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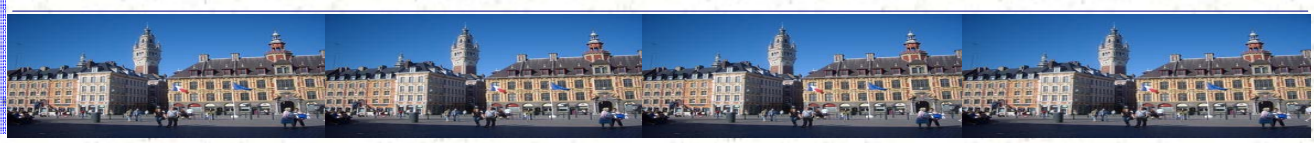

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Imaging Reconstruction of Internal Tissue Region Boundary by Analytic and Numerical Simulation

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Abstract

By the interaction between optic and biology born a new science, the biophotonic with their applications are already present in the medical diagnostic and therapy. In particular, near-infra-red (NIR) mammography imaging promising diagnostic tool for detecting breast cancers. The energy propagation in a highly scattering medium such human tissue can be modeled accurately by a time transport equation. By the regular Fourier transformation (time ? frequence) we obtain an equivalently elliptic complex partial differential equation (PDE) for spectrum intensity resolution using the simulation by 2D finite element methods and after that we apply the inverse fast Fourier transformation (IFFT) techniques to find the photon density in time domain. Analytical and Numerical results are presented.

A Generic Simulation Service for Distributed Multi-Agent Systems

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Abstract

Multi-agent systems are well suited for building large software systems. A great deal of these complex systems includes process flows that are concerned with time or are even time-critical. The activities of these process flows are often executed in distributed autonomous subsystems that have to be synchronized with respect to the superordinated task execution. To be able to build such systems and test their behaviour adequately, it is often advantageous and sometimes necessary to simulate them in the run-up to their practical use. Testing and simulation of process flows within multi-agent systems requires synchronization of the participating agents with respect to the global simulation time. In this paper, a design proposal and a service implementation for testing and simulation is presented, which takes care of the special requirements imposed by multi-agent settings. This so called time service is implemented as a FIPA-compliant agent, and can be used to couple heterogeneous subsystems implemented on different agent platforms.

Multidimensional Shooting Method for Nonlinear Boundary Value Problems

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Abstract

In this work we consider a finite set of boundary value problems defined on neighboring intervals. The solutions at the boundaries are assumed to be smooth. We introduce a multidimensional shooting method (backward and forward) to simultaneously solve for the solutions. The set of initial conditions are iteratively adjusted using one of the iterative methods such as the steepest descent technique. Application of this method to certain models will be presented. The convergence of the method is also discussed.

An invariant subspace method for large scale algebraic Riccati equation

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Abstract

We consider the Algebraic Riccati Equation (ARE) used to define the feedback solution of the linear quadratic regulator problem. A classical approach to compute the solution of ARE is to consider the invariant stable subspace of the Hamiltonian matrix associated to the equation. For large scale systems, the complete determination of this subspace is out of reach, and only a part of it can be computed. We show that the feedback operator is defined by considering only the controllable and observable modes of the system. By using this property, we discuss the choice of the stable invariant subspace of the Hamiltonian matrix. We introduce a low rank approximation of the solution of ARE which is a symmetric and positive semi-definite matrix. The feedback operator we obtain is a good approximation of the exact operator and stabilizes the system. We present the particular case of Lyapunov equation and Bernoulli equation ([1]). In this case, if the system has some unstable modes, we obtain, by using the same method, the exact unique stabilizing solution. A connection of this approach with model reduction is also presented. To illustrate the method, we give various examples of optimal control problems in fluid mechanics

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A Hybrid Direct-Iterative Method for Constrained Linear Systems from Implicit Structural Mechanics

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Abstract

Implicit structural mechanics requires minimizing $\|Ku - f\|_2$ subject to $Cu = g$, where K is an $n \times n$ stiffness matrix, u is an $n \times 1$ vector of translations and rotations, f is an $n \times 1$ vector of forces and C is an $r \times n$ full rank constraint matrix, where $r \leq n$.

With a direct elimination technique we use the r constraint equations to eliminate r of the n stiffness system equations, giving an $(n - r) \times (n - r)$ reduced linear system $\widehat{K}_{\mathcal{I},\mathcal{I}} u_{\mathcal{I}} = \widehat{f}_{\mathcal{I}}$ to solve for the independent degrees of freedom $u_{\mathcal{I}}$.

The solution of this reduced linear system is typically done using a direct solver. In part this is due to tradition, or the ill-conditioning of the system due to the use of shells, or the fact that many applications of interest are inherently 2-D or 2.5 dimensional (think of sheet metal forming or the shape of a car chassis) and so suited for direct methods. Eigenanalysis is another application which requires very accurate solutions to the intermediate linear systems, for which direct solvers are better suited than iterative solvers.

Nonetheless, there comes a point where direct solvers stumble. At present this point lies around 10M degrees of freedom in our applications. Here the storage for the factors force the application code to go out-of-core, which significantly slows down the solution process. The use of distributed memory computers has raised the upper size limit for a practical use of direct solvers, but our MPP codes still must go out-of-core for the largest problems.

We are interested in using a direct solver to solve a smaller linear system that remains in-core. Therefore our approach is a hybrid direct-iterative solver, where the reduced system $\widehat{K}_{\mathcal{I},\mathcal{I}} u_{\mathcal{I}} = \widehat{f}_{\mathcal{I}}$ is solved using a preconditioned conjugate gradient algorithm. The preconditioner is a direct solve of a further reduced system that remains in-core.

We partition the independent degrees of freedom into fine $u_{\mathcal{F}}$ and coarse $u_{\mathcal{C}}$ dof and construct constraints that define the fine dof in terms of the coarse dof, i.e., $u_{\mathcal{F}} + \widehat{C}_{\mathcal{F},\mathcal{C}} u_{\mathcal{C}} = 0_{\mathcal{F}}$. We use direct elimination to form the reduced system $\widetilde{K}_{\mathcal{C},\mathcal{C}} u_{\mathcal{C}} = \widetilde{f}_{\mathcal{C}}$. One step of the preconditioner requires projecting the force from the fine dof $f_{\mathcal{F}}$ onto the coarse dof $f_{\mathcal{C}}$, solving the second reduced system for $u_{\mathcal{C}}$, and then using the constraints to solve for the fine dof $u_{\mathcal{F}}$.

Physics-based metamodeling for parameterized PDE problems using space-parameter space Principal Component Analysis

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Abstract

In this work, we propose reduced-order models (ROM) to deal with parameterized PDEs, where the parameters are involved within the equation and the boundary conditions. The construction of POD (Proper Orthogonal Decomposition) modes in both physical space and parameter space allows to summarize high-dimensional discrete solutions with few coefficients, as described in [1, 2]. For numerical experiments and validation we consider several 2D nonlinear stationary convection-diffusion-reaction problems, first with two parameters and then with five ones. For these two applications it is shown that a 5×5 (respectively 13×6) coefficient matrix is sufficient to reproduce accurately the expected solution. This methodology can have advantages for specific Computational-Assisted Engineering problems, such as design analysis and optimal design. Moreover let us point out that the ROM that we propose include some Physics and owns a nonintrusive feature, which is of great advantage. Indeed this work is based on the ideas developed in [3], where a nonintrusive Physics-based-metamodeling formalism is discussed. Finally, an extension of these ROM concerns unstationary parameterized problems (see [2]).

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A fully automatic parallel GMRES solver preconditionned by a Multiplicative Schwarz iteration

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Abstract

The goal of the work [1, 2, 3] was to design a parallel solver adapted to large and sparse linear systems. One of the sought characteristics was to obtain a fully automatic code which minimizes the users involvement.
The method is the GMRES method preconditioned by a Multiplicative Schwarz iteration based on an algebraic domain decomposition with overlapping blocks. With domain decompositions, the most frequent option for a parallel preconditionner is to consider the Additive Schwarz iteration wich is intrinsically parallel, contrary to its multiplicative counterpart. In spite of that, the present option is to select the multiplicative version for its usually much better effect for speeding up the convergence.
Parallelism is obtained by pipelining the steps of the relaxation within the construction of the Arnoldi basis. This is obtained by an a priori construction of a basis of the Krylov space and it implies a special control on the roundoff errors. The final code does not involve global synchronization as usually done with the distributed inner products which often prevents an efficient parallelization. A special tool was also designed to obtain an adequate partitionning of the matrix.

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Memory and Cache Efficient Grid Generation Based on Sierpinski Curves for the Simulation of Dynamically Adaptive Problems

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Abstract

We present an approach to the numerical simulation of dynamically adaptive problems on recursively structured adaptive triangular grids. The intended application is the simulation of oceanic wave propagation (Tsunami simulation, e.g.) based on the shallow water equations. For the required 2D dynamically adaptive discretisation, we adopt a grid generation process based on recursive bisection of triangles along marked edges. The recursive grid generation may be described via a respective refinement tree, which is sequentialised according to a Sierpinski space-filling curve. This leads to a storage scheme for the adaptive grid that requires only a minimal amount of memory (less than 10 bytes per grid cell). Moreover, the sequentialisation and, hence, the locality properties induced by the space-filling curve are retained throughout adaptive refinement and coarsening of the grid. Explicit and implicit time-stepping techniques, as well as efficient multilevel solvers for linear systems arising from implicit time discretisation, are implemented using an inherently cache-efficient processing scheme, which is based on the use of stack and stream-like data structures and a traversal of the adaptively refined grid along the Sierpinksi curve. We demonstrate the computational efficiency of the approach by showing performance results for several test scenarios. We will also show first results of the implementation of a Discontinuous Galerkin method to solve the shallow water equations on dynamically adaptive grids.

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Block factorization of a Hankel matrix and Euclidean Algorithm

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Abstract

We propose the solution of a general Toeplitz linear system via matrix embedding and transformation in generalized Cauchy form. Some interesting results are shown in the rank deficient case.

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Jacobi method for Hamiltonian eigenvalue problem

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Abstract

We adapt the nonsymmetric Jacobi iteration to the special case of Hamiltonian structure. We describe a way to compute a Hamiltonian Schur form by using sequence of symplectic similarity transformations. Our purpose is to use new symplectic Givens rotations defined in a $\mathbb{K}$-module structure ($\mathbb{K} = \mathbb{R}^{2\times 2}$). The construction of those transformations are defined in parallel with the classical Givens rotations in the Euclidean spaces.

