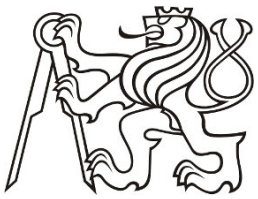

Department of Mathematics
Faculty of Civil Engineering
Czech Technical University in Prague

Preconditioning of Iterative Methods

Theory and Applications

A Conference in Honor of Ivo Marek

Book of Abstracts

July 1 – 5, 2013

Prague

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Foreword

Dear Participant,

Welcome to the PIM 2013 conference held on the premises of the Faculty of Civil Engineering, Czech Technical University in Prague, from July 1 to July 5, 2013. The acronym PIM stands for the first part of Preconditioning of Iterative Methods – Theory and Applications. Although this topic itself is worth scholarly disputation, the conference is also organized to honor Professor Ivo Marek on the occasion of his 80th birthday.

Ivo Marek graduated from Charles University in Prague in 1956 and began his career at the Nuclear Research Institute where he pursued the numerical modeling of processes in nuclear reactors. This research increased his interest in (numerical) linear algebra and operator theory; topics for which he is renowned.

In 1963, he joined the Faculty of Mathematics and Physics, Charles University, where he had spent more than 30 fruitful years. On the brink of retirement, he joined the Faculty of Civil Engineering, Czech Technical University in Prague, where he is still active both in research and in PhD courses.

The conference subtopics are based on Ivo's areas of interest and include:

i. preconditioning of sparse matrix problems, symmetric or non-symmetric, arising in large-scale real applications;
ii. multilevel preconditioning techniques, including multigrid, algebraic multilevel, and domain decomposition methods for partial differential equations;
iii. multilevel solution of characteristics of Markov chains.

The conference program consists of 15 plenary lectures, 28 contributed talks, and 8 posters. Around 90 participants from 20 countries registered for the conference.

The participants are given an opportunity to submit a research paper based on their PIM 2013 presentation for possible publication in either a special issue of Numerical Linear Algebra with Applications (NLAA; http://onlinelibrary.wiley.com/journal/10.1002/%28ISSN%291099-1506) or special PIM 2013 sections of Applications of Mathematics (AM; http://am.math.cas.cz/).

All submissions will be peer-reviewed. The former journal (NLAA) accepts manuscripts on topics related to numerical analysis, with emphasis on numerical linear algebra and its applications. The latter journal (AM) focuses mainly on mathematical methods for solving problems related to differential equations and their applications.

We hope that you enjoy your stay in Prague.

Sincerely,

Ivana Pultarová

on behalf of the PIM 2013 Organizing Committee

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Plenary Lectures

Preconditioning methods for high order strongly stable time integration methods with an application for a DAE problem

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A particular type of high order stable time integration method enables the use of large time-steps and is applicable also for differential-algebraic problems, without any order reduction. To solve the arising block matrix systems, an efficient preconditioning method is presented and analysed. The method is applied for the solution of a Biot-Wallis type of consolidation problem arising in poroelasticity.

Polynomial acceleration of GeneRank

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The ranking of genes plays an important role in biomedical research. The GeneRank method of Morrison, Breitling, Higham and Gilbert ranks genes based on the results of microarray experiments combined with gene expression information, for example from gene annotations. The algorithm is a variant of the well known PageRank iteration, and can be formulated as the solution of a large, sparse linear system. Due to the irregular structure of the underlying graph, sparse direct solvers suffer tremendous fill-in on this type of problem and thus cannot be recommended.

Here we show that classical Chebyshev semi-iteration can considerably speed up the convergence of GeneRank, outperforming other acceleration schemes such as conjugate gradients (CG). We also consider the use of polynomial preconditioning schemes for the CG algorithm.

This is joint work with Verena Kuhlemann.

Iterative methods around porous media flow and elasticity

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Processes in porous media, involving mechanical deformation and fluid flow in porous space, deserve more and more applications. Linear poroelasticity or nonlinear poromechanics are applied in soil and rock mechanics, but also in biomechanics, filtration technologies, fuel cells and others. In these fields, one needs demanded computations of coupled multiphysics problems, which require space and time discretization and efficient, parallelizable iterative methods with suitable preconditioners for the solution of the arising large scale systems.

For the iterative solution of such systems, we use Krylov type iterative methods with preconditioners, which exploit the natural block decomposition provided by the physics and saddle point structure of the matrices. The saddle point structure is provided by both multiphysics and mixed finite element discretization. In this contribution, we review such preconditioners and introduce some new variants based on the Schur complement. We also provide analysis and comparison of diagonal and block triangular variants and discussion on efficient implementation. Finally, we indicate some possible extension for solving more complicated models, which couples multiphase flow and more general mechanical behaviour.

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Structured preconditioners for Markov and Markov regenerative processes

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Modeling formalisms like queueing networks, stochastic Petri nets, stochastic automata or other formal description techniques are often used to specify models that describe Markov Processes or Markov Regenerative Processes. The matrices governing the process behavior have a very regular structure that can be interpreted as a block-strcutured matrix where every block is represented as a sum of Kronecker products of small component matrices. Steady state analysis of the processes requires the solution of a set of linear equations with a coefficient matrix of the mentioned type. Since the resulting systems of equations are huge for realistic examples, efficient solution methods are necessary.

The talk presents an overview of solution methods that exploit the structure of the coefficient matrix for building preconditoners. In particular preconditioning techniques are proposed that generate a preconditioner by modifying only the small matrices in the Kronecker products and not the global coefficient matrix. Those preconditioners, which are denoted as structured, can be generated efficiently and require only negligible memory compared to the solution vector. Preconditioning uses a Schur factorization of the component matrices. The talk discusses the advantages and disadvantages of using real or complex Schur factorizations in preconditioning. Finally, experimental results for several example models that are analyzed with different solution techniques are presented.

Eventually SDD matrices and their applications

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A matrix A is called *nonnegative* if it is entrywise nonnegative, and it is called *eventually nonnegative* if A^k is nonnegative for all sufficiently large integers k. An *M-matrix* A has the form $A = sI - B$, where B is a nonnegative matrix and $s \geq \rho(B)$, the spectral radius of B. If, in addition, $s > \rho(B)$, then A is a nonsingular M-matrix. Recently, several generalizations of M-matrices, based on replacing nonnegativity of B by conditions related to eventual nonnegativity of B, have been considered. Following the same path of generalization, we will discuss some possibilities to extend SDD class to *eventually SDD* one, and, then, apply the new classes to two important problems in applied linear algebra: eigenvalue localization and max norm estimation for the inverse of a given matrix.

Iterative aggregation–disaggregation for Markov chains: The Czech perspective

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Markov chains are widely used to model systems which evolve by visiting the states in their state spaces following the available transitions. In these models, the probability distribution of the next state of a system conditioned on its current state and the previous states it has visited depends only on its current state. In discrete time, this requires that the time spent in a state during a visit be geometrically distributed, whereas in continuous time it requires that the time spent in a state during a visit be exponentially distributed. Markov chains can be analyzed probabilistically for their steady-state and transient behavior using numerical linear algebra to improve existing systems or to devise new systems that meet certain requirements. One of the most effective methods for computing the steady-state probability distribution of a Markov chain is iterative aggregation–disaggregation. To be able to use this method, first a partitioning of the state space into subsets of states needs to be identified. Once this is done, the method proceeds iteratively in a two-level manner starting with an initial approximate solution to the original problem. At the coarse level, each subset of states is aggregated into a single state using the previous solution to the problem and an aggregated, smaller, but new problem is obtained and solved. Then this new solution at the coarse level is used to compute a hopefully better solution to the original problem at the fine level. The method is of a divide-and-conquer nature and can be extended to more than two levels. The objective for this iterative multi-level approximation is to converge relatively fast to the exact steady-state probability distribution of the Markov chain at hand with reasonable accuracy. This talk celebrates and tries to put into perspective the contributions of Ivo Marek and his collaborators over many years to this particular area.

The role of generalized matrix inverses in Markov chains

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Generalized matrix inverses play significant roles in solving for various key properties of finite, irreducible, Markov chains, in particular, the stationary distribution and the moments of the first passage time distributions. This arises from the observation that generalized matrices are used to solve systems of singular linear equations. In the context of Markov chains, we consider generalized matrix inverses of the singular Markovian kernel, I - P, where P is the transition matrix of the Markov chain.

We survey the application of generalized matrix inverses to such problems. We also establish that, under the aforementioned conditions, all generalized inverses of the Markovian kernel can be uniquely specified in terms of the stationary probabilities and the mean first passage times of the underlying Markov chain. Special sub-families include Meyer's group inverse of I - P, Kemeny and Snell's fundamental matrix of the Markov chain, and the Moore-Penrose g-inverse.

Eigenvalues of hollow, symmetric, nonnegative matrices

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An n-by-n matrix is called "hollow" if all it's diagonal entries are 0. A hollow, symmetric, irreducible, (entry-wise) nonnegative matrix (n-by-n, with $n > 2$) must have at least two negative eigenvalues, because of Perron-Frobenius; if only two, it must be nonsingular. Distance matrices and adjacency matrices of graphs are good examples. We were motivated to study such matrices by an initial desire to understand inequalities between diagonal entries and eigenvalues of LaPlacians. There are such inequalities that do not occur for general symmetric matrices. However, this study led many interesting places, which we will survey. For example, anywhere from 2 to $n-1$ nonpositive eigenvalues may occur, though 2 is extraordinarily rare for large n. When 2 occurs, it is associated with remarkable matrix structure. Very modest assumptions about the off-diagonal entries require the number of nonpositive eigenvalues to grow with n (eg adjacency matricies).

