Mathematisches Forschungsinstitut Oberwolfach

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Sparse Approximation of Non-Local Operators

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Preface

From February, 27, to March, 4, 2000, a half-size conference concerning the "Sparse Approximation of Non-Local Operators" was held at the Mathematisches Forschungsinstitut Oberwolfach. The organizers were Wolfgang Hackbusch (Leipzig), Tobias von Petersdorff (Maryland) and Stefan Sauter (Zürich).

Integral equations are a common example of nonlocal operators. The difficulty in the numerical treatment is the fact that standard discretisations lead to systems of linear equations with a fully populated matrix. Therefore, the work necessary to discretise and solve the systems no longer is proportional to the number of unknowns. This conference deals with various ways of approximating non-local operators not only resulting from integral equations, but also from the field of partial differential equations or molecular or gravitational dynamics.

For integral equations, there are the following important approaches:

- **Wavelet techniques** that make use of the local smoothness of the kernel involved and lead to a matrix compression by replacing small enough entries by zero.
- **Panel clustering techniques** that start from a given discretisation (e.g., Galerkin, collocation) of an integral equation and try to perform fast matrix-vector multiplications by the use of short expansions of the kernel in certain admissible clusters.
- **$\mathcal{H}$-matrix techniques** which generalise the ideas behind the panel clustering technique and allow approximate matrix operators (matrix-matrix multiplication and inversion).

Applications of these techniques were discussed in the field of partial differential equations (approximation of the inverse stiffness matrix) as well as for molecular dynamics or astronomical simulation, where the Coulomb potentials require a fast evaluation.

The wavelet approach is not only helpful for the fast numerical treatment, but also for the construction of discretisations. In the framework of wavelets the following question can be discussed easier than for other discretisation methods:

- **Adaptivity** and nonlinear approximation are directly connected with the existence and construction of fast methods.

Although the wavelet and panel clustering techniques are of different nature with different advantages and disadvantages, they have many details in common. This was also a topic of the evening discussions.

The quiet and stimulation atmosphere of the research institute and the excellent service provided a good basis for the conference to gain progress.

Abstracts of the Lectures

Attila Caglar, Michael Griebel (Universität Bonn)
Multilevel methods in computational chemistry

A major difficulty in Quantum-Mechanical or Molecular Dynamics simulation methods is the complexity of the long range force evaluation in each time step. To cope with this problem there exist various multiscale type methods, i.e. tree codes, multipole approximations, or multigrid techniques, which reduce the $\mathcal{O}(N^2)$ complexity of the naive approach to $\mathcal{O}(N \log N)$ or even $\mathcal{O}(N)$.

Our approach makes use of a variant of adaptive Barnes-Hut/Multipole methods. Here we obtain a (h, p)-type functionality of the method.

We discuss several expansion systems. For dealing with the adaptivity of the method, we use a hash-technique. A further reduction of execution time is possible by parallelization. Here however — especially for adaptive tree-type methods — the implementation is quite difficult and cumbersome. We present a parallel method with space-filling Hilbert curves.

We will give an overview on numerical methods for quantum and molecular dynamics simulations.

Wolfgang Dahmen (RWTH Aachen)
Adaptive approximation of operators

Given an operator equation $Lu = f$ where L is an isomorphism from some Hilbert space into its dual we are concerned with the design of adaptive schemes that exhibit in some sense (provable) asymptotically optimal complexity. The class of problems in mind covers a wide range of elliptic partial differential or singular integral equations as well as saddle point or other indefinite problems.

The first step is to transform the original problem into a discrete infinite system which is well posed in l_2 where now the system matrix is symmetric positive definite. This can be achieved e.g. by suitable wavelet least squares formulations.

In the second step a convergent iterative scheme for the inifinite dimensional problem is formulated. Starting with some finitely supported initial guess the idea is to apply now the infinite dimensional operator up to some dynamically upgraded accuracy to the current finitely supported iterate in an adaptive way.

Some properties of such application schemes are identified for which the scheme converges with asymptotically optimal complexity, i.e. for any desired accuracy an approximate solution is obtained at the expense of computational work and storage which stays asymptotically uniformly proportional to the minimal number of wavelet functions needed to recover the solution with that accuracy. The validity of the key properties is confirmed for several types of problems.

