convergence and allows for parallelization. The traditional tools for a good incomplete factorization are suitable reordering and dropping; here, we add local transformations on matrix and unknowns. It will be shown that this leads to a robust preconditioner, moreover some results will be shown for application to bordered systems which occur for example in the Jacobi Davidson method.

Pawan Kumar: "A Purely algebraic domain decomposition method for the incompressible Navier-Stokes equation"

In this talk, a Schur complement based approach is used for the solution of incompressible Navier-Stokes equation. The global Schur complement is approximated by Schur complements in patches. The approach leads to a parallel construction and solve process within a preconditioned iterative method. The method is particularly attractive for problems with high Reynolds numbers. The method is also compared with the existing state of the art methods.

Sebastiaan Breedveld: "Optimization in cancer treatment: indefinitely a problem?"

In radiation therapy, patients suffering from cancer are treated by irradiating the tumour with ionizing beams. The irradiation does not only "harm" cancerous cells, but also healthy tissue. The key is to design a treament plan that sufficiently irradiates the tumour to erradicate it, but also keeps the dose (harm done by irradiation) to the healthy tissue within limits, and generally as low as possible. The broad radiation therapy treatment planning problem falls in the category of a large scale combinatory non-convex multi-criteria optimization problem. The (non-convex) optimization part can be treated as a general mathematical solver, which is currently implemented as an interior-point method.

Solving a general constrained optimization problem eventually leads to solving the reduced Karush-Kuhn-Tucker system, which is an indefinite matrix. The class is large-scale: 500-5000 (or starting at 15.000 for other treatment modalities) descision variables, and at least 50.000 constraints. There are several challeging points in solving the indefinite system: 1) is the non-sparsity of the problem: explicit construction of the indefinite system is not possible. 2) precision of the solution: as solving the system is part of an interior-point solver, the system should be solved accurately in order for the optimization to converge properly. 3) preconditioner without constructing the system.

Currently, solving is done by further reducing the Karush-Kuhn-Tucker system to a dual-norm matrix. This is an expensive operation, as it involves matrix-matrix computations. One other approach is the L-BFGS-B method, but this is not yet implemented.

Implementation and numerical stability of saddle point solvers

Miroslav Rozložník

Institute of Computer Science
Academy of Sciences of the Czech Republic
CZ 182 07 Prague 8, Czech Republic
e-mail: miro@cs.cas.cz

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

Luca Bergamaschi, Dipartimento di Ingegneria Civile Edile e Ambientale
University of Padova, e-mail luca.bergamaschi@unipd.it

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.