Stochastic solution of large least squares systems in variational data assimilation

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The 4DVAR method of data assimilation requires the solution of a large nonlinear least squares problem. The Gauss-Newton or the Levenberg-Marquardt method require the solution of a large linear least squares system in each iteration. The solution can be cast as the output of the Kalman smoother for a linearized problem. A Monte-Carlo method, the ensemble Kalman smoother, is used as an approximate linear solver. The ensemble approach is computationally efficient and naturally parallel over the ensemble members, the linear least squares system is never formulated explicitly, and no tangent or adjoint operators are needed. The ensemble approximations converge stochastically to the exact solution of the linear least squares problem by a law of large numbers in the ensemble size. However, a small ensemble is sufficient for the approximate linear solver in the nonlinear iterative process.

Compartmental systems and IAD computations

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The following features of the compartmental systems are discussed:

- Stationary states and their computation
- Boundary layer phenomena
- IAD methods

Multilevel methods for strongly anisotropic problems

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Consider the following elliptic boundary-value problem:

$$
\begin{aligned}
&(1a) && -\nabla\cdot(\boldsymbol{a}(\boldsymbol{x})\nabla u(\boldsymbol{x})) &&= f(\boldsymbol{x}) && \text{in } \Omega,\\
&(1b) && u &&= 0 && \text{on } \Gamma_D,\\
&(1c) && (\boldsymbol{a}(\boldsymbol{x})\nabla u(\boldsymbol{x}))\cdot\boldsymbol{n} &&= 0 && \text{on } \Gamma_N.
\end{aligned}
$$

Here $\Omega \subset \mathbb{R}^2$ is a convex polygonal domain with boundary $\Gamma = \Gamma_D \cup \Gamma_N$, The coefficient matrix $\boldsymbol{a}(\boldsymbol{x}) = (a_{ij}(\boldsymbol{x}))_{i,j=1}^2$ is assumed to be symmetric positive definite. The main focus is on anisotropic problems, i.e., problems for which $\boldsymbol{a}(\boldsymbol{x})$ is ill-conditioned.

The Ritz-Galerkin method is used to approximate the solution of (1) using linear (conforming and non-conforming) or quadratic finite elements. The problem of finding the weak solution of (1) in V_h is equivalent to solving a system of linear algebraic equations $A\mathbf{u} = \mathbf{f}$, where A denotes the stiffness matrix, $\mathbf{f}$ the right hand side and $\mathbf{u}$ the vector of nodal unknowns.

A partitioning of the set $\mathcal{D}$ into a set $\mathcal{D}_{\rm f}$ of fine DOF and a set $\mathcal{D}_{\rm c}$ of coarse DOF is performed, i.e. $\mathcal{D} = \mathcal{D}_{\rm f} \oplus \mathcal{D}_{\rm c}$, where $\mathcal{D}_{\rm c}$ is associated with an augmented coarse grid. Then we define the preconditioner

$$
(2) \qquad B = \begin{bmatrix} I & -{B_{\rm ff}}^{-1}A_{\rm fc} \\ & I \end{bmatrix} \begin{bmatrix} {B_{\rm ff}}^{-1} & \\ & Q^{-1} \end{bmatrix} \begin{bmatrix} I & \\ -A_{\rm cf}{B_{\rm ff}}^{-1} & I \end{bmatrix},
$$

to approximate the inverse of A where Q is an assembly of Schur complements of properly scaled local (stiffness) matrices associated with a covering of the entire domain by overlapping subdomains, and $B_{\rm ff}$ is an approximation to the pivot block $A_{\rm ff}$ of A. Similar techniques have recently been applied successfully to piecewise bilinear approximations of problems with highly oscillatory coefficients.

Optionally, a (block) Gauss-Seidel smoother (for A) improves the preconditioner. This construction can be recursively extended to define a multilevel block-factorization. The use of the augmented coarse grid is the key to enhance the efficiency of the (block) smoother on the coarse level where Q plays the role of A. Based on these building blocks a nonlinear algebraic multilevel iteration (AMLI) method is defined.

The presented numerical results demonstrate the performance of the nonlinear W-cycle AMLI method for strongly anisotropic elliptic problems, including the case when the direction of dominating anisotropy is not aligned with the grid in this experiment.

A comparison between three implementations of the nonlinear W-cycle AMLI method is performed. Variant (1) is without additional global smoothing, variant (2) includes one symmetric point Gauss-Seidel (G-S) smoothing step while variant (3) makes use of one symmetric block Gauss-Seidel (G-S) smoothing step. Two inner generalized conjugate gradient (GCG) iterations are performed in the W-cycle on each coarse level except on the coarsest level where the problem is solved exactly.

Some robust results for high-frequency and high-contrast problems including strongly anisotropic channels are presented at the end.

Model reduction and preconditioned eigenvalue methods in noise analysis and noise reduction

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We discuss nonlinear parameter dependent eigenvalue problems arising in the the noise analysis of disk brakes. The problem of our partners in engineering and the car industry is to avoid squeaking of brakes in operation. To achieve this goal preconditioned iterative solution methods for the solution of nonlinear parameter dependent eigenvalue problems for the finite element models are studied. These are solved for a large set of parameters to achieve a parameter dependent small scale representation that can be used in noise reduction or compensation. We present some of the necessary analysis and several numerical results.

This is joint work with Sarosh Quraishi and Christian Schröder.

Challenges for the numerical solution methods when simulating multiphase flow problems

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Microstructure evolution in complex multiphase-multicomponent systems has been and is of significant importance for numerous industrial processes as well as for academic research, technology improvements and development of new materials and devices.

Phase transitions and morphological changes in microstructures take place in a variety of processes, such as spinodal decomposition, grain and crystal growth, solute drag, directional solidification, diffusion-controlled processes, reaction pathways controlling the structural evolution of complex material mixtures and many more. Today, a deeper understanding of the dynamics of those complex and coupled phenomena is to a large extent gained by computer simulations of the underlying processes, based on adequate mathematical models.

We discuss numerical simulations of multicomponent and multiphase systems, based on the so-called phase-field model. The major focus is on the arising algebraic structures and suitable preconditioned iterative methods to solve the arising nonlinear and linear systems of equations.

Functional analysis and algebraic iterative computations. There and back again.

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In mathematical modelling using partial differential equations, setting the mathematical model and its analysis is followed by discretization and by matrix computations for finding (an approximate) solution of the resulting finite dimensional algebraic problem. When such computations are performed iteratively, *preconditioning* is required in order to achieve a sufficiently accurate solution at an acceptable computational cost. Furthermore, *a posteriori* error analysis which takes into account algebraic errors and allows to construct appropriate stopping criteria becomes an inherent part of the algorithm.

This contribution recalls some views to iterative algebraic computations with emphasize on the interplay between modelling, discretization, analysis and computation. Efficiency of algebraic computations and their analysis depend on the knowledge of the context in solving the original infinite dimensional (physically motivated) problems. On the other hand, algebraic analysis can bring in issues such as non-asymptotic reasoning and investigation of numerical stability which can not be properly addressed by the functional analysis view.

After reviewing the whole concept we present particular examples illustrating individual points.

Preconditioned solution of the coupled Stokes-Darcy flow problem

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We consider the numerical description of the coupled Stokes-Darcy flow, i.e., of flow where one part of the domain is governed by a Stokes flow, and the other corresponds to porous media flow, along with coupling conditions on the interface. We propose the use of a constraint preconditioner for this problem. We provide spectral bounds for the preconditioned problems, which are independent of the size of the finite element mesh. We use both standard (continuous) finite elements for both flows, and also consider the case where the porous media flow is modeled with Discontinuous Galerkin methods. Numerical experiments illustrate our results, and comparisons with other saddle-point preconditioners found in the literature demonstrate the advantage of our approach. We also illustrate the high order convergence of the Discontinuous Galerkin method for this problem.

This is joint work with Prince Chidyagwai and Scott Ladenheim.

Enhancing eigenvector approximations of huge gyroscopic eigenproblems from AMLS with subspace iteration

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In this presentation we consider the problem to determine all eigenvalues in an interval $[0, \lambda_{\max}]$ and corresponding eigenvectors of a huge eigenvalue problem $Kx = \lambda Mx$, where K and M are the stiffness and the mass matrices of a finite element model.

A robust and efficient method is the subspace iteration method (SIM) which was developed about 40 years ago by Bathe [1]. At that time a typical task was to determine a small number of eigenmodes (10 to 20, e.g.) at the lower end of the spectrum, but today often hundreds of eigenpairs are needed for problems with millions of degrees of freedom [2,3].

Given a matrix V_0 containing approximations to the wanted eigenvectors the basic task in the jth step of SIM is to solve the block linear system $K\hat{V}_k = MV_{k-1}$ for $\hat{V}_k$ and to M-orthonormalize the columns of $\hat{V}_k$ to obtain the next

matrix V_k. Crucial for the success of SIM is to establish effective starting vectors V_0 and (in particular for huge problems) to solve the linear systems efficiently.

We propose to take advantage of automated multi-level sub-structuring (AMLS) for both tasks which combines block Gaussian elimination and modal reduction of sub-structures. Thus the size of the finite element model is reduced substantially yet yielding approximations to eigenmodes of moderate accuracy over a wide frequency range of interest. The essential steps of AMLS are the following ones: using a graph partitioning tool the original structure is divided into many substructures with multi levels. The stiffness matrix K is transformed into block diagonal form $\tilde{K}$ by block Gaussian elimination, and the eigenproblem is reduced by modal condensation of the substructure eigenproblems. These two steps are performed in an interleaving way to avoid the storage of the transformed mass matrix $\tilde{M}$, which would require plenty of extra storage.

Information from ASML is used in SIM exploiting the block-structure of $\tilde{K}$ but avoiding the use of the dense matrix $\tilde{M}$. To this end the current approximation $\tilde{V}_{k-1}$ is back transformed to V_{k-1} in the original FEM basis, V_{k-1} is multiplied by the original mass matrix M, MV_{k-1} is transformed to some matrix $\tilde{Z}_k$ in the AMLS basis, and finally $\tilde{K}\tilde{V}_k = \tilde{Z}_k$ is solved. Numerical experiments demonstrating the efficiency of this approach are given in the presentation, details are contained in the joint paper [3] with Pu Chen and Jiacong Yin, Peking University.