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Algebraic analysis of non-Galerkin type coarse grid operators in multigrid methods and examples for circulant matrices

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Abstract

In geometric multigrid methods it is common to rediscretize the problem on the coarser grid using the same type of discretization but a coarser grid spacing. As a result the number of arithmetic operations is constant per unknown on each level. These methods are optimal, i.e. $\mathcal{O}(N)$, for a broad class of problems.
In algebraic multigrid methods the Galerkin operator is used on the coarse grid. Its use is possible in geometric settings as well and it is known at least since the work of Nicolaides [4]. While it is optimal in the sense of the theory presented by Mandel [2], McCormick [3] and by Ruge and Stüben [5], its use has a downside. As the coarse grid operator is formed as the product of the restriction operator, the fine grid operator and the prolongation operator the operator complexity is growing, i.e. the number of arithmetical operations per unknown is growing, while the number of unknowns is reduced. While this will not necessarily harm optimality of the methods, the question arises if the additional work is necessary, as it does not occur in geometric multigrid methods. Motivated by the techniques presented in the work of Ashby and Falgout [1] we analyzed the implications of similar approaches on the two grid and multigrid convergence. We derived conditions on that the methods still converge and bounds for the convergence rate of the modified methods.
We will present our theoretical considerations as well as some multigrid methods for special classes of circulant matrices as an example.

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A thin plate spline-Lyapunov method for smoothing approximation problems

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Abstract

Variational methods in Computer Aided Geometric Design and Earth Sciences have received considerable attention, due to their efficiency and usefulness in the fitting and design of curves and surfaces. A wide range of minimization functionals derived from physical considerations have been studied these last years. In this talk, we introduce a new numerical method for solving the smoothing approximation problem by minimizing the energy related to thin plate splines [4, 1, 2]. Our approach is based in converting the original smoothing approximation problem to solving Lyapunov matrix equations. To solve those matrix equations, we use some matrix Krylov subspace methods such as global GMRES [5, 3]. Some applications are given for surface approximation fitting and restoration of images that have been degraded by an additive noise.

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About the distance to the nearest pencil

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Abstract

This work focuses on nonsquare matrix pencils $A - \lambda B$ where $A, B \in \mathcal{M}^{m \times n}$ and $m > n$. Traditional methods for solving such non-square generalized eigenvalue problems $(A - \lambda B)\underline{v} = \underline{0}$ are expected to lead to no solutions in most cases. We propose a different treatment: we search for the minimal perturbation to the pair (A, B) such that these solutions are indeed possible. This talk proposes insight into the characteristics of the described problems along with practical numerical algorithms towards their solution. We also present a simplifying factorization for such non-square pencils, and some relations to the notion of pseudospectra. We finish by introducing the correlation with dynamical systems and the notion of controllability.

On some properties of the bivariate Shepard operator of Bernoulli type

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Abstract

The Shepard method is a well suited method for multivariate interpolation of very large scattered data sets. It has the advantages of a small storage requirement and an easy generalization to additional independent variables, but it suffers from no good reproduction quality, low accuracy and a high computational cost relative to some alternative methods.
In [3] we have introduced a combined operator of Bernoulli type which diminishes the mentioned drawbacks. It is obtained using the classical Shepard operator and then a modified Shepard method, introduced by Franke and Nielson in [6]. They preserve the advantages and improve the reproduction qualities, have better accuracy and better computational efficiency.
We study the possibility to constrain the modified Shepard-Bernoulli to take nonnegative values, then to take values in the interval $[0, 1]$ and furthermore in an arbitrary interval $[a, b]$, $a > b$, $a, b \in R$, as it was studied in [1] for a certain class of Shepard operators.

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On the Newton-GMBACK method

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Abstract

GMBACK [3] is a Krylov solver for large linear systems

$$Ax = b, \quad A \in \mathbb{R}^{N\times N} \text{ nonsingular}, b \in \mathbb{R}^N,$$

which is based on backward error minimization properties. For a given subspace dimension $m \in \{1, \ldots, N\}$ and an initial approximation $x_0 \in \mathbb{R}^N$ having the residual $r_0 = b - Ax_0$, GMBACK finds $x_m^{GB} \in x_0 + \mathcal{K}_m = x_0 + \text{span}\{r_0, Ar_0, \ldots, A^{m-1}r_0\}$ by solving:

$$\left\|\Delta_m^{GB}\right\|_F = \min_{x_m \in x_0+\mathcal{K}_m} \|\Delta_m\|_F \quad \text{w.r.t. } (A - \Delta_m)x_m = b,$$

where $\|\cdot\|_F$ denotes the Frobenius norm of a matrix.
The minimum backward error is guaranteed (in exact arithmetic) to decrease as the subspace dimension is increased. We consider some test problems for nonlinear systems $F(y) = 0$, which we solve by the Newton-GMBACK method:

$$\left(F'(y_k) - \Delta_k^{GB}\right) s_k^{GB} = -F(y_k)$$
$$y_{k+1} = y_k + s_k,$$

$k = 0, 1, ...,$ y_0 given. We notice that in floating point arithmetic the mentioned property does not longer hold, and this leads to nonmonotone behavior of the errors. We study the causes of this behavior and we also propose some remedies.

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Calculating the H_∞-norm of large sparse systems via Chandrasekhar iterations and extrapolation

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Abstract

We consider the computation of the $\mathcal{H}_\infty$-norm ($\gamma^* := \|G(z)\|_\infty$) of a $p \times m$ real rational transfer function

$$G(z) := C(zI_n - A)^{-1}B + D \tag{1}$$

of a discrete-time system, where $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{p\times n}$, and $D \in \mathbb{R}^{p\times m}$, with $n \gg m, p$.

It is well known that γ^* is bounded if and only if $G(z)$ is stable. We therefore assume that the given quadruple $\{A, B, C, D\}$ is a real and minimal realization of a stable transfer function $G(z)$. The stability of $G(z)$ implies that all of the eigenvalues of A are strictly inside the unit circle, and hence that $\rho(A) < 1$, where $\rho(A)$ is the spectral radius of A.

Our result is related to the *bounded real lemma*, which states that $\gamma > \|G(z)\|_\infty$ if and only if there exists a solution $P \succ 0$ to the linear matrix inequality (LMI):

$$H(P) := \begin{bmatrix} P - A^TPA - C^TC & -A^TPB - C^TD \\ -B^TPA - D^TC & \gamma^2 I_m - B^TPB - D^TD \end{bmatrix} \succ 0. \tag{2}$$

This suggests that γ^* could be calculated by starting with an initial large value $\gamma > \gamma^*$ for which the LMI has a solution and iterate by decreasing γ until the LMI does not have a solution. The condition $H(P) \succ 0$ is equivalent to the existence of P as a solution of a special DARE. This solution P can be obtained from an iterative scheme known as the Chandrasekhar iteration:

$$P_{i+1} = A^TP_iA + C^TC - K_i^TR_i^{-1}K_i, \tag{3}$$

where $R_i := B^TP_iB + D^TD - \gamma^2 I_m$, and $K_i := B^TP_iA + D^TC$.

The closed loop matrix $A_{F_i} := A - BF_i$ (where $F_i := R_i^{-1}K_i$) has a spectral radius $\rho_i := \rho(A_{F_i})$ which determines essentially the convergence of the scheme (3). Since $A - BF_i$ is stable and converges to $A - BF_\gamma$ (where F_γ is the feedback corresponding to the DARE), one can track its spectral radius by the power method applied to $A - BF_i$.

Generalized Approximate Inverse Preconditioners for Least Squares Problems

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Abstract

This talk concerns constructing preconditioners for large sparse matrices $A \in R^{m\times n}, m \geq n$, using an approximate inverse idea. The objective is to solve the least squares problem

$$\min_{x\in R^n} \|b - Ax\|_2,\ A \in R^{m\times n},\ b \in R^m \tag{1}$$

by transforming it to

$$\min_{x\in R^n} \|Mb - MAx\|_2,\ A \in R^{m\times n},\ M \in R^{n\times m},\ b \in R^m \tag{2}$$

and then applying a Krylov subspace method.

Preconditioning techniques based on sparse approximate inverse for square sparse matrices have been well developed. One of them is well known as the Minimal Residual method(MR), which was proposed by Chow and Saad in 1998[2]. In this talk, we apply the MR method to a rectangular matrix A to construct a preconditioner M which minimizes the Frobenius norm of $I - MA$ approximately, and then use this M as a preconditioner for Krylov subspace methods.

We found out that M can be expressed in a form of $p_k(A^TA)A^T$, where $p_k(\cdot)$ is a polynomial of degree k. Based on this fact and theoretical results of [1] and [3], we showed that we can use GMRES to solve the preconditioned problem (2) using the preconditioner M and get a least-squares solution to the original problem (1) without breakdown. Moreover, since MA is symmetric, the MINRES method can be used instead of GMRES.

Our numerical experiments show that this preconditioner may be a little expensive, but it can help to reduce the number of iterations significantly, and the preconditioning time pays off in certain cases.

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Preconditioning Navier–Stokes problem discretized by a finite volume method

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Abstract

We focus on the Discrete Duality Finite Volume (DDFV) method whose particularity is to allow the use of unstructured or nonconforming meshes. We discretize the non-linear Navier-Stokes problem, using the rotational formulation of the convection term, associated to the Bernoulli pressure. With an iterative algorithm, we are led to solve a saddle–point problem at each iteration. Many efficient preconditioners are known for saddle–point problems arising from finite–element discretizations, but their adaptation to matrices issued from finite–volume discretizations is not trivial. For example, some preconditioners are not well defined on staggered grids [3]. Moreover, the rotational formulation of the convection is rarely used to test the performances of saddle–point solvers [4].
We will see that this system can be solved by an Uzawa method or by a pressure convection–diffusion type preconditioner [2, 3]. Both methods require a preconditioner for the Schur complement. In [1], Elman et al. introduce a preconditioner based on approximate commutators. This method can be viewed as an algebraic extension of the preconditioners based on formal commutators described in [3]. Then, Olshanskii and Vassilevski [4] introduced a variation of the Elman preconditioner whose performances, in finite elements, are independent of the mesh size for moderate Reynolds numbers.