Yuli Eidelman, Israel Gohberg (Tel Aviv University)
Algorithms for a new class of structured matrices

We consider a class of structured matrices arising in numerous applications. Such matrices are generalizations of two well-known classes: Band matrices and diagonal plus semiseparable matrices. These matrices may be treated as input output operators for discrete time varying linear systems with boundary conditions. The algebra of such operators is analysed, we show that this class is invariant under inversion.

Linear complexity multiplication and inversion algorithms are presented and their implementation is discussed.

Klaus Giebermann (Universität Bonn)
A multilevel representation of boundary integral operators

We consider a multilevel representation of boundary element matrices as they arise from the discretization of boundary integral equations by Galerkin's method. Our main emphasis lies in the numerical treatment of boundary integral equations defined on complex detailed two-dimensional manifolds in three-dimensional space. Although we do not assume that the underlying discretization has any hierarchical structure our method builds such a hierarchy by introducing various box coverings of the boundary. Each of these boxes is equipped with a suitable interpolation grid.

Thanks to the smoothness of the kernel function $k(x, y)$ for $x \neq y (x, y \in \mathbb{R}^3)$ we can approximate the application of the operator to a function in finite-dimensional space by a discrete interaction between the grid points and a local operator. The interaction on the "fine grid" is then approximated by an interaction on a coarse grid plus a local correction. This scheme provides us with a significant compression of the stiffness matrix without losing the asymptotic approximation property of Galerkin's method.

Lars Grasedyck (Universität Kiel)
$\mathcal{H}$-Matrices: Implementation and application to PDE's

A new class of hierarchically structured matrices, the so-called $\mathcal{H}$-matrices, has been introduced by W. Hackbusch. These matrices are sparse in the sense that only $\mathcal{O}(n \log n)$ data are needed to store an $n \times n$ $\mathcal{H}$-Matrix and $\mathcal{O}(n \log n)$ flops are necessary to evaluate them.

They allow an approximate addition, multiplication and inversion within the set of $\mathcal{H}$-matrices which are again of almost linear complexity $\mathcal{O}(n \log^{\kappa} n)$. Basic ingredients for the implementation of the arithmetics are given in detail.

Afterwards numerical results for the inversion of some elliptic PDE's are shown. It turns out that the $\mathcal{H}$-Inverse approximates these operators up to a desired accuracy. Finally the complexity and storage of $\mathcal{H}$-Matrices in concrete implementations are compared to those of full matrices.

Wolfgang Hackbusch (MPI Leipzig)
Matrix representations of type $\mathcal{H}$ and $\mathcal{H}^2$

Standard bases discretizations lead to full matrices when applied to non-local operators. Examples are the boundary element matrices for integral equations and the inverse of a finite element matrix. In these cases the hierarchical matrix representation (H-matrices) allow to compress the data to $\mathcal{O}(nk \log n)$ (matrix size n), where k (bound for the rank) is responsible for the introduced error. Moreover, this format allows a fast matrix-vector multiplication and matrix-matrix addition, multiplication and inversion.

If we fix the subspace $\mathcal{V}(b)$ for all blocks b and satisfy a compatibility condition, we obtain the $\mathcal{H}^2$-matrix format, which leads to better cost estimates. In both cases the choice of the rank linearly increasing from the small to the large blocks saves $\log n$-factors in the cost estimate.

Boris N. Khoromskij, Wolfgang Hackbusch (MPI Leipzig)
Towards $\mathcal{H}$-matrix approximation of linear complexity

We discuss a systematic approach to optimize data sparsity of $\mathcal{H}$-matrices that are appropriate for approximation of nonlocal (integral) operators on spatial domains in R^d, $d = 2, 3$. The typical kernel function is defined by the fundamental solution of the elliptic operator $\mathcal{L}$ with constant coefficients. The first idea is to reduce the integration over the product of two admissible clusters to the integrals over the product of their boundaries due to the basic property of the Green's function. In this way, we build kernel expansions (of reduced order) supported only on the product of boundaries of geometrical clusters. With variable order expansions, this leads to the $\mathcal{H}$-matrix approximation of linear complexity, $O(N)$, for both the memory needs and the matrix-vector multiplication. In particular, our approach generalizes the familiar multipole expansions. In the case of a tensor product FE ansatz space, we discuss "very sparse" fully separable expansions approximating the matrix blocks with *sublinear* storage demands $O(n_\tau^{1/d} \log^{2d} N)$, where N is the problem size and n_τ denotes the blocksize. Finally, we consider blended FE and polynomial approximations of kernels implying the representation of matrix blocks via the tensor-product of Toeplitz and rank-k matrices.