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Contributed Talks

Preconditioning of Krylov subspace methods using recycling in Lattice QCD

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Many applications in computational science and engineering require the solution of sequences of slowly changing linear systems. We focus on problems arising in Lattice QCD simulations. While computing masses of elementary particles, we have to solve a linear system with a Dirac operator in each time step of the hybrid Monte-Carlo simulations. This operator changes just slightly from time step to time step. While recycling subspace information from the previous system like described in [1] reduces the number of necessary matrix-vector multiplications, the systems are still expensive to solve. To overcome this limitation, we include preconditioning in our implementation.

We will present the approach and the results obtained, including the use of a Schwarz preconditioner.

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On the problem of interface weights in domain decomposition methods

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In many domain decomposition methods, an important question is how to average a discontinuous function at the interface between adjacent subdomains. Two standard approaches commonly found in literature are: (i) arithmetic average, based simply on counting number of subdomains at an interface unknown, and (ii) weighted average, with weights derived from diagonal stiffness of subdomain Schur complements with respect to the interface. Its simplification represents approximation of the diagonal of the Schur complement by the diagonal of the original matrix, also known as the *stiffness scaling* [3]. (The applicability of the so called *ρ-scaling*, see e.g. [3] or [4] for theoretical analysis, is limited to the case of material coefficients constant on each subdomain, which is not preserved in our examples and consequently this approach is not included in this study.)

In our work we study performance of these standard choices on a series of two-dimensional numerical experiments with the Poisson equation. In addition to the standard approaches, two new methods are included – averaging based on a unit jump on the interface, and a new approach based on a unit load applied on boundary of a subdomain, both described in [1]. Regular and irregular subdomains were used for testing, and also jumps in material coefficients were present, with different alignment with respect to interface. The Balancing Domain Decomposition by Constrains (BDDC) method [2] is used for this study.

No approach is shown to be universally superior to others. The two new approaches are shown to be competitive with the standard ones; in certain situations they can be preferable.

Acknowledgements

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National Supecomputing Center – new opportunities and challenges

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We first briefly recall the development of HPC in Ostrava from the early modest results in iterative solution of large (by then standards) problems motivated by the needs posed by mining engineering, with grateful acknowledgement of the role of the birthday person and his summer schools, to establishing the systematic research in HPC related fields within the National Supercomputing Center. The traditional research was transformed toward the development of scalable massively parallel algorithms for the solution of problems of computational mechanics and other fields. A true breakthrough is related to the participation in the Partnership for Advanced Computing in Europe (PRACE) project. The project supports access to the European supercomputer centers, including Tier 0. Both the senior and young researchers from the HPC related research programs participated in the specialized workshops, got new skills, implemented powerful software, and entered the international cooperation. The scope of the research was extended by new highly qualified staff, often hired abroad. For example, the numerical research includes the multiscale problems, multiphysics problems, aposteri error estimates, and adaptive discretization. The group working in molecular dynamics was strengthened by the young staff of physicists and computer scientists. The solution of external problems by the fast boundary element methods found applications in magnetooptics. Interesting applications of dynamic systems were found in economy and mechanics, in particular in the analysis of rotor dynamics. An overview of the research will be accompanied by applications.

DG for fluid-structure interaction problems

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The contribution will be concerned with the simulation of viscous compressible flow in time dependent domains. The motion of the boundary of the domain occupied by the fluid is taken into account with the aid of the ALE (Arbitrary Lagrangian-Eulerian) formulation of the Euler and Navier-Stokes equations describing compressible flow. They are discretized in space by the discontinuous Galerkin (DG) finite element method using piecewise polynomial discontinuous approximations. For the time discretization BDF method or DG in time is used. Moreover, we use a special treatment of boundary conditions and shock capturing, allowing the solution of flow with a wide range of Mach numbers. As a result we get an efficient and robust numerical process. The applicability of the developed method will be demonstrated by some computational results obtained for flow induced vibrations of an airfoil with two degrees of freedom.

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A philosophical note on the origin of smoothed aggregations

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We derive the smoothed aggregation two-level method from the variationalobjective to minimize the *final error* after finishing the entire iteration. This contrasts to a standard variational two-level method, where the coarse-grid correction vector is chosen to minimize the error after coarse-grid correction procedure, which represents merely an intermediate stage of computing. Thus, we enforce *the global minimization of the error*. The method with smoothed prolongator is thus interpreted as a qualitatively different, and more optimal, algorithm than the standard multigrid.

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Double preconditionings of IDR(s)Stab(ℓ) method for gaining both convergence rate and accuracy of approximated solutions

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We consider to solve a linear system of equations $A\boldsymbol{x} = \boldsymbol{x}$, where A is a given large sparse $N \times N$ nonsymmetric matrix and $\boldsymbol{x}$, $\boldsymbol{b}$ are solution, right-hand side vectors of order N, respectively. Sonneveld and van Gijzen proposed IDR(s) methods and IDR Theorem in 2007. This iterative method has a property that it requires at most $N + N/s$ matrix-vector multiplications to compute an exact solution in exact arithmetic mode. As variants of Bi-CG method, Sleijpen *et al.* derived IDR(s)Stab(ℓ) method as extension of BiCGStab(ℓ) method, and Tanio *et al.* derived also GBi-CGSTAB(s, ℓ) method by adapting polynomial of high order degree of ℓ to Bi-CG(s) and GBi-CG(s).

Concerning IDR(s) method, it is well known that, for large parameter s, there occasionally occurs spurious convergence phenomenon, i.e., the residual

computed in the algorithm being small, though the true residual is not small. As well as IDR(s) method, IDR(s)Stab(ℓ) and GBi-CGSTAB(s, ℓ) methods have the same property that spurious convergence occasionally occurs during iteration process.

In our talk, we propose double preconditioning strategies for IDR(s)Stab(ℓ) and GBi-CGSTAB(s, ℓ) methods in order to gain both convergence rate and accuracy of approximated solutions We present the numerical results that our preconditioning strategies work effectively in Table 1(a)-(c). "TRR" means True Relative Residual of $\log_{10}(||\boldsymbol{b} - A\boldsymbol{x}_{k+1}||_2/||\boldsymbol{b} - A\boldsymbol{x}_0||_2)$ for the converged approximated solutions $\boldsymbol{x}_{k+1}$. From this Table 1, we see that double preconditioning strategies is very effective in view of convergence rate and improvement of accuracy of the approximated solutions.

Table 1: Numerical results of IDR(s)Stab(ℓ) method for matrix dc3.
(a)without preconditioning

s	ℓ	IDR(s)Stab(ℓ)			new IDR(s)stab(ℓ)		
		itr.	time	TRR	itr.	time	TRR
4	1	824	3.78	-7.67	932	**3.39**	**-9.74**
4	2	854	4.60	-7.38	957	4.20	-9.76
4	4	904	5.79	-7.24	956	5.17	-9.71
4	6	1,024	7.83	-5.38	1,002	6.57	-9.75
4	8	1,084	9.58	-5.50	1,010	7.83	-9.71

(b)with ILU(0) preconditioning

s	ℓ	IDR(s)Stab(ℓ)			new IDR(s)stab(ℓ)		
		itr.	time	TRR	itr.	time	TRR
4	1	369	2.52	-7.13	404	**2.38**	**-10.91**
4	2	414	3.08	-6.15	435	2.80	-10.63
4	4	444	3.84	-6.04	451	3.43	-10.87
4	6	424	4.19	-2.63	457	4.01	-11.31
4	8	484	5.35	-0.69	444	4.43	-8.88

(c)with modified Eisenstat-SSOR preconditioning

s	ℓ	IDR(s)Stab(ℓ)			new IDR(s)stab(ℓ)		
		itr.	time	TRR	itr.	time	TRR
4	1	374	2.11	-10.47	374	**1.78**	**-10.78**
4	2	384	2.34	-9.77	397	2.06	-10.71
4	4	384	2.79	-9.21	385	2.45	-10.73
4	6	394	3.36	-6.87	394	2.95	-10.68
4	8	364	3.51	-5.16	404	3.49	-10.63

A smoothed aggregation MG method with small coarse space.

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We describe a general technique of aggressive coarsening in the framework of smoothed aggregation multilevel methods for the solving of elliptic type problems. This technique can be viewed as an alternative to domain decomposition method since as in this class of methods, it results in the solving of small coarse grid problem associated with parallel sub-domain solvers. The method, using a transformed Chebyschev polynomial (smoother) $S = pol(A)$, changes the original problem $A\mathbf{x} = \mathbf{f}$ into $S^2 A\mathbf{x} = \mathbf{S^2 f}$. This problem is solved by a general multilevel method, with a small coarse space. The previous procedure is combined with a smoothing on the original problem $A\mathbf{x} = \mathbf{f}$, using the smoother associated to the error propagation operator S. We prove a general convergence result and apply it to a variational two-level method and a variational multigrid. In both cases, we prove that the convergence rate is independent of the first and second level resolution. Concerning computational costs, the proposed method is asymptotically superior to domain decomposition methods and opens the possibility for a better level of parallelism. Numerical experiments will be presented to assess the efficiency of the method. We will show in particular that in contrast to standard multigrid methods that require semi-coarsening to conserve their efficiency, this method can be efficient even for problems with anisotropies. For instance, for the following elliptic problem :

$$-\left(\frac{\partial^2}{\partial x^2} + \varepsilon\frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) u = f \text{ on } \Omega = (0,1)^3,\ u = 0 \text{ on } \partial\Omega. \tag{1}$$

the table below shows a mild dependence of the convergence rate on the degree of anisotropy (ε).