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On Algorithms to Find an Overlapping Partitioning of a Graph and Applications to Preconditioning

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Abstract

Additive and multiplicative Schwarz preconditioners are known to be an efficient class of preconditioners for problems involving a geometric domain. They are based on decomposing the domain into a set of overlapping subdomains, in such a way that the restrictions of the original problem to the parallel subdomains are easily solvable. Algebraic Schwarz preconditioners work without an underlying geometric domain by restricting the linear operator to overlapping subsets of the coordinates. A good choice of these overlapping subsets is essential for the usefulness of the preconditioner. The graph formulation of the problem is to find an overlapping partitioning of the nodes of the graph of the linear operator.

The algorithms presented to find overlapping partitionings share the idea of starting with finding a non-overlapping partitioning. For this task XPABLO (eXtended PArametrized Block Ordering) is used. Note that the non-overlapping partitionings found by XPABLO can be used to construct block Jacobi and block Gauss-Seidel preconditioners; see [1]. Each subgraph in this partitioning is then grown to include nodes overlapping with other subgraphs. The algorithms use structural and numerical properties of the underlying matrix to find the nodes to be added to each subgraph. Several strategies to control the amount of overlap added to each subgraph are presented.

Numerical experiments show how these algebraic Schwarz preconditioners perform and how their performance compare to and improve on the performance of XPABLO-based block diagonal and block triangular preconditioners.

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Performance evaluation of IDR

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Abstract

The IDR(s) method proposed by P. Sonneveld and M. van Gijzen[**?**] showed excellent characteristics compared with the conventional iterative methods in terms of convergence rate and amount of needed memory.
In this article, we evaluate performance of IDR(s) method compared with that of GMRES(k) method for various problems in Florida Sparse Matrix Collection. In particular, we estimate performances for some problems unsolved by these iterative methods with usual ILU(0) decomposition as preconditioner.
In Table **??**, we present convergence of ILU(0) preconditioned IDR(s) and GMRES(k) methods with accelerated parameter γ (≥ 1.0) for diagonal entries for matrices Li and Xenen2.
Parameter s of IDR(s) method varies from 1 upto 10, and examined parameter k of GMRES(k) method are 10, 20, 50, 100, 150 and 200. "pre-t", "itr-t" and "tot-t" as shown in Table **??** mean CPU times in seconds of preconditioing, iteration and in total, respectively. Similarly, "mem. [MB]" means needed memory in Mega-bytes. The bold figure represents the least CPU time for each matrix. Table **??** verifies that IDR(s) method works well compared with GMRES(k) method in view of CPU time and amount of necessary memory.

matrix	γ	method	$s(k)$	itr.	pre-t [sec.]	itr-t [sec.]	tot-t [sec.]	ratio	mem. [MB]	ratio
Li	1.0	IDR	all	max	-	-	-	-	-	-
		GMRES	all	max	-	-	-	-	-	
	1.1	IDR	10	max	-	-	-	-	54.41	1.00
		GMRES	200	max	-	-	-	-	83.98	1.54
	1.2	IDR	7	806	0.73	13.20	13.93	1.00	52.85	1.00
		GMRES	200	2914	0.74	81.75	82.49	5.92	83.98	1.59
	1.3	IDR	4	466	0.74	7.10	**7.84**	1.00	51.29	1.00
		GMRES	200	2904	0.75	75.34	76.09	9.71	83.98	1.64
Xenon2	1.0	IDR	all	max	-	-	-	-	-	-
		GMRES	all	max	-	-	-	-	-	-
	1.1	IDR	2	399	1.10	23.54	**24.64**	1.00	159.78	1.00
		GMRES	50	389	1.12	29.39	30.51	1.24	211.46	1.32
	1.2	IDR	4	375	1.08	23.96	25.04	1.00	166.99	1.00
		GMRES	50	452	1.11	34.44	35.55	1.42	211.46	1.27
	1.3	IDR	2	398	1.10	23.85	24.95	1.00	159.78	1.00
		GMRES	100	431	1.13	39.68	40.81	1.64	271.59	1.70

Table1: Numerical results of IDR(s) and GMRES(k) methods for matrices Li and Xenon2.

Parallel resolution of sparse linear systems by mixing direct and iterative methods

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Abstract

Parallel sparse direct solvers are now able to solve efficiently very large three-dimensional linear systems but require a lot of memory to store the factors. Iterative methods on the other hand require much less memory but often fail to solve ill-conditioned method. We propose a hybrid method to make the most of these two classes of method by combining them and building a robust parallel solver, able to solve difficult problems in a effective way by using notably few memory and dense block matrix operations (BLAS).

Our approach is to build a decompositions of the adjacency graph of the system into small "domains" usually of a few hundreds or thousand nodes with overlap. The subsytems corresponding to interior domains are factored exactly; those small subsystems are independent and can be solved in parallel. Thanks to the exact solution of this part of the system, solving the whole system amounts to solve the Schur complement system on the interface between subdomains.

A krylov subspace method is used to solve this subsystem preconditioned with an ILU factorization of the whole Schur complement. The special ordering of the unknowns and the block fill-in pattern in the factors of the Schur complement are chosen to control memory usage, exhibit parallelism and take advantage of dense block computation.

The talk will present some algorithms and the performance of our parallel solver `HIPS` (Hierarchical Iterative Parallel Solver) and a comparison of different build-in strategies : for example we are also able to use ILUT method during the Schur matrix computation to drop even more terms and the resulting drop of computation volume can in some case balance the lost of BLAS acceleration.

Improving the parallel performance of a domain decomposition preconditioning technique in the Jacobi-Davidson method for large scale eigenvalue problems

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Abstract

Most computational work in Jacobi-Davidson [1], an iterative method for large scale eigenvalue problems, is due to a so-called correction equation. In [2, 3] a strategy for the computation of (approximate) solutions of the correction equation was proposed. The strategy is based on a domain decomposition preconditioning technique in order to reduce wall clock time and local memory requirements.

However, there is more to gain. This talk discusses the aspect that the original strategy in [2, 3] can be improved by taking into account that, for approximate solves of the correction equation by a preconditioned Krylov method, Jacobi-Davidson consists of two nested iterative solvers. For ease of presentation, consider the standard eigenvalue problem $\mathbf{A}\,\mathbf{x} = \lambda\,\mathbf{x}$ with an approximate eigenvalue θ, computed by Jacobi-Davidson so far, and preconditioner $\mathbf{M} \approx \mathbf{A} - \theta\,\mathbf{I}$. In the innerloop of Jacobi-Davidson a search subspace for the (approximate) solution of the correction equation is built up by powers of $\mathbf{M}^{-1}\,(\,\mathbf{A} - \theta\,\mathbf{I}\,)$ for fixed θ. In the outerloop a search subspace for the (approximate) solution of the eigenvalue problem is built up by powers of $\mathbf{M}^{-1}\,(\,\mathbf{A} - \theta\,\mathbf{I}\,)$ for variable θ. In [2, 3] the domain decomposition preconditioning technique was applied to the innerloop. But, as θ varies slightly in succeeding outer iterations, one may take advantage of the nesting by applying the same technique to the outerloop.

For large scale eigenvalue problems this aspect turns out to be nontrivial. In the talk, the impact on the parallel performance will be shown by results of scaling experiments on linux clusters (up to 200 nodes). This is of interest for large scale eigenvalue problems that need a massively parallel treatment.

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Nonnegative Matrix Factorization and Underapproximation

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Abstract

Nonnegative Matrix Factorization (NMF) is a recent compression technique which allows interpretation of nonnegative data. After recalling some well-known ideas about NMF, we present a new efficient algorithm based on the method of alternating variables (also called coordinate descent method). While it has fast convergence and low complexity, it generates sparse and accurate solutions.
Afterwards, we introduce a similar problem : Nonnegative Matrix Underapproximation (NMU). We show that NMU is equivalent to the maximum edge biclique problem in bipartite graphs, which is NP-complete. However, for a positive matrix, it is possible to solve the rank-one problem for specific cost functions. This can be used to build recursively an underapproximation of a desired rank. We then present a global approach to solve the NMU problem using Lagrangian relaxation and adapting the NMF algorithms. NMU is particularly well-suited to achieve part-based representation, for example in facial feature extraction. It can also be used to initialize classical NMF algorithms: as it has already been observed, judicious initializations allow to speed up the convergence and improve the solution compared to random ones.

Keywords: Nonnegative Matrix Factorization, Coordinate Descent Method, Maximum Edge Biclique Problem, Part-based Representation, Image Processing, Text Mining, Initialization.

Parallel algebraic additive Schwarz preconditioners for Schur complement systems in 3D

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Abstract

In this work we investigate the parallel scalability of variants of additive Schwarz preconditioners for three dimensional non-overlapping domain decomposition methods. To alleviate the computational cost, both in terms of memory and floating-point complexity, we investigate variants based on a sparse approximation or on mixed 32- and 64-bit calculation. The robustness of the preconditioners is illustrated on a set of linear systems arising from the finite element discretization of elliptic PDEs, and from structural mechanical problem through extensive parallel experiments on up to a thousand processors. Their efficiency from a numerical and parallel performance view point are studied. Consequently the size of the linear systems varies from 8 millions to 43 millions unknowns.

The research activity of the first two authors was partially supported within the framework of the ANR-CIS project Solstice (ANR-06-CIS6- 010)

Extremal rational functions on discrete sets and superlinear convergence of the ADI method

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Abstract

The ADI iterative method may be used to solve the Sylvester equation
$AX - XB = C$, which occur for instance for partial realization problems in linear control theory.

The convergence analysis of the ADI method shows that the rate of convergence — in case of choice of optimal parameters — may be described with help of the Zolotarev quantity

$$Z_n(E_N, F_N) := \min \left\{ \frac{max_{z\in E_N} |r(z)|}{min_{z\in F_N} |r(z)|}, r \in \mathcal{R}_{n,n} \right\}$$

where $\mathcal{R}_{n,n}$ is the set of all rational functions with numerator and denominator of degree at most n and E_N, F_N are discrete sets, such as the spectra of A and B, respectively. In practical problems, often the matrices A, B of order N are stemming from the discretization of some partial differential equation, the quantity N being related to a stepsize, which implies that E_N, F_N for $N \to \infty$ have some asymptotic distribution described by some measures σ_A, σ_B.