Angela Kunoth (Universität Bonn)
Wavelet least square methods for boundary value problems

For the numerical solution of stationary operator equations, least square methods will be considered. The primary focus is the combination of the following conceptual issues: the selection of appropriate least square functionals, their numerical evaluation in the context of wavelet methods and a natural way of preconditioning the resulting systems of linear equations.

First the problem is formulated in a general setting to bring out the essential driving mechanisms. Special cases that fit into this framework are a transmission problem that

involves differential and integral operators, and saddle point problems where an elliptic partial differential equations is to be solved subject to side conditions.

One primary motivation has been the well-known fact that a major obstacle in the context of least square methods based on finite element discretizations is the evaluation of certain norms such as the H^{-1}–norm. In this regard the fact that weighted sequence norms of wavelet coefficients are equivalent to relevant function norms arising in the least squares context are exploited. Truncating the (infinite) wavelet series appropriately leads to stable Galerkin schemes.

This talk is based on:

W. Dahmen, A. Kunoth, R. Schneider,
Wavelet least square methods for boundary value problems, IGPM–Preprint #175, RWTH Aachen, September 1999.

Anita Mayo (T.J. Watson Research Center, IBM)

On particle-mesh methods for the evaluation of fields induced by vortex sheets and the solution of integral equations

Velocity fields induced by vortex sheets are often evaluated using mesh based methods known as particle mesh (PM) methods. In this talk we present new results on the accuracy of the standard PM methods. Specifically, although it has long been known that sandard particle mesh calculations are mesh and angle dependent, in this talk we provide precide results on the nature of this dependence. In particular, we introduce a technique that can be used to determine the amount by which the weights for spreading the vorticity to the mesh in a given method differ from correct weights. By correct weights we mean those which provide potential values which are correct up to truncation error. We show that this difference between the weights is often a fixed fraction of the correct weights. We also give examples where a standard particle mesh method provides the correct weights when the mesh is oriented one way, and we also show exactly what the errors in the weights and potential are if the mesh is oriented differently. In addition, we give examples where merely translating (and not rotating) the mesh changed the error in the weights. Although this changing of the errors in the weights changes the errors in the potential function, these errors in the potential need not be large. We show that even when the weights differ from ones that provide the correct potential by an amount that is $\mathcal{O}(1/h)$, the potential values obtained can still be $\mathcal{O}(h)$ accurate.

We also show why an alternative mesh method can provide more accurate, and less mesh dependent results. Essentially, this method gives a procedure for spreading the vorticity to the nearby mesh points as accurately as needed.

In addition, we study the accuracy of the interpolation formulas obtained by choosing the weights for interpolating the velocity onto the vortex sheet to be equal to the weights used for spreading the vorticity to the mesh in the standard particle mesh methods. We show that this commonly used procedure sometimes provides better results than one might expect, and that, in some cases, we obtain first order accurate approximations to the

average velocity at points on the sheet after interpolating. We also show why the method we propose can always give more accurate (second or fourth order) results.

Finally, we apply the methods discussed to the mesh based solution of certain integral equations.

Peter Oswald (Bell Laboratories, Lucent Technologies)
Multilevel matrix compression and nonlinear approximation

Several generalizations of the $\mathcal{H}$-matrix concept are discussed. We emphasize the connection to new, unsolved problems on m-term approximation. We also propose to pay more attention to algorithmical realizations beyond the area of boundary integral equations. In the introduction, a brief review of work by S. Kapur (`http://www.research.bell-labs.com/user/kapu`) and D. Long on capacitance extraction codes for chip design is given.

Sergei Pereverzev (Kiev's Mathematical Institute and University of Kaiserslautern)
Sparse approximation for regularization of ill-posed inverse problems

The aim of the talk was to describe how the idea of sparse approximation can work in case of ill-posed inverse problems. In particular an adaptive strategy for discretizing Tikhonov-Phillips regularization method with a posteriori parameter selection is proposed.

For a rather general situation we have obtained a sparse matrix structure which still leads to optimal convergence rates but requires substantially less scalar products for computing a finite dimensional approximation compared with a standard Galerkin scheme.

Andreas Rathsfeld (TU Chemnitz)
Quadrature algorithms for fast wavelet methods in BEM

Wavelet compression has been shown to be an efficient tool to design fast algorithms for the numerical solution of integral equations if the underlying domain of integration is the union of a small number of parametrization patches. Using well established compression strategies, the main problem is to develop the right adaptive quadrature rules for the assembling of the stiffness matrices and the corresponding fast implementation.