512 000 dofs, coarse space 512 dofs, $deg(S) = 7$, $H/h = 9$.		
ε	rate of conv	no. iter.
1000	0.321	19
100	0.241	15
10	0.137	11
1	0.131	11
0.1	0.221	14
0.01	0.317	19
0.001	0.300	18

Applications of AMG methods based on aggressive coarsening and polynomial smoothing

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In this contribution, we present numerical results obtained by using the novel multigrid methods based on aggressive coarsening and polynomial smoothing. The focus will be on real-world problems arising in nuclear engineering, including the numerical modeling of reactor cores of the two Czech nuclear power plants as well as the research reactor located at the Czech Technical University in Prague. One of the important problems encountered in practical computational nuclear engineering is the solution of large-scale eigenvalue problems with complicated geometries and material data leading to unacceptably slow convergence rates of standard iterative methods. The novel evolving coarse-space method, presented in an accompanying contribution, is particularly suitable for solving these kinds of problems with very strict calculation time constraints.

Acknowledgment

This work was sponsored by the Technology Agency of The Czech Republic Grant TA01020352 and The Office of Naval Research Global Grant N62909-11-1-7032.

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Numerical experiments of preconditioned iterative Krylov methods and multigrids methods for an elliptic partial differential equation in generalised coordinates

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The solutions to the Laplace equation

$$\frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0 \quad \text{in} \quad \Omega \tag{1}$$

are sought in the domain shown in Figure 1 with the Dirichlet boundary conditions.

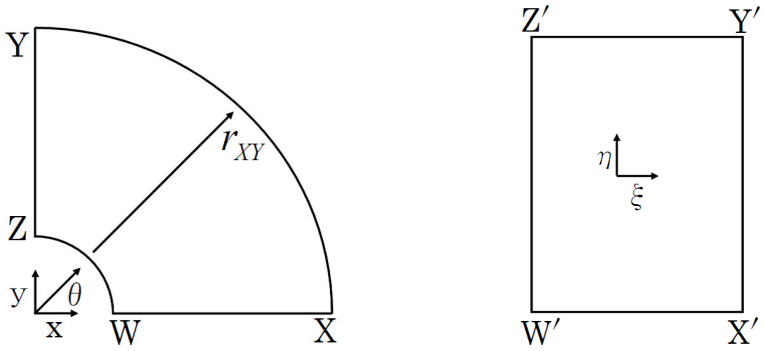

Figure 1 Solution domain for the Laplace equation.

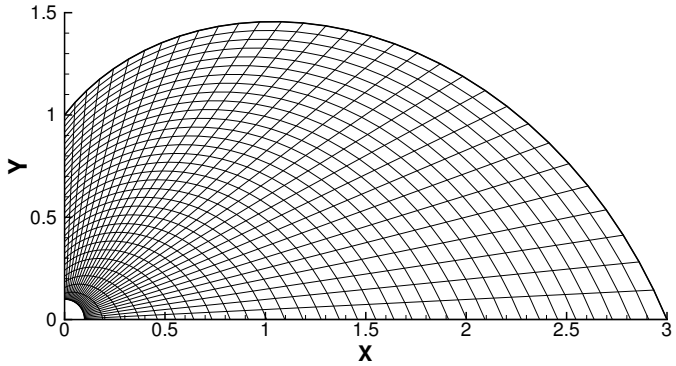

Figure 2 Deformed solution domain and grid.

The solution domain is deformed by moving the point X as shown in Figure 2. The Laplace equation in generalised coordinates ξ, η becomes

$$-\left\{\left(\frac{\nabla^2 \xi}{J}\right)\phi\right\}_\xi - \left\{\left(\frac{\nabla^2 \eta}{J}\right)\phi\right\}_\eta + \left\{\left(\frac{\alpha}{J}\right)\phi\right\}_{\xi\xi} + \left\{\left(\frac{\beta}{J}\right)\phi\right\}_{\xi\eta} + \left\{\left(\frac{\gamma}{J}\right)\phi\right\}_{\eta\eta} = 0$$

The equation is discretized using three-point centered difference scheme. The resulting linear system $A\mathbf{x} = \mathbf{b}$ is solved. The non-zero entries of A are $a_{k,k-I-1}, a_{k,k-I}, a_{k,k-I+1}, a_{k,k-1}, a_{k,k}, a_{k,k+1}, a_{k,k+I-1}, a_{k,k+I}, a_{k,k+I+1}$. The system is solved by iterative Krylov methods and multigrid methods. Iterative Krylov methods include BCG, CGS, BCGSTAB, BCGTAB2, GPBCG, BCGSafe, BCR, CRS, BCRSTAB, BCRSTAB2, GPBCR, BCRSafe, GMRES. They are preconditioned by ILU and MILU. Multigrid methods are geometric multigrid (discretization coarse grid approximation, Galerkin coarse grid approximation) and algebraic multigrid. Table 1 shows the CPU time on a common workstation for the methods on a 768^2 grid. The result shows that MILU greatly improves the efficiency of the iterative Krylov methods.

Table 1: CPU time (s) on a 768^2 grid

Method	Preconditiong or Approximation	$r_x = 1$	$r_x = 2$	$r_x = 3$
BCG	ILU	92	78	68
	MILU	26	20	18
BCR	ILU	136	114	98
	MILU	37	31	26
CGS	ILU	64	52	46
	MILU	19	13	12
CRS	ILU	68	57	50
	MILU	17	14	12
BCGSTAB	ILU	71	60	50
	MILU	18	16	12
BCRSTAB	ILU	75	62	55
	MILU	20	15	13
GPBCG	ILU	90	79	66
	MILU	22	18	16
GPBCR	ILU	111	78	70
	MILU	23	18	16
BCGSTAB2	ILU	96	79	70
	MILU	26	18	16
BCRSTAB2	ILU	97	83	73
	MILU	26	19	16
BCGSafe	ILU	83	72	61
	MILU	20	16	14
BCRSafe	ILU	96	72	64
	MILU	21	17	15
GMRES(k) k=30	ILU	459	337	272
k=20	MILU	34	30	27
Geometric MG	DCA (7-grid)	8.6	117	∞
	GCA (7-grid)	9.5	8.0	8.0
Algebraic MG	–	8.7	8.5	8.9

Multilevel ILU preconditioning for iterative solution of general sparse linear systems

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We consider the problem of numerical solution of sparse unsymmetric non-singular linear systems using threshold-based Incomplete LU preconditioned BiCGStab iterations. We present a multilevel ILU preconditioning (MLILU) based on (recursive) reordering and 2×2 block splitting, which guarantees strong diagonal dominance in the leading block of a possibly large dimension.

The idea of the method is due to Saad [4]; however, we use a different procedure for the construction of such reordering and splitting, which was first presented in [1] and is essentially based on 2-side scaling of the matrix which approximately equilibrates its row and column norms. Based on [1, 2], some theoretical evidence supporting the proposed algorithm is given, including the upper bounds for the fill-in for the ML-ILU triangular factors.

Results of numerical testing on sample matrices from the University of Florida are given. Moreover, we present some results obtained for hard-to-solve linear systems arising in real-life oil and gas simulation.

Table 1. Total solution time (s) for test problems with matrices from University of Florida collection

matrix	n	nz(A)	$t_{PARDISO}$	t_{MLILU}
language	399130	1216334	1191.3	6.7
torso3	259156	4429042	49.4	9.5
ohne2	181343	6869939	44.0	14.0
atmosmodl	1489752	10319760	1291.0	61.1
rajat31	4690002	20316253	58.0	67.2

In Table 1, our fast and reliable implementation of the MLILU-BiCGStab solver is compared with the well-known PARDISO package based on highly optimized direct sparse LU-decomposition (the timings for the latter were taken from [3]). Note that the timings for MLILU were obtained on a slower desktop PC AMD compared to that of PARDISO using one Intel Xeon core.

A simple coarse-grained parallel version of the algorithm, which has satisfactory efficiency for a moderate number of processors, is also discussed.

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Additive Schur complement approximation: Theory and applications

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The method of additive Schur complement approximation (ASCA) has been introduced in [1] and more recently studied in context of high-frequency high-contrast problems, cf. [2]. In this talk we present its theoretical analysis in the framework of auxiliary space preconditioning. Moreover, a multilevel algorithm is proposed that recursively extends a general two-level method based on exact two-level block factorization of local (finite element stiffness) matrices related to a partitioning of the domain into overlapping or non-overlapping subdomains. The size and the overlap of the subdomains control the sparsity of the coarse-grid operator which is defined via ASCA. The robustness of the proposed method for high-contrast multiscale problems is proved and demonstrated by numerical experiments. Further, aspects of parallelization and possible applications of auxiliary space multigrid methods are discussed.

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Skew-symmetric preconditioners for strongly nonsymmetric linear equation systems [1]

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Any matrix A can naturally be expressed as a sum of symmetric matrix A_0 and skew-symmetric matrix A_1. This splitting is named symmetric - skew-symmetric spliting (SSS).

Consider the linear equation system

$$Au = f, \tag{1}$$

where A is non-symmetric matrix, u is the vector of unknown, f is the vector of the right part is considered.

Iterative method based on symmetric - skew-symmetric splitting was firstly proposed for this business by Gene Golub [1].

If A_0 is a positive definite than matrix A is named positive real. We will name matrix A strongly non-symmetric if

$$\|A_0\|_* << \|A_1\|_*$$

where$\|\&\|_*$ is some matrix norm.

It is well known, that difficulties to solve such linear equation systems grows up because matrix can lose property of diagonal dominant. Skew-symmetric iterative methods (SSIT) for these cases have been proposed [2].