In this talk we give the N-th root asymptotics for $Z_n(E_N, F_N)$ for $n, N \to +\infty$ such that $n/N \to t \in (0, 1)$, provided that the families of discrete sets $(E_N)_N$, $(F_N)_N$ have an asymptotic distribution. To our knowledge, the Zolotarev problem for discrete sets has not been considered before. It is well-known from [1] that the superlinear convergence of the conjugate gradient method is closely related to nth root asymptotics of discrete orthogonal polynomials and to a constrained equilibrium problem in logarithmic potential theory for positive measures. For the discrete Zolotarev problem, we show that one has to consider a constrained condenser, that is, a constrained equilibrium problem in logarithmic potential theory for signed measures.

As a consequence, we are able to quantify in an asymptotic sense the rate of super-linear convergence of the ADI method in case of "favorable" asymptotic eigenvalue distributions. We illustrate our findings by discussing some model problems stemming from the discretisation of the Poisson equation.

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A new quasi-Newton secant method for arbitrary black-box linear problems

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Abstract

A new quasi-Newton secant method for solving the linear system of equations $K(p) = 0$ in a matrix-free manner is presented :

$$p_{s+1} \quad = \quad p_s - (\hat{K}'_s)^{-1} K(p_s)$$

It builds an approximate Jacobian $\hat{K}'_s$ based on input-output combinations of a black-box system K. The method that we present in the paper is based on a novel coupling technique using reduced-order models for fluid-structure interaction problems [1]. We adapt it to solve linear problems (representative of the local convergence of non-linear problems), and show that the consecutive approximate Jacobians, and their inverse, can be obtained by a rank-one update, and present analytical foundations to the method and a convergence analysis.
The basic idea of the method can be summarized as follows: define

- $v_i^s = p_s - p_i \;\; (i = 0, \ldots, s-1)$ and
  $V_s = [v_0^s \; v_1^s \; \ldots \; v_{s-1}^s] \in I\!R^{n \times s}$
- $w_i^s = K(p_s) + p_s - K(p_i) + p_i \;\; (i = 0, \ldots, s-1)$ and
  $W_s = [w_0^s \; w_1^s \; \ldots \; w_{s-1}^s] \in I\!R^{n \times s}$

and construct $\hat{K}'_s$ as $\hat{K}'_s = W_s (V_s^T V_s)^{-1} V_s^T - I$.
The method is shown to be theoretically convergent in $n + 1$ steps, i.e. not counting numerical errors. Line searches, which are common for most quasi-Newton methods are shown to have no long term effect on the convergence. No particular conditions, like positive definiteness, are imposed on the system matrix. Compared with other similar methods (like Broyden, SR1, Pearson, BFGS, PSB) using a rank-one update it is shown to be greatly superior for non positive definite matrices.

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An Iterative Scheme for Multilayer Flows in Porous Media

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Abstract

In this work we present an efficient and accurate iterative scheme for the resolution of the flow velocity of fluid in multilayer porous media. The porous layers are of different characteristics, thus introducing discontinuity at the interface regions. The flow velocity and shear stress are assumed to be continuous at the interface between the layers. The method is based on the nonlinear shooting method for boundary value problems which transforms the problem to solving a sequence of initial value problems. Newton's method is used as the iteration mechanism. Accuracy of the algorithm is validated by examples for which exact solutions are known. Convergence of the algorithm is discussed.

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Block versus global extended Arnoldi methods for Sylvester matrix equations

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Abstract

In this talk, we compare two projection methods for solving Sylvester matrix equations of the form $AX - XB = C$ where $A \in \mathbb{R}^{n\times n}$ is a large and sparse matrix and $B \in \mathbb{R}^{n\times s}$ with $s \ll n$. The two proposed methods are based on the use of the block extended Arnoldi process and the global extended Arnoldi process respectively. Both the two process- the block one and the global one-, use the inverse of the matrix A to enrich the classical block and matrix Krylov subspaces. Hence, the generated sequences of approximation subspaces contain information on both the matrix A and and its inverse A^{-1}, by adding two vectors at the time, one multiplied by A, and one by A^{-1}. We also show how to obtain low rank approximate solutions to the Sylvester matrix equation $AX - XB = EF^T$, where $E \in \mathbb{R}^{n\times r}$, $F \in \mathbb{R}^{s\times r}$ are matrices of rank r with $r \ll n$ and $r \ll s$. For this second matrix Sylvester equation, we also show how to get approximate solutions in a factored form. We end this talk by reporting some numerical experiments.

Keywords. matrix Sylvester equation, low rank approximate solutions, extended block Krylov subspaces, extended matrix Krylov subspace, Arnoldi process, projection methods,

How to make Simpler GMRES and GCR more stable

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Abstract

In this contribution we analyze the numerical behavior of several minimum residual methods. Two main approaches are compared: the one that computes the approximate solution in terms of a Krylov space basis from an upper triangular linear system for the coordinates, and the one where the approximate solutions are updated with a simple recursion formula. We show that a different choice of the basis can significantly influence the numerical behavior of the resulting implementation. While Simpler GMRES [2] and ORTHODIR [4] are less stable due to the ill-conditioning of the basis used, the residual basis is well-conditioned as long as we have a reasonable residual norm decrease. These results lead to a new implementation, which is conditionally backward stable, and, in a sense they explain the experimentally observed fact that the GCR [3] (also known as ORTHOMIN [4]) method delivers very accurate approximate solutions when it converges fast enough without stagnation.

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Multilevel Methods for Nonsymmetric Discontinuous Galerkin Methods

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Abstract

The application of discontinuous Galerkin methods to elliptic or parabolic problems dates back to the 1970's, see e.g. [1]. More recently their application to elliptic and parabolic problems has gained interest again due to new developments, see [2]. As a consequence, solution methods for the arising discrete problems became a field of active research. Multilevel methods for conforming as well as for many nonconforming discretizations are well-established. For discontinuous Galerkin methods multilevel- theory and practice are less developed. For the symmetric case multilevel methods have been analyzed e.g. in [3]. The non-symmetric situation has been treated only on a less rigorous level, see e.g. [4].

In this contribution we discuss a multilevel solver for discontinuous Galerkin discretizations. It is based on overlapping block-iterative schemes. We apply the methods to different non-symmetric discontinuous Galerkin discretizations of the Poisson equation, namely the OBB-, NIPG- and the IIPG-scheme, see e.g. [5]. The solution behavior is investigated with respect to the penalty parameter and the problem size. It is shown that for certain combinations the resulting schemes are of optimal complexity.

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On a local multilevel scheme for the 2D incompressible Navier-Stokes equations with domain decomposition

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Abstract

We aim to integrate incompressible Navier-Stokes equations describing the motion of a fluid in a domain $\Omega \in \mathbb{R}^2$. General and open boundary conditions and mixed finite elements are used. The velocity and pressure fields, the unknowns of the problem, can be splitted into small and large scales by using hierarchical basis.

A autoadaptative multilevel approach is studied and implemented here: when a coarse level of discretization is chosen, we solve only the equation for the large scale components. But, the effect of the small scales cannot be neglected, this would introduce to much error. Deriving bounds on the error introduced, we obtain estimates on the lengths of time during which the interaction terms can be frozen.

Also, it has been shown that the notion of small and large scales should be local, the small scales can have a negligible or important effect, depending on their positions and on the time. One possibility to define a localized decomposition is to consider a decomposition of the domain Ω and, on each subdomain, to use hierarchical basis.

Following the FETI ideas, the original problem is reduced to the interface problem which is formulated as a dual one by the introduction of the stress vector, the dual variable of the velocity. This vector, which components are interpreted as Lagrange multipliers, enforce the compatibility at interface nodes.

A "dual" Schur method is implemented on a parallel computer with distributed memory, where each subdomain was assigned to an individual processor. Some numerical results for the lid-driven cavity test and the flow past an obstacle, for Reynolds numbers corresponding to periodic regimes, confirm our approach.

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A domain decomposition method for the resolution of an eigenvalue problem in neutron physics

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Abstract

The simulation of the neutron transport inside a nuclear reactor leads to the computation of the lowest eigen pair of a simplified transport operator T [1]. The numerical strategy at our disposal today presents two drawbacks. On the one hand, the memory requirement is so high that certain case studies cannot be carried out on standard workstations. On the other hand, the solver is based on a conforming cartesian mesh, which does not allow us to locally refine the mesh in zones of interest. The computation of the lowest eigen pair of T is done by computing the highest eigenmode of T^{-1} with the power algorithm. At each iteration, a block Gauss-Seidel algorithm is used to solve a linear system of the form $Ax = b$. For our application, one Gauss-Seidel iteration is already sufficient to ensure the right convergence of the power algorithm. For the resolution of the linear system, we propose a non overlapping domain decomposition based on the introduction of Lagrange multipliers in order to deal with different numerical approximations (mesh size, finite element order) between two adjacent subdomains [2]. The method performs well on simple test cases provided that the linear system is solved sufficiently accurately. Furthermore, we present results from parallel computations on up to 100 processors for an industrial test case.

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Feedback control algorithms for large linear systems

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Abstract

Let us consider a large linear system, e.g. coming from the discretization of partial differential equations. Using an iterative solver, let us describe the evolution of the error with a dynamical, discrete-time linear system, controlled by an output feedback, see e.g. [1]. The choice of the control technique, i.e. of the controller, a matrix, is fundamental; it can be simply noted that it acts as the inverse of a preconditioner. We consider the application of well established techniques taken from the automatic control theory, to the iterative solution of large linear systems. Therefore, there is an intimate connection with the design of preconditioners. In general, an effective technique is the *pole-placement*, which for discrete-time systems can lead to a *deadbeat* condition, i.e. to guarantee that the error vanishes in a finite number of iterations, but for large dimensions the computational cost is too high. The construction of preconditioners with a partial pole-placement technique [3] can be found in [2], which we refer for comparison. We propose two techniques, at opposite sides: *partial deadbeat control* and *PID autotuning*. In the first, computationally expensive, the characterization of the control action is quite difficult, since the controller is the result of an inverse eigenvalue problem, while the behaviour of the error dynamics is simply imposed by choosing the desired locations for the eigenvalues of the closed loop system matrix. In the second, computationally cheap, the control action is simply proportional to the residual, its integral and its derivative, while the error dynamics are not easily predictable. Here can help the *autotuning*: the optimal parameters of the control algorithm are determined iteratively, according to the computed residual. In this way, it determines a-posteriori the unknown relation between the desired dynamics for the error and the variable PID control law. We show some preliminary results for both techniques.