For a piecewise linear collocation scheme, we shall discuss three different quadrature algorithms corresponding to different smoothness assumptions on the kernel function of the integral operator. In particular, it turns out that, for the convergence of one of these methods, a finite degree of smoothness together with the usual Calderón-Zygmund estimates of the kernel function are sufficient. Finally, we present a numerical example.

Sergej Rjasanow, Mario Bebendorf (Universität des Saarlandes)
Adaptive cross approximation of boundary element matrices

We consider the problem of approximating a general asymptotically smooth function in two three-dimensional variables, typically arising in integral formulations of boundary value

problems, by a sum of products of two functions in each variable. From these results an iterative algorithm for the low-rank approximation of blocks of large unstructured matrices generated by asymptotically smooth functions is developed. This algorithm uses only few entries of the original block and since it has a natural stopping criterion the approximative rank is not needed in advance.

Stefan Sauter (Uni Zürich)
Variable order panel clustering

The panel clustering method is an approximate sparse representation of integral equations. It is based on the approximation of the integral kernel on "admissible" surface blocks by suitable expansions. The "variable-order" panel clustering method employs an h-p approximation of the kernel. On small blocks, the expansion order is constant while on larger blocks this order is increased.

The computational complexity of the algorithm is $O(N)$ where N denotes the number of degrees of freedom. The classical matrix-oriented representation of integral operators has complexity $O(N^2)$.

Reinhold Schneider (TU Chemnitz)
Multi-scale bases for boundary integral equations

Wavelet bases give rise to quasi-sparse representations of boundary integral operators (or e.g. pseudodifferential operators). Appropriate biorthogonal wavelet bases on surfaces, manifolds and domains can be constructed by "grid" refinement strategies. With these bases at hand one can show a convergence result and optimal complexity of the Wavelet-Galerkin-method. Numerical examples demonstrate this result in the asymptotic.

In practice, e.g. for complex geometries, the discretization from which refinement is induced requires still too many degrees of freedom. To overcome this deficiency, a coarsening strategy is developed. We build wavelet bases on the surface with e.g. vanishing multipole moments.

Ernst Stephan (Universität Hannover)
Schwarz preconditioners for the hp-version of the BEM

We consider screen problems (with a hypersingular or a weakly singular integral equation on an open surface Γ) as model problems. For the hypersingular equation the preconditioner is based on a three-level decomposition of the underlying ansatz space, the levels being piecewise bilinear functions on a coarse grid, piecewise bilinear functions on a fine grid, and piecewise polynomials of high degree on the fine grid.

We prove that the condition number of the preconditioned linear system is bounded by $\max_j (1 + \log(H_j p_j / h_j))^2$ where H_j is the diameter of an element Γ_j on the coarse grid, h_j is the size of the elements of the fine grid on Γ_j and p_j is the maximum of the polynomial degrees used in Γ_j. For the weakly singular integral equation where no continuity of test and trial functions across the element boundaries has to be enforced, the method works for

non-uniform degree distributions as well. We comment also on various adaptive algorithms. Numerical results supporting the theory are reported.

W.L. Wendland (Universität Stuttgart)
Some basic properties of integral operators as pseudodifferential operators

Boundary integral operators and non-local operators are mostly classical pseudodifferential operators defined either by the fundamental solution or a parametrix or Levi functions. The decisive properties of these operators are characterized by corresponding pseudo-homogeneous expansions of the kernels of corresponding general integral operators. These expansions are decisive for the mapping and smoothness properties of these non-local operators which one needs for appropriate discretizations.

The lecture is based on:

G.C. Hsiao, Wolfgang L. Wendland: Boundary Integral Equations (in preparation).