Let us approach (1) by considering the iterative methods of the following form:

$$y^{n+1} = Gy^n + \tau B^{-1} f, \quad G = B^{-1}(\omega)(B(\omega) - \tau A), \tag{2}$$

where f, $y_0 \in H$,H is an n-dimensional real Hilbert space, f is the right part of (1), A, $B(\omega)$ are linear operators (matrices) in H, A is given by equation (2), $B(\omega)$ is invertible, y_0 is an initial guess, y_k is the k-th approach, $\tau, \omega > 0$ are iterative parameters, u is the solution that we obtain, $e^k = y^k - u$ and $r^k = Ae^k$ denote the error and the residual in the k-th iteration, respectively.

Consider the next choice of operator B. The class of triangular skew-symmetric iterative methods is defined by (2) with the matrix B being chosen as

$$B(\omega) = B_c + \omega((1+j)K_L + (1-j)K_U), \quad j = \pm 1,\ B_c = B_c^*. \tag{3}$$

The class of product triangular skew-symmetric iterative methods is defined by (2) with the matrix B being chosen as

$$B = (B_C + \omega K_U)B_C^{-1}(B_C + \omega K_L), B_c = B_c^*, \tag{4}$$

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where $K_L + K_U = A_1, K_L = -K_U^*$, $B_C = B_C^*$.

Operator B_C can be chosen arbitrarily, but has to be symmetric. These methods are from class of SSIT and called as two-parameters triangular(TTM) and product triangular (TPTM) method. Convergence of TTM and TPTM has been considered and proved. We compare TTM to the conventional SOR procedure and TPTM to the conventional SSOR procedure.

For the check of TPTM behavior, the standard 5-point central difference scheme on the regular mesh has been used for approximation of the convection-diffusion equation with Dirichlet boundary conditions and small parameter at the higher derivatives in the incompressible medium and it's transformation by regular ordering to strongly non-symmetric linear equation systems. In the case of central difference approximation of the convective terms operator A can naturally be expressed in a sum of symmetric positive definite operator A_0, which is a difference analogue of the Laplace operator and skew-symmetric operator A_1, which is a difference analogue of the convective terms.

Numerical experiments show that in considered particular cases the behavior of methods is closely related to the technique of choosing the matrix B_C.

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The evolving coarse-space method for generalized eigenvalue problem

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We introduce a two-level method with evolving coarse-space for finding smallest eigenvalue and the corresponding eigenvector for mutual eigenvalue problem $\mathbf{Ax} = \lambda\mathbf{Bx}$. We suppose that matrix $\mathbf{A}$ is invertible and the eigenvalue is real and positive. Solving of such type of problems are important in nuclear reactor criticality calculations for example.

For $\mathbf{x}$ being the fine-level approximation of the solution, the coarse-space $V = V(\mathbf{x})$ is constructed so that $\mathbf{x}$ satisfies $\mathbf{x} \in V$. This is achieved by adding the vector $\mathbf{x}$ as a first column of the prolongator. (The columns of the prolongator P form a computationally relevant basis of the coarse-space $V = \mathrm{Range}(P)$.) The cost of enritching the coarse-space V by the current approximation $\mathbf{x}$ is a single dense column of the prolongator that has to be updated each iteration.

The efficiency of presented method will be demonstrated on several numerical experiments. The computations were performed on GPU Nvidia Tesla M2090.

Acknowledgment

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Characterization of worst-case GMRES

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The GMRES method for solving the linear algebraic system $Ax = b$ with the initial guess $x_0 = 0$ generates a sequence of iterates x_k, so that the corresponding kth residual $r_k \equiv b - Ax_k$ satisfies

$$\|r_k\| \;=\; \min_{p\in\pi_k} \|\, p(A)b \,\|\,. \tag{1}$$

Here $\|\cdot\|$ denotes the Euclidean norm, and π_k denotes the set of polynomials of degree at most k and with value one at the origin. For simplicity, suppose that $\|b\| = 1$.

A common approach for investigating the GMRES convergence behavior is to bound the right hand side in (1) independently of b. For each iteration step k the *best possible bound* on the GMRES residual norm that is independent of b is given by maximizing the right hand side of (1) over all unit norm vectors,

$$\|r_k\| \;=\; \min_{p\in\pi_k} \|\, p(A)b \,\| \;\le\; \max_{\|v\|=1} \min_{p\in\pi_k} \|\, p(A)v \,\| \;\equiv\; \Psi_k(A)\,. \tag{2}$$

The quantity $\Psi_k(A)$ is called *the kth worst-case GMRES approximation*. The upper bound given by (2) is sharp in the sense that for each given A and k there exists a unit norm initial vector b so that the corresponding kth GMRES residual vector satisfies $\|r_k\| = \Psi_k(A)$.

The focus of this talk will be on mathematical characterizations of the worst-case GMRES approximation problem on the right hand side of (2). It will be shown that initial vectors for which the value $\Psi_k(A)$ is attained satisfy an intriguing algebraic equality, which has been called the "cross equality". Moreover, it will be shown that for given A and k there may exist different polynomials from the set π_k and corresponding different initial vectors which attain the same worst-case value $\Psi_k(A)$. The non-uniqueness of worst-case GMRES is somewhat surprising, since the closely related "ideal GMRES" approximation problem always has a uniquely defined solution. It represents one of the challenges in the numerical and mathematical analysis of the worst-case GMRES problem.

The talk will be based on joint work with Vance Faber and Petr Tichý [1].

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Auxiliary space multigrid method for flows in porous media

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We consider the mixed finite element approximation of Darcy's law in porous media where the flux and the pressure variables are approximated in the lowest-order Raviart-Thomas space and the space of piece-wise constant functions, respectively. The arising indefinite system is solved by the MINRES method using a block-diagonal symmetric positive definite preconditioner. The application of the latter is accomplished by applying an auxiliary space multigrid method to solve the subproblem related to the flux component. The key for achieving uniform convergence is to use an additive Schur complement approximation (ASCA), which has been studied earlier for conforming discretizations of scalar elliptic problems, [1, 2]. Based on a proper covering of the domain by overlapping subdomains the ASCA and thus the resulting method is robust with respect to arbitrary jumps of the (piecewise constant) permeability. Numerical experiments demonstrating the performance of the proposed multigrid algorithm are conducted.

This is a joint project with Johannes Kraus from RICAM-ÖAW, Austria and Svetozar Margenov from IICT-BAS, Bulgaria.

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A low-rank tensor method for large-scale Markov Chains

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A number of practical applications lead to Markov Chains with extremely large state spaces. Such an instance arises from models for calcium channels, which are structures in the body that allow cells to transmit electrical charges to each other. These charges are carried on a calcium ion which can travel freely back and forth through the *calcium channel*. The state space of a Markov process describing these interactions typically grows exponentially with the number of cells. More generally, Stochastic Automata Networks (SANs) are networks of interacting stochastic automata. The dimension of the resulting state space grows exponentially with the number of involved automata. Several techniques have been established to arrive at a formulation such that the transition matrix has Kronecker product structure. This allows, for example, for efficient matrix-vector multiplications. However, the number of possible automata is still severely limited by the need of representing a single vector (e.g., the stationary vector) explicitly. We propose the use of low-rank tensor techniques to avoid this barrier. More specifically, an algorithm will be presented that allows to approximate the solution of certain SANs very efficiently in a low-rank tensor format.

This is a joint work with Prof. Daniel Kressner (École Polytechnique Fédérale de Lausanne, Switzerland).

TRACEMIN-Fiedler: Reducing the weighted bandwidth of a matrix in parallel

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Fiedler vector [2] is an indispensable tool in spectral graph analysis. It essentially maps each graph node onto the real line in such a way that heavily connected nodes are kept close together. Specifically assuming, for simplicity, an undirected graph G with positive edge weights and A its (symmetric, nonnegative) adjacency matrix, we define its weighted Laplacian L as a matrix

with entries $l_{ii} = \Sigma_k a_{ik}$ on the diagonal and $l_{ij} = -a_{ij}$ otherwise. The Fiedler vector x_F is then L's eigenvector corresponding to its *second smallest* eigenvalue $\lambda_2 > 0$, i.e. $Lx_F = \lambda_2 x_F$. Note that the *smallest* eigenvalue for L always vanishes and corresponds to the case when we assign the same coordinate to all graph nodes - for single component graphs - or the nodes of each of the components in the general case of multiple component instances. In the case of k components, $\lambda_1 = 0$ will generally pair to k linearly independent eigenvectors x_i with $Lx_i = 0, i = 1, \ldots, k$ so the non-trivial Fiedler vector x_F will be the $(k+1)^{th}$ eigenvector in this ascending eigenvalue ordering, $x_F = x_{k+1}$. It easily follows that $x^\top Lx$ is non-trivially minimized for normalized $x = x_F$ in all cases, and this accounts for the aforementioned collocation property of x_F for heavily connected nodes.

In particular, we advocate the use of the Fiedler vector as a tool for the symmetric permutation of the matrix of coefficients A in a linear system of the form $Ax = b$, with the intention of moving heavy elements closer to the diagonal. So we target the reduction of the effective matrix bandwidth in order to identify an envelope for the construction of efficient preconditioners used in the subsequent iterative solution of the permuted system. By employing a preprocessing transformation $A \leftarrow (|A| + |A^\top|)/2$, the coefficient matrix can be viewed as the adjacency matrix of a positively weighted, undirected graph. In this setting our intention translates, for each nonzero a_{ij}, to keeping $|i - j|$ minimal, i.e. closer to the diagonal, for any nodes i, j that are heavily connected. On the other hand as mentioned, the Fiedler vector will assign coordinates to nodes to keep essentially $|x_{F,i} - x_{F,j}|$ small for such heavily connected pairs (collocation property). It is exactly this fact that drives our approach for selecting the ordering computed in x_F as an intuitively attractive, bandwidth-reduction permutation [1].