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Balanced Incomplete Factorization based on AISM

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Abstract

A new incomplete algorithm to factorize a positive definite symmetric matrix into triangular factors, LDL^T factors and their inverses, at the same time, is presented. The method use the approach based on the Sherman-Morrison formula [3] to compute an approximate inverse of the matrix.
In this algorithm the direct and inverse factors directly influence each other throughout the computation, and if the dropping strategies of [2] are used a balance in the factors is achieved, helping to control the conditioning of the factors.
The new approximate LDL^T factorization is called Balanced Incomplete Factorization (BIF). Experimental results show that this factorization is very robust and may be useful in solving difficult ill-conditioned problems by preconditioned iterative methods. The new approach exhibits shorter setup times than RIF [1], a method of a similar and very high level of robustness.

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Numerical resolution of elliptic problems in perforated domains

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Abstract

The modelling of composite materials or fluid particle flows calls for efficient solvers of Poisson-like problems on domains with (possibly many) holes or inclusions. After a description of the native difficulties of the problem, we will give an overview of the several methods which have been proposed to address this challenge, and present in detail some of them, paying a special attention to numerical efficiency and conditionning aspects. Among the methods we plan to present, let us mention the direct approach, based on a boundary-fitted (and therefore unstructured) mesh, and fictitious domain methods (based on a global mesh which covers the whole region of interest), like the Penalty Method, the Fat Boundary method, and some new variants of the Saddle Point approach à la Glowinski.

The parametrized Lanczos method for multiple right-hand side

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Abstract

The solution of the parametrized system

$$Ax = f \quad \text{with} \quad A = K - \omega^2 M \tag{1}$$

with K real symmetric, and M symmetric positive definite arises in applications, including structural engineering and acoustics. The parameter ω is often the frequency (or the wave number) and lies in $[\omega_{\min}, \omega_{\max}]$, which is the frequency interval where the numerical model is valid. Usually, $\omega_{\max}$ is determined by the level of mesh refinement. In many cases, $\omega_{\min} = 0$. The solution x is called the frequency response function.

The traditional method in engineering is modal superposition where (1) is projected on the eigenvectors associated with the eigenvalues of

$$Ku = \lambda M u \tag{2}$$

in $\Lambda = [\lambda_{\min}, \lambda_{\max}]$, where $\lambda_{\min} \ll \omega_{\min}^2$ and $\lambda_{\max} \gg \omega_{\max}^2$. This method is usually experienced as very efficient when the eigenvectors and eigenvalues are available, since (1) is transformed to a diagonal linear system. The practical problem is that it is not always clear how $\lambda_{\min}$ and $\lambda_{\max}$ need to be chosen. For example, when $\omega_{\min} = 0$, we use $\lambda_{\min} = 0$ and $\lambda_{\max} = \eta\omega_{\max}^2$ with $\eta \in [2, 10]$.

Efficient methods for solving (1) have been developed over the last decade, in the context of iterative linear system solvers for parametrized problems [**?**] [**?**], and the Padé via Lanczos method in the context of modelreduction [**?**] [**?**] [**?**].

In this paper, we study the use of eigenvectors to precondition the Lanczos method from [**?**] for solving (1). Modal superposition is used as a preconditioner to the parameterized Lanczos method. This work is an extension of recycling Ritz vectors for the solution of linear systems with multiple right-hand sides to parameterized linear systems with multiple right-hand sides. We show a numerical example arising from structural analysis.

A Multigrid Method for Evolution Problems with Adaptive Local Refinement

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Abstract

We present a multigrid solver for a multilevel adaptive finite element approximation of evolution partial differential equations (PDEs).

The principle of the adaptation procedure, called CHARMS, is to refine/unrefine primarily basis functions instead of meshes. More precisely, a parent/child relationship is stated between basis functions belonging to Lagrange finite element spaces associated with successively nested grids. The elementary refinement (resp. unrefinement) is then defined by the replacement of parents (resp. children) by their children (resp. parents).

At a given time t_n, the history of the time marching procedure, which involved many adaptation stages, leads to a multilevel approximation space V_J of functions belonging to different levels from the coarsest (level 1) to the finest (level J). Then a Galerkin method is used on the basis of V_J to approximate the unknowns at time t_n. The multilevel structure of V_J is further exploited to design efficient preconditioners of the arising linear system: the multigrid framework is applied on coarsened auxiliary embedded spaces $V_1 \subset \cdots \subset V_{J-1} \subset V_J$. A coarse space $V_{\ell-1}$ is obtained from the immediately finer space V_ℓ by replacing all basis functions of level ℓ by their parents. The intergrid transfer operators are deduced from the natural injection $V_{\ell-1} \to V_\ell$ which is easily derived from the algebraic relationships between parent/child basis functions. Thus, the auxiliary spaces V_ℓ are deduced from V_J but not from the adaptation procedure which leads to V_J.

Attractive features follow from this methodology:

- the same subdivision pattern is uniformly applied to all meshes ;
- the generated grids are nonconforming but the multilevel finite element approximation spaces remain conforming by construction ;
- apart from the prolongation matrices, the multigrid algorithm if fully expressed in a pure algebraic setting ;
- A large independence is maintained between the particular PDEs, the adaptation procedure, the discretization scheme and the algebraic solver.

The capabilities of the presented numerical scheme are illustrated on various examples, including the direct numerical simulation of multiphase flows with diffuse interface methods.

Algebraic Analysis of V-cycle multigrid

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Abstract

We develop the analysis of V-cycle multigrid, targeting results that are applicable to both geometric and algebraic multigrid methods. On one hand, we reformulate the classical abstract Successive Subspace Correction (SSC) theory (presented in [1][2]) adopting it to the algebraic multigrid framework and improving the convergence rate estimate [3]. The resulting theory has a degree of freedom, denoted by a set $\{G_k\}$ of matrices. We investigate some particular choices for this set.

On the other hand, the well-known classical result due to Hackbusch (see [4]) is extended to any reasonable smoother's scaling. We also show that, when a particular set $\{G_k\}$ is used in the reformulated SSC theory, the resulting bound can be compared directly to the extended Hackbusch's result. The comparison of two bounds reveals their complementarity.

Finally, using the reformulated SSC and Hackbusch's theories, we extend the classical scope of Fourier analysis and show how it may be used to accurately predict the actual convergence of V-cycle multigrid.

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Preconditoners for problems with extreme contrast in the coefficients.

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Abstract

When the coefficients of a problem have jumps of several orders of magnitude and are anisotropic, many preconditioners and domain decomposition methods suffer from plateaus in the convergence due to the presence of very small isolated eigenvalues in the spectrum of the preconditioned linear system. We investigate how adequate interface conditions can cope with this problem. Numerical results are given and compared with other approaches.

Optimal Schur methods (Neumann-Neumann or FETI type methods) for systems of PDEs

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Abstract

We focus on domain decomposition methods for systems of PDEs (versus scalar PDEs). The Smith factorization (a "pure" algebra tool) is used systematically to derive new domain decompositions methods for symmetric and unsymmetric systems of PDEs: the compressible Euler equations, the Stokes and Oseen (linearized Navier-Stokes) problem. We will focus on the Stokes system. In two dimensions the key idea is the transformation of the Stokes problem into a scalar bi-harmonic problem. We show, how a proposed domain decomposition method for the bi-harmonic problem leads to a domain decomposition method for the Stokes equations which inherits the convergence behavior of the scalar problem. Thus, it is sufficient to study the convergence of the scalar algorithm. The same procedure can also be applied to the three-dimensional Stokes problem.

An aggregation-based algebraic multigrid method

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Abstract

Algebraic multigrid (AMG) methods are among the most efficient preconditioning techniques for large linear systems arising from discretized PDEs. In this talk, we revisit the simplest and cheapest AMG scheme, based on so-called coarsening by aggregation. We show that the basic two–grid scheme has convergence rate independent of the grid size. This is proved by developing the Fourier analysis of several aggregation–based two–grid schemes for a model anisotropic problem [1]. With a proper choice of the coarsening, the convergence rate is also uniformly bounded with respect to the anisotropy ratio. To further obtain grid independent convergence with a truly *multi*grid method, we consider so-called K–cycle multigrid [2], in which Krylov subspace acceleration is used at every level. This makes multigrid methods significantly more robust, and optimal convergence properties can be proved under mild conditions on the two–grid convergence rate. This approach is combined with an automatic aggregation scheme for which the size of most aggregates is equal to 4, independently of the problem peculiarities [3]. Numerical experiments indicate that the resulting method is efficient and can be more robust than classical AMG methods. These experiments include challenging convection–diffusion problems with high Reynolds number and varying convective flow, as well as some problems from industrial chemistry. We also discuss the parallelization of the method. The aggregation algorithm parallelizes in a natural way, and the method achieves good algorithmic scalability. Timing results indicate that satisfactory speed up can be obtained even on a relatively slow network, providing that the load per processor is kept significant.

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Adaptively tuned IDR(s) method on parameter s

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Abstract

P. Sonneveld and M. van Gijzen devised the IDR(s) method from an extended IDR theorem[1]. The IDR(s) method has excellent property compared with the conventional iterative methods in terms of efficiency of convergence and necessary amount of memory. However, we rarely meet with stagnation of the relative residual 2-norm of the IDR(s) method during the iteration process. In the present article, we propose a strategy for adaptively tuning of parameter s of the IDR(s) method when its residual 2-norm stagnates in the course of iteration process.

We describe briefly an outline of adaptively tuning technique for parameter s of the IDR(s) (abbreviated as AT_IDR(s)) method.

- Let s_{min} be an initial value of parameter s, and s_{max} be maximum value of parameter s.
- Detect stagnation of relative residual 2-norm of IDR(s) method as below.
  - Compute $\sigma_n = \frac{|||\boldsymbol{r}_{n+1}||_2 - ||\boldsymbol{r}_n||_2|}{||\boldsymbol{r}_n||_2}$
  - If a state of $\sigma_n < \delta$ lasts in a succession of $sentinel$ times, we regard that stagnation of IDR(s) method occurred.
- When the above stagnation occurred, in case of $s < s_{max}$, then we make increment as parameter $s = s+1$.
- When the above stagnation didn't occur, in case of $s > s_{min}$, then we set $s = s_{min}$.