List of Participants

Mario Bebendorf	bebendorf@num.uni-sb.de
Steffen Börm	sbo@numerik.uni-kiel.de
Attila Caglar	caglar@iam.uni-bonn.de
Wolfgang Dahmen	dahmen@igpm.rwth-aachen.de
Yuli Eidelman	eideyu@math.tau.ac.il
Klaus Giebermann	gieberma@iam.uni-bonn.de
Ivan Graham	igg@maths.bath.ac.uk
Lars Grasedyck	lgr@numerik.uni-kiel.de
Wolfgang Hackbusch	wh@mis.mpg.de
Ralf Hiptmair	hiptmair@na.mathematik.uni-tuebingen.de
Boris Khoromskij	bokh@mis.mpg.de
Angela Kunoth	kunoth@iam.uni-bonn.de
Ulrich Langer	ulanger@numa.uni-linz.ac.at
Anita Mayo	amayo@watson.ibm.com
Peter Oswald	poswald@research.bell-labs.com
Sergei Pererzev	serg-p@mail.kar.net
Tobias von Petersdorff	tvp@math.umd.edu
Andreas Rathsfeld	andreas.rathsfeld@mathematik.tu-chemnitz.de
Sergei Rjasanov	rjasanow@num.uni-sb.de
Stefan Sauter	stas@amath.unizh.ch
Reinhold Schneider	reinhold@mathematik.tu-chemnitz.de
Christoph Schwab	christoph.schwab@sam.math.ethz.ch
Ernst Stephan	stephan@ifam.uni-hannover.de
Wolfgang L. Wendland	wendland@mathematik.uni-stuttgart.de

Tagungsteilnehmer

Mario Bebendorf
Fachbereich 9 - Mathematik
Universität des Saarlandes
Postfach 151150
66041 Saarbrücken

Dr. Steffen Börm
Institut für Informatik und
Praktische Mathematik
Universität Kiel
Hermann-Rodewald-Str. 3/1
24118 Kiel

Attila Caglar
Institut für Angewandte Mathematik
Universität Bonn
Wegelerstr. 6
53115 Bonn

Prof. Dr. Wolfgang Dahmen
Institut für Geometrie und
Praktische Mathematik
RWTH Aachen
Templergraben 55
52062 Aachen

Dr. Yuli Eidelman
Department of Mathematics
School of Mathematical Sciences
Tel Aviv University
Ramat Aviv, P.O. Box 39040
Tel Aviv 69978
ISRAEL

Dr. Klaus Giebermann
Institut für Angewandte Mathematik
Universität Bonn
Wegelerstr. 4
53115 Bonn

Dr. Ivan G. Graham
School of Mathematical Sciences
University of Bath
Claverton Down
GB-Bath Somerset BA2 7AY

Prof. Dr. Lars Grasedyck
Institut für Informatik und
Praktische Mathematik
Universität Kiel
Hermann-Rodewald-Str. 3/1
24118 Kiel

Prof. Dr. Wolfgang Hackbusch
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr. 22 - 26
04103 Leipzig

Dr. Ralf Hiptmair
Mathematisches Institut
Universität Tübingen
Auf der Morgenstelle 10
72076 Tübingen

Dr. Boris Khoromskij
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr. 22 - 26
04103 Leipzig

Dr. Angela Kunoth
Institut für Angewandte Mathematik
Universität Bonn
Wegelerstr. 6
53115 Bonn

Dr. Andreas Rathsfeld
Weierstraß-Institut für
Angewandte Analysis und Stochastik
im Forschungsverbund Berlin e.V.
Mohrenstr. 39
10117 Berlin

Prof. Dr. Ulrich Langer
Institut für Analysis und Numerik
Universität Linz
Altenbergstr. 69
A-4040 Linz

Dr. Sergej Rjasanow
Fachbereich 9 - Mathematik
Universität des Saarlandes
Postfach 151150
66041 Saarbrücken

Prof. Dr. Anita Mayo
IBM Corporation
Thomas J. Watson Research Center
P. O. Box 218
Yorktown Heights , NY 10598
USA

Prof. Dr. Stefan A. Sauter
Institut für Mathematik
Universität Zürich
Winterthurerstr. 190
CH-8057 Zürich

Prof. Dr. Peter Oswald
Lucent Technologies
Bell Laboratories
600 Mountain Avenue
Murray Hill , NJ 07974-0636
USA

Prof. Dr. Reinhold Schneider
Fakultät für Mathematik
Technische Universität
Chemnitz
09107 Chemnitz

Prof. Dr. Sergei Pereverzev
Fachbereich Mathematik
Universität Kaiserslautern
67653 Kaiserslautern

Prof. Dr. Christoph Schwab
Seminar für Angewandte Mathematik
ETH-Zentrum
Rämistr. 101
CH-8092 Zürich

Prof. Dr. Tobias von Petersdorff
Department of Mathematics
University of Maryland
College Park , MD 20742
USA

Prof. Dr. Ernst P. Stephan
Institut für Angewandte Mathematik
Universität Hannover
Postfach 6009
30060 Hannover

Prof. Dr.-Ing. Wolfgang L. Wendland
Mathematisches Institut A
Universität Stuttgart
70550 Stuttgart