We have developed TRACEMIN-Fiedler [4], a parallel algorithm based on Trace Minimization [5], which is a symmetric eigenvalue problem solver, to compute x_F of L. This is based on the idea that L, if projected on the subspace spanned by the eigenvectors corresponding to its smallest eigenvalues will be a diagonal matrix with minimal trace, i.e. the sum of these smallest eigenvalues. So in search for these eigenvectors, and x_F in particular, we iteratively compute corrections perpendicular to the current basis, however always trying to minimize the associated trace in doing so; this minimization in turn necessitates solving a saddle point problem for the correction at each iteration step. Although, solving a large linear system at each iteration might seem expensive one can take advantage of the following: (i) the cofficient matrix is the Laplacian matrix with a strong diagonal, (ii) sparse matrix vector multiplication can be computed in parallel and (iii) those saddle point linear systems only need to be solved approximately. TRACEMIN-Fiedler is implemented in Fortran, using both message passing and shared address space paradigms (enabled respectively by MPI calls and OpenMP directives). It compares favorably with MC73_FIEDLER [3], the state-of-the art serial code in Harwell Subroutine Library (HSL) being heav-

ily optimized for the Fiedler vector computations. Experiments demonstrate over two orders of magnitude speedup in time-to-permutation, in some matrix instances and cluster configurations, while retaining the bandwidth-reduction properties of computed x_F's induced permutation (accuracy).

Our initial implementation was designed for matrices whose graph has a single component. We have added the ability to handle multi-component graphs through two additional modules: (i) a *preprocessing* module that identifies the graph components and treats each of them as a separate matrix, i.e. of a single-component graph support; in doing so, it also avoids the overhead of having to call into TRACEMIN-Fiedler even for small component matrices, utilizing standard sequential eigensolvers instead, (ii) a *postprocessing* module that composes Fiedler-induced permutations as returned by the eigensolvers with the component-revealing one captured at preprocessing, to produce the final permutation.

We experiment with a set of matrices covering a broad spectrum of application domains and ranging in size between some hundreds of thousands to a few millions of nodes. Preliminary tests indicate that our updated codes can now address multicomponent graphs at a fraction of time compared to the state-of-the-art approaches, also at competitive quality rates. Being parallel, these codes do not suffer the scalability problems of MC73_FIEDLER and thus they could be used for the efficient generation of bandwidth-reduction permutations for large systems of linear equations.

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Numerical solution of the incompressible Navier-Stokes equations by multigrid method

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We propose some approaches for solving the incompressible Navier-Stokes equations.

We consider classical formulation of the Navier-Stokes equation:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} + \frac{\partial P}{\partial x} - \frac{1}{Re}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) = f_1,$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} + \frac{\partial P}{\partial y} - \frac{1}{Re}\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) = f_2,$$

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = f_3,$$

where Re is Reynolds's number, $V = (u\ (x,\ y,\ t),\ v(x,\ y,\ t))$ is the velocity and P is the pressure.

To approximate the time derivative method of characteristics is used. Space discretization is carried out by finite element method. It's used a mixed formulation, when a combinations of simple finite elements – bilinear for velocities and constant elements for pressure are applied [1].

After discretization we obtain a linear algebraic equation system with a symmetric matrix which has a spectrum with alternating signs. We use multigrid method for solving this system. Multigrid methods are proving themselves as very successful tools for the solution of the algebraic equation systems associated with discretization of boundary-value problems. MGM is not a fixed multigrid algorithm. There is rather a multigrid technique fixing only the framework of the algorithm. The efficiency of the multigrid algorithm depends on the adjustment of its components to the problem in question [2].

Some numerical results are presented.

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Partitioning reachable state space into product state spaces for multilevel methods

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Discrete event dynamic systems with interacting subsystems can be specified with various high-level formalisms and then mapped to a multi-dimensional Markov chain. The reachable state space of such a Markov chain is usually a proper subset of its product state space [2]. Efficient implementation of multilevel methods requires the set of reachable states to be represented as a union of Cartesian products of subsets of subsystem state spaces. Currently there are only ad hoc methods that can be used to this end. In this talk, we discuss how a given multi-dimensional reachable state space can be automatically partitioned into Cartesian products of subsets of subsystem state spaces using ideas from combinatorics [1].

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Reaching a consensus: A nonlinear case

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Historically, the idea of reaching consensus through repeated averaging was introduced by DeGroot [1], for a structured, time-invariant, and synchronous environment. For reasons of self-exposition, it is convenient to first provide a linear model for an estimate-modification process of a structured, time-invariant, and synchronous environment which was presented in [1] and [3].

Consider a group of m individuals, each of whom can specify his or her own subjective probability distribution for the unknown value of some parameter θ. Suppose the m individuals must act together as a team or committee.

For $i = 1, \cdots, m$, let $x_i^{(0)}$ denote the subjective probability distribution that individual i assigns to the parameter θ. The subjective distributions, $x_1^{(0)}, \cdots, x_m^{(0)}$, will be based on the different backgrounds and different levels of expertise of the members of the group. It is assumed that if individual i is informed of the distributions of each of the other members of the group, he/she might wish to revise his/her subjective distribution to accommodate this information. In the DeGroot's model [1], it was assumed that when individual i makes this revision, his/her revised distribution is *a linear combination of the distributions* $x_1^{(0)}, \cdots, x_m^{(0)}$. Let P_{ij} denote the weight that individual i assigns to $x_j^{(0)}$ when he/she makes this revision. It was assumed that the $P_{ij} \geq 0$ and $\sum\limits_{j=1}^{m} P_{ij} = 1$. So, after being informed of the subjective distributions of the other members of the group, individual i revises his/her own subjective distribution from $x_i^{(0)}$ to $x_i^{(1)} = \sum\limits_{j=1}^{m} P_{ij} x_j^{(0)}$.

Let $\mathbb{P}$ denote the $m \times m$ matrix whose (i,j)th element is P_{ij}. It is clear that $\mathbb{P}$ is a stochastic matrix since the elements are all non-negative and the rows sum to one. Let $x^{(0)} = (x_1^{(0)}, \cdots, x_m^{(0)})$ and $x^{(1)} = (x_1^{(1)}, \cdots, x_m^{(1)})$ be vectors. Then the vector of revised subjective distributions can be written as $x^{(1)} = \mathbb{P}x^{(0)}$.

The critical step in this process is that now the above revision is iterated. It is assumed that after individual i is informed of the revised subjective distributions, $x_1^{(1)}, \cdots, x_m^{(1)}$ of the members of the group, he/she revises his/her subjective distribution from $x_i^{(1)}$ to $x_i^{(2)} = \sum\limits_{j=1}^{m} P_{ij} x_j^{(1)}$. The process continues in this way.

Let $x^{(n)}$ denote the subjective distribution of individual i after n revisions. Then $x^{(n)} = \mathbb{P}x^{(n-1)} = \mathbb{P}^n x^{(0)}$. DeGroot states [1] that a consensus is reached if

and only if all m components of $x^{(n)}$ converge to the same limit as $n \to \infty$.

In [2], Chatterjee and Seneta consider a generalization of DeGroot's model in which the individuals can change their weights P_{ij} at each iteration.

In this paper, we shall consider *a nonlinear model for an estimate-modification process of a structured, time-varying, and synchronous environment.* Namely, we suppose that every individual makes a revision of his/her subjective distribution as *a nonlinear combination of the previous distributions.* More precisely, in our nonlinear model, after being informed of the subjective distributions of the other members of the group, individual i revises his/her own subjective distribution from $x_i^{(0)}$ to $x_i^{(1)} = \sum\limits_{j,k=1}^{m} P_{ijk} x_j^{(0)} x_k^{(0)}$, where $\mathcal{P} = (P_{ijk})_{i,j,k=1}^{m}$ is a triple stochastic cubic matrix with non-negative entries i.e., $P_{ijk} \geq 0$ and $\sum\limits_{i=1}^{m} P_{ijk} = \sum\limits_{j=1}^{m} P_{ijk} = \sum\limits_{k=1}^{m} P_{ijk} = 1$ for any $i, j, k = \overline{1, m}$. In our nonlinear model, the individuals can change their weights P_{ijk} at each interaction.

In our nonlinear model for an estimate-modification process, we showed that if in some interaction all weights P_{ijk} are positive then consensus can be reached in the environment.

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Block Krylov subspace recycling: Theory and application in a Newton iteration

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We address the solution of a sequence of families of linear systems. For the ith family, there is a base coefficient matrix A_i, and the coefficient matrices for all systems in the ith family differ from A_i by a multiple of the identity, i.e.,

$$A_i x_i = b_i \quad \text{and} \quad (A_i + \sigma_i^{(\ell)} I) x_i^{(\ell)} = b_i \quad \text{for} \quad \ell = 1 \dots L_i,$$

where L_i is the number of shifts at step i. This is an important problem arising in various applications.

The recycled GMRES method (RGMRES) [1] is an extension of GMRES in which the minimum residual projection is performed over an augmented Krylov subspace. The formulation of RGMRES allows for minimization of the residual over arbitrary augmented subspaces. For solving a sequence of linear systems, this allows us to use a subspace of the search space generated when solving system i to augment the Krylov subspace generated for system $i + 1$.

We extend the machinery of RGMRES to minimize the residuals of the shifted systems by direct projection. All approximations come from the same augmented Krylov subspace, but for each shifted system, the approximation is chosen such that the residual is orthogonal to a different constraint space. The constraint spaces are chosen such that the approximations can be computed efficiently. Upon convergence of the iteration for the base system, the shifted system approximations have improved, but the iterations will not necessarily have converged. In this situation, the method can be called recursively for the remaining unconverged systems. We present analysis of this method and numerical results involving systems arising in lattice quantum chromodynamics.

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On preconditioning of saddle point systems arising from interactions of incompressible fluid flow with structure

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The coupled problems describing the interactions of fluid flow with elastic structure are of great importance in many engineering applications. In the technical practice typically the determination of the stability of the system is of interest only, and thus the problem is modeled only in linear regime. Recently, the research focuses also on numerical modeling of nonlinear coupled problems. In this case the efficient approximation of very complex coupled problem is needed. The mathematical model consists of fluid flow description, structure motion equations and the interface conditions.