In Table 1, we present convergence of IDR(s) and AT_IDR(s) methods for six test matrices. Let number of $sentinel$ be 20, and δ be 0.1. Parameter s varies from 1 upto 10, and we set $s_{max} = s + 2$. In Table 1, "conv. cases" means number of successful converged cases. Table 1 verifies that number of successful converged cases of AT_IDR(s) method is much more than that of the original IDR(s) method. Table 1 demonstrates that the proposed AT_IDR(s) method can avoid the stagnation of residual, and converge efficiently.

Table 1: Convergence of IDR(s) and AT_IDR(s) methods for six test matrices.

Matrix	Method	conv. cases	ave. itr.	ave. time[sec.]
Airfoil2D	IDR(s)	0	-	-
	AT_IDR(s)	**9**	259	**0.88**
Memplus	IDR(s)	0	-	-
	AT_IDR(s)	**10**	526	**1.31**
Sme3Dc	IDR(s)	1	4354	314.14
	AT_IDR(s)	**10**	1447	**107.88**
Trans5	IDR(s)	0	-	-
	AT_IDR(s)	**10**	275	**6.15**
UTM5940	IDR(s)	0	-	-
	AT_IDR(s)	**6**	383	**0.38**
ViscoPlastic2	IDR(s)	0	-	-
	AT_IDR(s)	**10**	1477	**7.94**

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Un algorithme pararéel modifié pour les ODEs d'ordre deux

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Résumé

L'algorithme pararéel est une méthode d'integration en parallèle introduite par Lions, Maday et Turinici ([**?**]) pour calculer la solution approximative de l'équation :

$$u'(t) = f(u(t)),\ t \in (0,T),\ u(0) = u_0, \tag{1}$$

avec $f : \mathbb{R}^M \to \mathbb{R}^M$ et $u : \mathbb{R} \to \mathbb{R}^M$. L'intervalle de temps $(0,T)$ est décomposé dans N sous-intervalles $\Omega_n = (T_n, T_{n+1})$. En utilisant un propagateur $G(t_n, t_{n-1}, x)$ qui donne une approximation grossière de la solution de l'équation (1) avec condition initiale $u(t_{n-1}) = x$ et un propagateur $F(t_n, t_{n-1}, x)$ qui donne une approximation plus fine, l'algorithme commence avec une approximation initiale U_0^n, pour $n = 0, ..., N$, obtenue par example à l'aide du propagateur grossier G

$$U_{n+1}^0 = G(t_{n+1}, t_n, U_n^0), \qquad U_0^0 = u_0,$$

et pour chaque iteration $k = 0, 1, ...$ on améliore l'approximation par :

$$U_{n+1}^{k+1} = G(t_{n+1}, t_n, U_n^{k+1}) + F(t_{n+1}, t_n, U_n^k) - G(t_{n+1}, t_n, U_n^k).$$

Dans [**?**], [**?**], [**?**] les autheurs ont montré que l'algorithme pararéel produit un speed-up pour les ODEs d'odre un mais la méthode n'a pas le même potentiel pour les ODEs d'ordre deux. On s'intéresse à résoudre en parallèle le système d'ordre deux :

$$Mq'' + Dq' + Kq = f(t),\ q(t_0) = q_0,\ q'(t_0) = q_0'. \tag{2}$$

L'inefficacité de l'algorithme classique pour (2) a comme cause un phénomène de résonance quand on calcule $G(t_{n+1}, t_n, U_n^{k+1} - U_n^k)$. En suivant une idée de Farhat et al. ([**?**]) on va modifier l'algorithme pararéel classique : on approxime l'évolution de $U_n^{k+1} - U_n^k$ de manière plus exacte en utilisant le propagateur F pour la partie de $U_n^{k+1} - U_n^k$ dont on sait son evolution et le propagateur G pour la partie restante. Une analyse mathématique pour cette méthode est donnée.

Domain Decomposition and Symmetric Eigenvalue problems

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Abstract

In this lecture, we consider several approaches for solving large symmetric eigenvalue problems when the operator is defined via a domain decomposition technique. We focus primarily on those methods that are most suitable for parallel computing platforms. We assume that the operator is defined on the union of overlapping subdomains. Further, we assume that for each subdomain it is possible to compute eigenpairs of the restriction operator. The eigenvalues sought could be at either end of the spectrum or in the interior as well. We outline the difficulties encountered when using some of the most common approaches for handling the symmetric eigenvalue problem, and describe in detail our preferred scheme for refining a set of approximate eigenpairs [1, 2, 3]. In addition, we describe an alternative scheme based on the Lanczos algorithm without reorthogonalization but with a special procedure for discarding spurious eigenvalues. We compare our solvers with the Lanczos scheme with full and partial reorthogonalization using a shift-and-invert procedure. We conclude with a summary outlining the relative advantages or flaws of these approaches.

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Non-linear minimization method comparison for data assimilation for nuclear reactors

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Abstract

Xenon-135 is a nuclear fission product which is known to be at the origin of undesired neutron density axial oscillations of about one day period in pressurized water reactors. Xenon dynamics coupled to the fission product Iodine-135 dynamics are a non linear phenomenon which represents a challenge for oscillation prediction.
In order to improve xenon estimation in nuclear plants, several models have been proposed. These models require gauging in the form of parameter estimation such as presented in [1]. We investigate the feasibility of using data assimilation methods such as variational methods for a better estimation of initial 1D concentrations of Xenon and Iodine. The goal of variational methods is to minimize difference measure between the model and the data represented by a cost function.
Cost function spaces are quite small for our studies (around one hundred degrees of freedom) which will not be the case for industrial 3D studies. We compare three different minimization methods: Gauss-Newton [2], limited BFGS method [3] and an 4DVAR incremental approach where in the inner loop one minimizes the cost function linearized in a point updated until convergence of the outer loop. Our results show that the third method converges to the global minimum in very few iterations whereas the other two methods exhibit slow convergence or stall. We investigate the reasons of the failure of the first two methods.

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Multilevel preconditioning for solving the Helmholtz equation

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Abstract

In this study, we focus on developing an efficient solver for electromagnetic and acoustic scattering problems. In order for a finite difference (or finite element) discretization to satisfy a given accuracy, it is necessary for the number of grid points to grow quadratically in the wavenumber ([1]). We will focus on solving discretized Helmholtz equation by Krylov methods with a novel efficient preconditioner for various values of the wavenumber. During the two last decades, many researchers contributed to the development of this field, which remains of great interest for a variety of applications ([2], [3], [4]). This study is designed to prove that multilevel preconditioning can be a method of choice to solve large-scale indefinite linear complex system arising from finite difference discretization of our boundary value problem ([5]). Moreover, from an approximate solution of the Helmholtz equation, it is possible to build a specific multilevel method being well adapted to our problem.

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LSTRS: MATLAB Software for Large-Scale Trust-Region Subproblems and Regularization

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Abstract

We describe a MATLAB implementation of the method LSTRS for the large-scale trust-region subproblem:

$$\min \quad \frac{1}{2}x^T Hx + g^T x \ \text{ subject to } \ \|x\|_2 \leq \Delta, \tag{1}$$

where H is an $n \times n$, real, large, symmetric matrix, g is an n-dimensional real vector, and Δ is a positive scalar. Problem (1) arises in connection with the trust-region globalization strategy in optimization. A special case of problem (1), namely, a least squares problem with a norm constraint, is equivalent to Tikhonov regularization for discrete forms of ill-posed problems.

LSTRS is based on a reformulation of the trust-region subproblem as a parameterized eigenvalue problem, and consists of an iterative procedure that finds the optimal value for the parameter. The adjustment of the parameter requires the solution of a large-scale eigenvalue problem at each step. The method relies on matrix-vector products only and has low and fixed storage requirements, features that make it suitable for large-scale computations. In the MATLAB implementation, the Hessian matrix of the quadratic objective function can be specified either explicitly, or in the form of a matrix-vector multiplication routine. Therefore, the implementation preserves the matrix-free nature of the method. The MATLAB implementation offers several choices for the eigenvalue calculation and it also allows the users to specify their own eigensolver routine.

We present a brief description of the LSTRS method and describe the main components and features of the MATLAB software. We include comparisons with state-of-the-art, large-scale techniques for problem (1). We present examples of use of the software as well as results from the regularization of large-scale discrete forms of ill-posed problems.

Numerical behavior of inexact saddle point solvers

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Abstract

For large–scale saddle point problems, the application of exact iterative schemes and 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. In this talk we study numerical behavior of several iterative Krylov subspace solvers applied to the solution of large-scale saddle point problems. 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. We concentrate on the question what is the best accuracy we can get from inexact schemes solving either Schur complement system or the null-space projected system when implemented in finite precision arithmetic. The fact that the inner solution tolerance strongly influences the accuracy of computed iterates is known and was studied in several contexts.

In particular, for several mathematically equivalent implementations we study the influence of inexact solving the inner systems and estimate their maximum attainable accuracy. When considering the outer iteration process our rounding error analysis leads to results similar to ones which can be obtained assuming exact arithmetic. The situation is different when we look at the residuals in the original saddle point system. We can show that some implementations lead ultimately to residuals on the the roundoff unit level 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 the generic and actually the cheapest implementations deliver the approximate solutions which satisfy either the second or the first block equation to the working accuracy. In addition, the schemes with a corrected direct substitution are also very attractive. We give a theoretical explanation for the behavior which was probably observed or it is already tacitly known. The implementations that we pointed out as optimal are actually those which are widely used and suggested in applications.

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Preconditioning techniques for highly indefinite systems

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Abstract

Many practical situations require the solution of highly indefinite linear systems of equations. Among these are systems which arise from the Helmholtz equation or the very irregularly structured systems that are obtained from circuit simulation for example. This talk will discuss preconditioning techniques which emphasize robustness. One such technique is based on combining two-sided permutations with a multilevel approach. The nonsymmetric permutation technique exploits a greedy strategy to put large entries of the matrix in the diagonal of the upper leading submatrix. This leads to an effective incomplete factorization preconditioner for general nonsymmetric, irregularly structured, sparse linear systems. The algorithm is implemented in a multilevel fashion and borrows from the Algebraic Recursive Multilevel Solver (ARMS) framework. Preliminary parallel implementations using a Domain Decomposition framework will also be discussed. Illustrations with the Helmholtz equations and problems arising from an application in quantum transport will be reported.