In this paper the problem of the numerical solution of fluid-structure interactions shall be considered with the main attention paid to the flow problem, its linearization and efficient solution of the arising system of linear equations obtained by finite element approximation of structural and flow models, cf. [2]. The solution of the saddle point system is complicated particularly for the considered case of high Reynolds numbers, and the use of advanced stabilization, cf. [1]. The choice of suitable preconditioner is discussed and the multilevel method is applied. The practical implementation of the method in the finite element based solver is considered and the comparison of the performance on a number of two- and three dimensional cases is discussed.

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BDDC for mixed-hybrid formulation of flow in porous media with combined mesh dimensions

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A detailed description of flow in porous media is essential for building mathematical models with applications in, e.g., oil and gas recovery or nuclear waste disposal. In order to set up a reliable geomodel, one needs to have a good knowledge of the problem geometry and input parameters. The flow of water in granite rock, which represents one of the suitable sites for nuclear waste deposit, is conducted by the complex system of vugs, cavities and fractures with various topology and sizes. These alter the effective permeability, and therefore should be accurately accounted for in the geomodel. In the presented approach, the fractures are assumed to contain debris and they are modeled as porous media with specific permeabilities. The discretization is performed using the mixed-hybrid finite element method (FEM) with the lowest order Raviart-Thomas (RT0) elements. The resulting meshes are therefore unstructured, and they combine different spatial dimensions (line elements in 1D, triangles in 2D, and tetrahedrons in 3D) to model the effect of fractures. The systems of linear equations obtained from the FEM discretization are often very large and typically ill-conditioned due to mixing of spatial dimensions, large jumps in permeability coefficients and presence of elements of considerably different sizes. The matrices have a saddle-point structure

$$\begin{bmatrix} A & \mathcal{B}^T \\ \mathcal{B} & -C \end{bmatrix}, \tag{1}$$

where A is symmetric and positive definite on the kernel of $\mathcal{B}$, and C is symmetric and positive semi-definite. The 'penalty' block $C \neq 0$ arises from connecting meshes of different spatial dimensions.

We adapt the Balancing Domain Decomposition by Constraints (BDDC) [2, 4] method to this type of problems. A new scaling operator in the BDDC method suitable for the studied problems is also proposed. The mixed-hybrid formulation allows to modify the saddle-point problem to the one which is symmetric and positive definite. We eliminate the block A and 'a bit more' and introduce a symmetric and positive definite Schur complement with respect to interface Lagrange multipliers, which correspond to a part of block C. The reduced system is solved by the preconditioned conjugate gradient (PCG) method, and the BDDC method is used as the preconditioner. We take advantage of the special structure of the blocks in matrix (1) studied in detail in [3], and in particular in [1].

We describe our parallel implementation of the method and study its performance on several benchmark and real world problems. The extensions have been incorporated into our open-source solver library *BDDCML*, which has been combined with the *Flow123d* package for subsurface flow simulations. Numerical experiments confirm efficiency and scalability of the developed approach on up to 1024 computer cores (see Fig. 1).

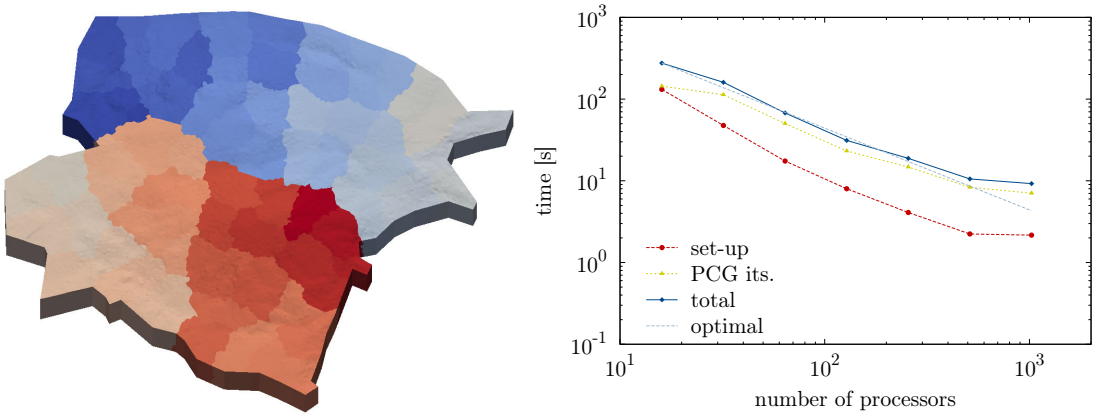

Figure 1 A problem of a candidate site for a nuclear waste deposit: Example division into 64 subdomains (left) and computing times for increasing number of CPU cores (right). Unstructured mesh contains 2.1 million elements and 15 million unknowns. Data by courtesy of Jiřina Královcová.

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Application of the conjugate gradient method applied to a matrix equation arising in learning machine dPLRM for cancer diagnosis

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We develop a novel method for cancer diagnosis of biological specimens based on the mass-spectrometry data obtained by the PESI (the Probe electrospray ionization) inutriment. By applying the learning machine dPLRM(dual Penalized Logistic Regression Machine) to the training data set, we were able to diagnose RCC, HCC and MEC. The algorithm of the machine solves a matrix nonlinear optimization problem by the CG-Newton method applied to an interesting matrix equations.

Parallel block Jacobi SVD solvers

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The Singular Value Decomposition (SVD) is one of the basic matrix decompositions with a very rich field of applications such as signal and image processing, data retrieval, statistical data analysis, which are solved e.g. by means of least squares and total least squares techniques. At the same time, the SVD is one of the most complex algorithms in linear algebra; for a matrix of order n it requires $O(n^3)$ floating-point operations and $O(n^2)$ memory locations (when computing its full version with both left and right singular vectors). This high arithmetic complexity has led to various algorithms that differ in main principles, matrix pre-processing and accuracy of computed results when using the floating-point arithmetic. For example, some algorithms compute only a partial SVD with a subset of singular values close to some target. Most algorithms compute singular values only with a guaranteed *absolute* accuracy, so that computed tiny singular values may not have any accurate digits at all.

The Jacobi method [5] was originally used by Jacobi in year 1846 for the iterative solution of a linear system of equations of order eight that was derived by applying the least-squares method to the measured positions of eight known planets at that time (Mercury, Venus, Earth, Mars, Jupiter, Saturn, Uranus, Neptune). The linear system was of the form $(H-\lambda I)x = 0$ with H symmetric, so in our terminology it was actually the eigenvalue problem, since the solution

yielded both λ (the eigenvalue) and x (the eigenvector). The generalization for the computation of the SVD of a rectangular matrix followed by Hestenes in [4]. It also became clear that, in contrast to the Eigenvalue Decomposition (EVD) of square matrices, there exist two methods of the SVD that differ in a way the matrix is diagonalized: either explicitly by applying two orthogonal transformations from left and right (the *two–sided* method), or implicitly by applying the orthogonal transformations only from right (the *one–sided* method). The one–sided variant is faster than the two–sided one due to the decrease of the number of matrix–matrix multiplications.

Serial Jacobi SVD methods have some excellent numerical properties, especially they are able to compute singular values with a high *relative* accuracy. However, they are inherently slow due to the necessary matrix updates via orthogonal transformations. This is the main reason why they were essentially abandoned in 1950's. The interest switched into the SVD computation by means of matrix bidiagonalization and recently also to some projection methods like the Jacobi–Davidson SVD algorithm. However, recent development and work of Drmač, Hari and Veselić have shown that the one–sided serial Jacobi method with some very clever improvements (e.g., special ordering of annihilation and matrix preprocessing) can be competitive to the well–known LAPACK SVD algorithm of Golub and Rench based on the matrix bidiagonalization; see [1, 2, 3].

Our work on the improvement of efficiency of the parallel two–sided block–Jacobi method in last 13 years started with the generalization of an original Jacobi idea of nullifying the largest magnitude element of a symmetric matrix in each iteration step. We have formulated this approach for a block partitioning of a large matrix and adapted it for the distributed memory paradigm of parallel computation where individual processors communicate by interchanging messages. Thus, a new *dynamic ordering* was born, which takes into account the actual status of the matrix off–diagonal norm. Since then, some other new ideas, like *optimal data transfer*, *optimal data layout* and *matrix preprocessing*, were subsequently applied to enhance the performance. We also got a new insight into its convergence properties in dependence of the distribution of singular values. Recently, all these ideas, especially a new dynamic ordering based on the estimation of principal angles between subspaces, were also used for the parallel one–sided block–Jacobi method. This approach resulted in a significant decrease of the number of parallel iteration steps needed for the convergence of both methods.

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An overview of multilevel methods with aggressive coarsening and massive polynomial smoothing

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We review our two–level and multi–level methods with aggressive coarsening and polynomial smoothing. Our methods can be percieved as a cheaper and more flexible (in multilevel case) alternative to the domain decomposition methods. Also, our polynomial smoothers (that is, the sequence of the Richardson's iteration) can be performed using up to $n = ord(A)$ processors and allow therefore for a better level of parallelism than the domain decomposition methods.

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Preconditioning of large-scale saddle point systems arising in Riccati feedback stabilization of coupled flow problems

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In order to explore boundary feedback stabilization of coupled flow problems, we consider the Navier-Stokes equations that describe instationary, incompressible flows for moderate Reynolds numbers coupled with a diffusion convection equation. Using a mixed finite element discretization, we get a differential-algebraic system of differential index two. We show how to reduce this index with a projection method [2] to get a generalized state space system, where a linear quadratic control approach can be applied [3]. This leads to large-scale saddle point systems which have to be solved in a threefold nested iteration. For obtaining a fast iterative solution of those non-symmetric systems we derive efficient block preconditioners based on the approaches due to Wathen et al. [1, 4]. We use some algebraic `multigrid` method for the $(1,1)$-block and a *Chebyshev* semi iteration to approximate the *Schur*-complement in the preconditioner. We demonstrate the feasibility of the arising nested iteration with some recent numerical results.