A new SR-algorithm for solving real algebraic Riccati equation

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Abstract

The aim of this paper is to present a new SR-factorization, based on a variant of SRDECO or SROSH algorithms and then, to derive a new symplectic QR-like algorithm for solving real algebraic Riccati equation.

Keywords. Skew-symmetric inner product, symplectic Householder transformations, SR factorization, structure and symplectic orthogonality preservation, Hamiltonian eigenvalue problem, numerical stability.
MSC : 65F15, 65F50

Analysis of FETI methods for multiscale PDEs

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Abstract

In this talk we consider a Poisson-type equation in two and three dimensions with a highly varying coefficient, i. e.,

$$-\nabla \cdot [\alpha \nabla u] = f \quad \text{in } \Omega\,,$$

and with some Dirichlet and/or Neumann boundary conditions on $\partial\Omega$. We are interested in solvers of the underlying finite element system which are robust with respect to the variation in $\alpha(\cdot)$ as well as to mesh refinement. A great success has been made with FETI-type domain decomposition methods: If the domain Ω can be decomposed into regular subdomains Ω_i where $\alpha(\cdot)$ is constant (or at least only slightly varying) on each of the subdomains, one can construct robust preconditioners for the iterative solution of the discretized PDE. It has been shown that the condition number of the preconditioned system behaves like

$$\mathcal{O}(\max_i (1 + \log(H_i/h_i))^2)\,,$$

where H_i denotes the subdomain diameter and h_i the subdomain mesh size. This estimate is independent of the values of α, and in particular of the jumps across subdomain interfaces.

In the present work, we generalize these standard results on FETI methods. We have two applications in mind: (i) the case of coefficient jumps not aligned with the subdomain interfaces, and (ii) highly varying coefficients within the subdomains. The latter situation appears for example when considering Newton linearizations of nonlinear magnetic field problems. We propose modifications of the standard FETI preconditioners which depend only (very mildly) on the variation of the coefficients near the interfaces. If we assume for each subdomain Ω_i, that the coefficient varies only mildly near the boundary, i. e., $\frac{\alpha(x)}{\alpha(y)} \le \alpha_i^*$ for all x, y that are less than η_i away from the boundary $\partial\Omega_i$, but varies arbitrarily otherwise, we can even give a rigorous analysis. In this case we can show that the condition number can be bounded by

$$C \max_i \left(\alpha_i^* \left(\frac{H_i}{\eta_i}\right)^2 (1 + \log(H_i/h_i))^2\right),$$

both in 2D and 3D. Provided the minimum of α in each subdomain Ω_i is attained in the boundary layer, this bound can be improved to linear dependence on H_i/η_i. This is confirmed in numerical experiments.

Stochastic Finite Elements and Fast Iterative Solvers

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Abstract

Simulation of the motion of an incompressible fluid and the transport of chemicals in porous media is a very challenging problem. In deterministic groundwater flow modelling, inputs such as material properties, boundary conditions and source terms are assumed to be known exactly. The so-called Stochastic Finite Element Method provides a framework for incorporating statistical information about spatial variability in material parameters so that more comprehensive information about the flow can be obtained. Instead of perform- ing multiple deterministic simulations, one large calculation is performed incorporating assumed statistics of the random inputs. The output can be post-processed to determine probabilistic information such as the expected concentration of a chemical in the ground- water at a nuclear waste storage site. This methodology will be reviewed in the talk with a particular focus on computational efficiency. If stochastic finite element methods are to be competitive with traditional Monte Carlo methods based on multiple realisations then we need fast and robust linear algebra techniques to solve the large indefinite systems that arise. We describe a generic block preconditioning technique for such systems with the property that the eigenvalues of the preconditioned matrices are contained in intervals that are bounded independently of the mesh size. An attractive feature is that the basis of the preconditioning is a readily available building block; namely, a scalar diffusion solve based on an algebraic multigrid V-cycle.

This is ongoing work with Oliver Ernst and Elisabeth Ullmann from Freiberg and with Catherine Powell from the University of Manchester. It is supported by the DAAD and British Council under ARC collaborative project grant 1279.

On Bi-CGSTAB and IDR(s)

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Abstract

We will discuss the relation between IDR(s) [2] and Bi-CGSTAB [3] and we will show how the IDR ideas can be incorporated in Bi-CGSTAB and visa versa. The BiCGstab(ℓ) [1] variant has some computational advantages that will be illustrated as well.

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The IDR-theorem

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Abstract

The *Induced Dimension Reduction*-theorem is the basis for the IDR(s) algorithms, a recent family of Krylov methods for solving large sparse non-symmetric linear systems. The IDR-theorem is about a *sequence of spaces* instead of a sequence of (Krylov-)vectors, in contrast with the theoretical background for other Krylov solvers.

The IDR-theorem can be formulated as follows: Let there be given a square $N \times N$ real matrix $\boldsymbol{A}$, an arbitrary nonzero vector $\boldsymbol{x}$ in $\Re^N$, and a sequence of non-zero numbers $\omega_1, \omega_2, \omega_3, \ldots$. Let $\mathcal{G}_0 = \mathcal{K}(\boldsymbol{A}, \boldsymbol{x})$, the full Krylov subspace associated with $\boldsymbol{A}$ and $\boldsymbol{x}$, and let $\mathcal{S}$ be an arbitrary proper subspace of $\mathcal{G}_0$. Then the sequence of spaces $\mathcal{G}_j$ constructed by the mapping process

$$\mathcal{G}_j = (\boldsymbol{I} - \omega_j \boldsymbol{A})(\mathcal{G}_{j-1} \cap \mathcal{S})$$

satisfies

1. $\mathcal{G}_j$ is a **proper subspace** of $\mathcal{G}_{j-1}$ for $1 \leq j \leq M$ for some $M \leq N$
2. $\mathcal{G}_j \equiv \mathcal{G}_{j-1}$ for $j > M$

The shrinking property of the space-sequence was originally proved using a dimension argument, which explains the chosen name. If $\mathcal{S}$ is chosen randomly, then $\mathcal{G}_M = \{\boldsymbol{0}\}$ with probability 1.

This theorem, which has been published in [1] is about 30 years old now. Although it is rather simple to read an understand, and also easily proved, the relation between the theorem and iterative linear solvers appears to be not at all obvious. Interested collegues put the question "How do you arrive at such an idea to found an algorithm?"

The author has had the same question about a lot of mathematical ideas of others, and seldom got answers from them, often because they lived in famous centuries, and weren't available anymore. Nevertheless, in his opinion as a teacher, these questions should be answered. Therefore in this lecture will be described the 'birth' of the theorem, the first practical use, an explanation for its early abandonment, and the reason for its recent reanimation.

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Iterative methods for anisotropic diffusion of speckled medical images

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Abstract

The goal of the proposed talk is to compute accurate and fast anisotropic diffusion of images affected by a specific noise, called speckle. This multiplicative and locally correlated noise is due to destructive interference of signals reflected from scatters within a single resolution cell. It is common in ultrasound and optical coherence tomography medical images. It reduces their contrast and the quantity of information perceived, leading to inaccurate medical decisions. Most existing techniques to reduce speckle ([**?**, **?**, **?**, **?**]) suffer one or several of these limitations: insufficient noise attenuation, insufficient edge preservation, instability or slowness of the method. In a previous work [**?**], we proposed a robust, speckle reducing anisotropic diffusion that adresses the first two limitations, i.e. insufficient noise attenuation and edge preservation. The proposed talk deals with all the mentioned previous limitations by solving the following non linear boundary values problem of diffusion (see [**?**]) in a rectangular domain $\Omega = [0, a] \times [0, b]$ with Neumann boundary conditions

$$\begin{cases} \frac{\partial u}{\partial t} - div(c.grad(u)) = 0, \text{ everywhere in } \Omega, 0 < t \leq T, \\ \frac{\partial u(x,y,t)}{\partial n}_{|\partial\Omega} = 0, \quad \forall t \in [0, T] \text{ (Boundaries Conditions)}, \\ u(x, y, 0) = u_0(x, y), \text{ (Initial Conditions)}, \end{cases}$$

where $\partial\Omega$ is the boundary of the domain Ω, $u = u(x, y, t)$ is the intensity, $T > 0$, is a strictly positive real number and in which the positive coefficient of diffusion $c = c(x, y, t, u)$ depends of the intensity u. In this original study, we propose a time marching semi-implicit discretization scheme in which the consistency and the stability of the global scheme is studied. Moreover, at each time step, it is necessary to solve a large linear algebraic systems by iterative methods such as (S.S.O.R. preconditionned) conjugate gradient method, or Schwarz alternating method which allows decreasing the ellapsed time by using parallel facilities. For both previous iterative methods, we analyse convergence (see particularly [**?**]-[**?**], [**?**] and [**?**]). Experimental sequential results concerning synthetic, ultrasound and optical coherence tomography medical images are also presented.

On the convergence of Algebraic Optimizable Schwarz Methods with applications to elliptic problems

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Abstract

The Schwarz method can be used for the iterative solution of elliptic boundary value problems on a large domain Ω. One subdivides Ω into smaller, more manageable, subdomains and solves the differential equation in these subdomains using appropriate boundary conditions. Schwarz-Robin methods use Robin conditions on the artificial interfaces forinformation exchange at each iteration. Optimized Schwarz Methods (OSM) are those in which one optimizes the Robin parameters. While the convergence theory of classical Schwarz methods (with Dirichlet conditions on the artificial interface) is well understood, the overlapping Schwarz-Robin methods still lack a complete theory. In this paper, an abstract Hilbert space version of the OSM is presented, together with an analysis of conditions for its convergence. It is also shown that if the overlap is relatively uniform, these convergence conditions are met for Schwarz-Robin methods for two-dimensional elliptic problems, for any positive Robin parameter. In the discrete setting, we obtain that the convergence rate $\omega(h)$ varies like a polylogarithm of h. Numerical experiments show that the methods work well and that the convergence rate does not appear to depend on h.

Inexact Krylov Subspace Methods for PDEs and Control Problems

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Abstract

In many circumstances, a known good preconditioner is not easily computable. Instead, an approximation to it is available. This is the case, for example, when the preconditioner has an inverse associated with it, such as in Schur complements (e.g., in saddle point problems), or in the reduced Hessian in some control problems. The application of the preconditioner implies then an iterative solution of a linear system. In these cases, the question is: how accurately to solve the (inner) iteration? In our work on Inexact Krylov methods, we have shown that the inner iterations can be solved progressively less accurately, as the underlying Krylov method (e.g., GMRES) converges to the overall solution. Computable inner stopping criteria were developed to guarantee convergence of the overall method. We will discuss these criteria, and illustrate its application to several problems. Currently, we are applying these ideas to parabolic control problems, where the reduced Hessian has two different inverses; and thus two inner iteration criteria

Algebraic Multigrid Methods for (Multilevel) Structured-plus-banded Uniformly Bounded Hermitian Positive Definite Linear Systems

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Abstract

In the past few years a lot of attention has been paid in the multigrid solution of multilevel structured (Toeplitz, circulants, Hartley, sine (τ class) and cosine algebras) linear systems whose coefficient matrix is Hermitian positive definite and banded in a multilevel sense. In the present communication we review the optimality theoretical results of available algebraic multigrid procedures. Moreover, we analyze in depth a suitable procedure modification in order to handle Hermitian positive definite structured-plus-banded uniformly bounded linear systems. In such a way, several linear systems arising is applications, as elliptic PDEs with various boundary conditions and image restoration problems, can be efficiently solved in linear time (with respect to the size of the algebraic problem). As a conclusion, a wide set of numerical tests is presented and discussed.

A generalized projected CG method with applications to Bubbly flow problems

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Abstract

For various applications, it is well-known that a two-level conjugate gradient method is an efficient method for solving large and sparse linear systems. A combination of traditional and projection-type preconditioners is used to get rid of the effect of both small and large eigenvalues of the coefficient matrix. The resulting projection methods are known in literature, coming from the fields of deflation, domain decomposition and multigrid. At first glance, these methods seem to be different. However, from an ab- stract point of view, it can be shown that some of them are closely related to each other and some of them are even equivalent. The aim of this talk is to compare these two-level PCG methods both theoretically and numerically. We investigate their equivalences, robustness, spectral and convergence properties. We end up with a suggestion of a two-level preconditioner, that is as robust as the abstract balancing preconditioner and nearly as cheap and fast as the deflation preconditioner.

Aitken acceleration of the convergence of the Schwarz method with Neumann- Dirichlet conditions on artificial boundaries to solve problem of Darcy flow with strong contrast on the permeabilities

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Abstract

The Aitken-Schwarz DDM [3] accelerates the convergence to the solution of the Schwarz DDM at the artificial interfaces using the Aitken acceleration technique. This uses the purely linear convergence property of the Schwarz due to the Dirichlet to Neumann linear mapping for elliptic problem [4]. Numerical efficiency on large 3D elliptic problems with separable operators can be found in [1]. For non separable operator, the explicit construction of the error operator at the artificial interfaces with respect to a nonuniform Fourier orthogonal basis associated to the interface discretisation is developed. We then have a framework to develop an adaptive construction of the acceleration matrix according to numerical *a posteriori* estimate of the Fourier mode behavior of the solution at artificial interface [2]. Result on the robustness of this kind of preconditionning of DDM has been validated on the Darcy problem with large contrasts in the permeability coefficients and on some test problems characterized by typical difficulties in Domain Decomposition.

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Application of the shifted-Laplace preconditioner for iterative solution of a higher order finite element discretisation of the vector wave equation

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Abstract

Radar cross section prediction techniques are used to determine the radar signature of a military platform when the radar signature can not be determined experimentally. For jet aircraft the radar cross section for forward observation angles is dominated by the contribution of the open ended cavity formed by the engine air intake. This cavity is characterized by its large depth, curved centerline and nonuniform cross section, for which the scattering characteristics can not by analyzed by asymptotic methods. Jin et al. [1] have published a numerical method based on a higher order finite element discretisation of the Maxwell equations, where the resulting linear system is solved by means of a (direct) frontal solution method . Because application of the frontal solution algorithm is prohibitively expensive for the analysis of large cavities, alternative approaches have been investigated, based on an iterative nonstationary linear solver. 'Standard' preconditioning techniques are generally not very effective for improving the convergence rate of the iterative solution of the discretised Maxwell equations at high wave numbers. Relatively recently the *shifted Laplace* preconditioner was introduced by Erlangga (see e.g. [2]) for very efficient preconditioning of iterative solution of the discretised Helmholtz equation. This technique has been extended from the scalar Helmholtz equation to the Maxwell vector wave equation. The details of this extension will be discussed and initial results obtained with this preconditioning strategy for the solution of the Maxwell vector wave equation for the analysis of cavity scattering are presented.

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Some graph optimization problems in data mining

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Abstract

Graph-theoretic ideas have become very useful in understanding modern large-scale data-mining techniques. We show in this talk that ideas from optimization are also quite useful to better understand the numerical behavior of the corresponding algorithms. We illustrate this claim by looking at two specific graph theoretic problems and their application in data-mining. The first problem is that of reputation systems where the reputation of objects and voters on the web are estimated; the second problem is that of estimating the similarity of nodes of large graphs. These two problems are also illustrated using concrete applications in data-mining.

IDR-based algorithms

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Abstract

The IDR theorem provides a new way for constructing iterative algorithms for solving nonsymmetric linear systems of equations. The talk will explain how such an IDR-based algorithm, which we called IDR(s) [3], can be constructed. It will also explain which freedom there is to develop algorithmic variants. The efficiency of IDR(s) will be demonstrated with test problems from different application areas. Comparison with established methods like GMRES [1], Bi-CGSTAB [4], and BiCGstab(ℓ) [2] shows a competitive and often superior performance for IDR(s) for important problem classes.

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Deflation acceleration of block ILU preconditioned Krylov methods.

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Abstract

We are using a Finite Element Method [Sepran] to solve various CFD problems, originating from industrial and biological applications. For many applications we are moving from two dimensional problems to three dimensional models. For this problems the memory and CPU time requirements are very high. Therefore we need fast parallel iterative methods in order to compute the solution in reasonable time.

For the parallelization of the Finite Element simulation, the grid is decomposed in a number of subgrids. Every element is only part of one subdomain. The construction of the FEM matrix is done per subdomain. Note that these subdomain-matrices are singular for subdomains, which are not connected to a Dirichlet or Robins boundary. The right-hand-side vector is also formed in this way. In order to obtain the global right-hand-side vector we sum up the local right-hand-side vectors in interface points. We use a preconditioned Krylov solver for the linear system. All the vectors used in the solver are stored as global vectors.

Preconditioned Krylov solvers consists of four building blocks: vector update, inner product, matrix vector product and preconditioner vector product. For the parallel implementation we use Fortran and MPI. The parallelization of the vector update is straightforward. For the inner product we first form the local inner products keeping into account that the interface values are used more than once. Thereafter a global inner product is formed. The matrix vector product is first done per block. Then the results on the interfaces are sent to the neighboring blocks and summed up. Finally for the preconditioner we use a block variant. We have to keep in mind that some of the subdomain-matrices are singular. The resulting method works fine but is not scalable. When the number of subdomains increases the number of iterations increases. In order to make the method scalable we add a deflation technique. Other second-level preconditioners are: additive coarse grid correction and abstract balancing. We give some theoretical and numerical comparisons of these acceleration methods.

On iterative solvers combined with projected Newton methods for reacting flow problems

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Abstract

The numerical modeling of laminar reacting gas flows in CVD (Chemical Vapor Deposition) processes commonly involves the solution of convection-diffusion-reaction equations for a large number of reactants and intermediate species. These equations are stiffly coupled through the reaction terms, which typically include dozens of finite rate elementary reaction steps with largely varying rate constants [2].

In this paper various numerical schemes for transient simulations of laminar reacting gas flows are compared in terms of efficiency, accuracy and robustness. It is concluded that, for time-accurate transient simulations of the stiff chemistry problems in CVD the conservation of the non-negativity of the species concentrations is much more important, and much more restrictive towards the time step size, than stability. For this reason we restrict ourselves in the remainder of this paper to the first order Euler Backward method.

Since the positivity of the solution is very important, the use of Newton methods to solve the non-linear problems is only feasible in combination with direct solvers. If iterative methods are used, it appears that the approximate solutions may have small negative elements. In order to prevent this, we use a projected Newton method [1]. This method is known in optimization applications, but it is not well known in the area of reacting flows. Since the number of reacting species is high (over 50 species) the resulting linear systems are large and sparse. Iterative methods are suitable candidates to solve such systems. We use preconditioned Krylov methods as solvers. In this paper various preconditioners are presented and compared. Choosing the best preconditioners combined with the projected Newton method enables us to solve problems on a $50 \times 50 \times 50$ grid with 50 chemical species.

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On the Inexactness Level of Robust Levenberg-Marquardt Methods

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Abstract

Recently, the Levenberg-Marquardt (LM) method has been used for solving systems of nonlinear equations with nonisolated solutions. Under certain conditions it converges Q-quadratically to a solution. The same rate has been obtained for inexact versions of the LM method. In this paper the LM method will be called robust if the magnitude of the regularization parameter occurring in its subproblems is as large as possible without decreasing the convergence rate. For robust LM methods the paper shows that the level of inexactness in the subproblems can be increased significantly. As an application, the local convergence of a projected robust LM method is analyzed.

Quantum Chemistry: a Challenge for Numerical Analysis

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Abstract

The basic equation of almost all quantum chemistry is the Schrödinger equation. It decribes a system of electrons and nuclei that interact by Coulomb attraction and repulsion forces. The much slower motion of the nuclei is usually separated from that of the electrons. This results in the electronic Schrödinger equation, the problem to find the eigenvalues and eigenfunctions of the electronic Schrödinger operator. Solutions of this equation depend on $3N$ variables, three spatial dimensions for each of the involved N electrons. Approximating the solutions is thus inordinately challenging, and it is conventionally believed that a reduction to simplified models, such as those of the Hartree-Fock method or density functional theory, is the only tenable approach. We will indicate why this conventional wisdom need not to be ironclad: the unexpectedly high regularity of the solutions, which increases with the number of electrons, the decay behavior of their mixed derivatives, and their antisymmetry enforced by the Pauli principle contribute properties that allow these functions to be approximated with an order of complexity which comes arbitrarily close to that for a system of one or two electrons, depending on the spin configuration. The hope is that such properties can help to develop true discretizations of the Schrödinger equation and to incorporate recent concepts from numerical analysis into the fascinating and important field of quantum chemistry.