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Homogenization method for periodic media based on Fast Fourier Transformations: Finite element formulation and error estimates

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Recent experimental and theoretical advances in microstructural characterization of heterogeneous media open novel possibilities in predictive "bottom-up" modeling of engineering materials. There are currently a variety of techniques being utilized to acquire a comprehensible digital representation of materials' structure. With regard to the format of input data, the pixel- or voxel-based methods appear to be a convenient choice for computational simulations of such materials.

Exactly with these applications in mind, Moulinec and Suquet introduced in [1] an efficient numerical approach to the numerical homogenization of deterministic periodic media based on the Fast Fourier Transforms. The method builds on an iterative solution to an integral equation of the Lippman-Schwinger type for the unit cell problem, with a kernel whose action can be efficiently evaluated in the Fourier space. Since then, several improvements of the basic scheme have been proposed, successfully applied to diverse problems, see e.g. overviews in [2, 3, 4]. The aim of this contribution is to summarize our recent results on the analysis and extensions of the Moulinec-Suquet scheme [4].

Our analysis rests of a variational formulation of the unit cell problem and the Helmholtz decomposition of the periodic fields. By utilizing a certain projection operator, related to the kernel of the integral equation, we show that the weak form is equivalent to the integral formulation. This allows us to demonstrate that the original scheme [1] is equivalent to the Galerkin discretization of the unit cell problem, with trigonometric polynomials [5] as the basis functions. Utilizing the approximation theory available in [5] and standard tools of finite element analysis, we obtain the convergence of the approximate solutions to weak solution, along with convergence rates for sufficiently smooth data. Moreover, using similar arguments, we show that the resulting non-symmetric system of linear equations can be solved by the Conjugate Gradient algorithm, as first experimentally observed in [2] and later studied in [3]. The trigonometric basis functions can be also conveniently applied to obtain guaranteed two-sided bounds on the homogenized coefficients, thereby generalizing the results of Dvořák [6].

This is a joint work with Jaroslav Vondřejc (University of West Bohemia in Pilsen) and Ivo Marek.

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Poster Session

Probabilistic approach to improve the reliability and the availability

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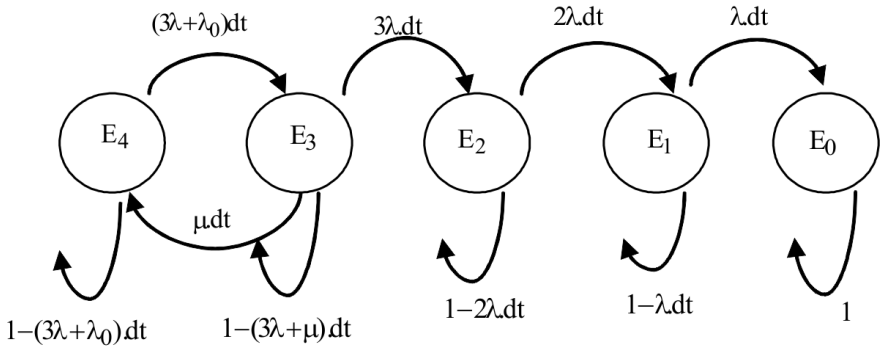
The industrial machines are often programmed to function for long uninterrupted periods. Their reliability and their availability depend mainly on their working regimes as well as their servicing and repairing methods i.e. their maintainability. Better reliability and availability cannot be conceived without a deep study of the various states in which the system of machines can be at the time t and $t + dt$. The Markov chains constitute a powerful computational tool for the reliability and availability in the sense that the hypothesis of the constant repair and failure rate is justified for complex systems, when we investigate the reliability and the average availability of a park of machines.

In this paper, it is first of all, a question of evaluating these two parameters (Reliability and Availability) then judging the necessary need of improving them in order to increase the productivity of machines and to implement the adequate means to reach this goal.



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Aggregation of coarse unknowns within the BDDC method

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Balanced domain decomposition methods for numerical solution of partial differential equations exploit solutions to certain (small) coarse problems in order to reduce the non-local parts of the error. Base functions of the coarse problem are polynomials on each element, continuous on each subdomain and fulfill the minimal energy condition on every subdomain. These base functions are defined by an appropriate dual space. We consider two kinds of degrees of freedom: values at corners and averages of nodal values along interfaces between every pair of neighboring subdomains. The resulting coarse spaces can be large enough and thus a further level of coarsening can be beneficial. We examine several aggregation strategies of the algebraic multigrid for the coarse problems for the diffusion equation and for the elasticity equation. For the elasticity equation a special type of aggregation can be more advantageous than that generally accepted.

The total least squares problem with multiple right-hand sides

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The *total least squares (TLS) techniques*, also called *orthogonal regression* and *errors-in-variables modeling* have been developed independently in several areas. For a given linear (orthogonally invariant) approximation problem

$$AX \approx B, \qquad \text{where} \qquad A \in \mathbb{R}^{m\times n}, \quad B \in \mathbb{R}^{m\times d}, \quad X \in \mathbb{R}^{n\times d},$$

the TLS formulation aims at a solution of a modified problem

$$(A+E)X = B+G \qquad \text{such that} \qquad \min \|[G,E]\|_F.$$

The algebraic TLS formulation has been investigated for decades, see the early works [3], [2, Section 6], [8]. In [4] it is shown that even with $d = 1$ (which represents a problem with the *single right-hand side* $Ax \approx b$, where b is an m-vector) the TLS problem may not have a solution and when the solution exists, it may not be unique. For $d > 1$, the classical book [9] analyzes only two representative cases characterized by the special distribution of singular values of the extended matrix $[B, A]$. A general case is not analyzed—it is considered only as a perturbation of one of the special cases. The so called *classical TLS algorithm* given in [9] computes some output X for any data A, B, but the relationship of the output X to the original problem is, however, not clear.

The single right-hand side problem has been recently revisited in the paper [7]. Here it is shown that the problem does not have a solution when the *collinearities among columns of A are stronger than the collinearities between $\mathcal{R}(A)$ and b*. An analogous situation may occur for $d > 1$, but here *different columns of B may be correlated with different subsets of columns of A*. In our contribution we try to fill this gap and investigate existence and uniqueness of the solution of the TLS problem with $d > 1$ in full generality. We suggest a classification of TLS problems revisiting and refining the basic generic-nongeneric terminology, see [5].

A core reduction concept introduced in [7] makes a clear link between the original data and the output of the classical TLS algorithm for the problems with the single righ-hand side (see also [5]). Therefore the core reduction is an appropriate tool for understanding the TLS problem with $d = 1$. In this contribution we introduce an extension of the core reduction for multiple right-hand sides problems. Following [7], we employ the SVD of A which allows us to define the *core problem* and show its fundamental properties. Then we show how the core problem can be obtained by the *band generalization of the Golub-Kahan iterative bidiagonalization* proposed for this purpose by Åke Björck, see,

e.g., [1]. We show, together with other results in progress (see [6]), that both approaches (based on the SVD of A and on the band algorithm) give the same core problem up to an orthogonal transformation. Using the core reduction, we illustrate some particular difficulties which are present in the TLS problems with $d > 1$.

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Efficient tridiagonal preconditioner for the matrix-free truncated Newton method

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In this contribution, we study an efficient tridiagonal preconditioner, based on numerical differentiation, applied to the matrix-free truncated Newton method for unconstrained optimization. It is proved that this preconditioner is positive definite for many practical problems. The efficiency of the resulting matrix-free truncated Newton method is demonstrated by results of extensive numerical experiments.

Reliability study for a mechanism aided by asynchronous actuator powered by asynchronous diesel generator

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The modern electric facilities are equipped by a great number of different mechanisms and devices actioned by Asynchronous electric Motor (ASM), the power of these motors is equal to the power of the generating devices, where their most complicated working regime is the starting when their power is equal to the power of the generating devices.

In this regime we can have an overcharge of the generating devices by the active and reactive power.

For this reason, this article is dedicated to the study of the starting methods of asynchronous motors that action the mechanisms and that are powered by Asynchronous Generating Diesel (AGD) with a limited capacity of DRY value and a given couple of resistance.

Skew-symmetric preconditioners for Krylov subspace methods

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Linear systems with large sparse non-symmetric matrices arise in many application. It is therefore important to be able to solve them rapidly and efficiently. Although there are a lot of techniques for solving non-symmetric linear systems, strongly non-symmetric systems are studied not enough. The special class of triangular and product triangular methods for solving strongly non-symmetric systems was constructed. The basic idea was put forward by prof. Krukier [1]. He suggested to use the skew-symmetric part of the matrix and only required the matrix to be positive real. Previously, the technique have been used for construction of iterative methods. Now we used it for preconditioning of Krylov subspace methods, that allowed us to combine the advantages of the two classes of methods [2].

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Street type LED armature modeling and analysis

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By the technological advances in solid-state lighting, the conventional lighting systems are transformed into high-efficiency and low-cost LED light source systems. One of the favorite application areas of this energy efficiency system is road lightings. In recent years, many countries like Japan, Italy, etc. converted their lightening systems to LED lightening systems which provide nearly 75 percent energy conservation. However, the biggest problem in these systems is overheating. The produced over heat by the high power LED must be dissipated effectively by a heat sink, else temperature at the armature will increase together with this the LEDs will not work effective and their life will be shorter, so the armature will be broken down. Because of this reason, before manufacture a LED armature making its heat analysis will be many beneficial. In this study a street type LED armature is modeled, and its energy and heat analysis are performed by a computer aided program. Also the armature is tested in laboratory by using thermocouples and thermal camera. At the end of the study the results are compared and the convergence of computer simulation is observed.

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