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Algorithms for the Arithmetic of Dense Matrices from BEM/FEM

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The mini-workshop was organized by Wolfgang Hackbusch, Leipzig. There were 16 participants, of which 13 held one talk and one gave two talks. The main topic was the construction of algorithms and structures to reduce the complexity and storage amount for the representation and arithmetics of dense matrices that arise in BEM and FEM.

1 The abstracts in chronological order

Lars Grasedyck: Arithmetics of $\mathcal{H}$-Matrices

The (hierarchical) partitioning of an $n \times n$-matrix M can be used as a method to identify subblocks $M|_b$ of the matrix, that allow an (approximate) low rank representation. Once the hierarchical structure is fixed, one can define (approximate) arithmetics within the set of these so-called $\mathcal{H}$-matrices.

It turns out that under rather simple assumptions (sparsity and near-idempotency) the storage requirements as well as the complexity for the $\mathcal{H}$-matrix operations

- matrix times vector
- matrix plus matrix
- matrix times matrix
- inversion of a matrix

are almost linear, that is proportional to $n\log(n)^\kappa$, where $\kappa \in \{1, 2, 3\}$. The addition and multiplication can be performed as the bestapproximation of the exact result within the set of $\mathcal{H}$-matrices with respect to the frobeniusnorm.

Michael Lintner: Solution of the 2D wave equation with hierarchical matrices

The 2D wave equation is discretized with linear finite elements and the exponential Gautschi method. The resulting three-term-recursion for the discrete solution yields a restriction of the time step by the spatial mesh size like the CFL-condition in the case of explicit methods. This is due to the fact that some sine-like matrix functions within the Gautschi algorithm are no longer representable by hierarchical matrices for large enough step size, which is probably caused by the nearly equal distribution of their eigenvalues for that case.

Mirjam Köhl, Sergej Rjasanow: Simultaneous multifrequency analysis for the Helmholtz equation

In this talk a new numerical method for the multifrequency analysis for the Helmholtz equation is introduced.

We consider the 3D exterior Dirichlet boundary value problem (BVP) for the Helmholtz equation:

$$\begin{aligned} \Delta\, u(x) + \kappa^2\, u(x) &= f(x)\,, \quad x \in \Omega^c \subset \mathbb{R}^3\,, \\ u(x) &= g(x)\,, \quad x \in \Gamma = \partial\Omega \end{aligned}$$

and $u(x)$ satisfies the Sommerfeld radiation conditions.

Furthermore we assume that the wave number κ is real.

The associated boundary integral equation (BIE) is discretized by using the collocation method.
The resulting system of linear equations depends on the wave number κ.

$$A(\kappa) f(\kappa) = g(\kappa)$$

Using the one-dimensional inverse Fourier transform with respect to κ, we obtain the following results:

- The transformed collocation matrix $\check{A}(\xi)$ is real and has a sparse structure leading $O(M^2 N)$ units of required memory, where M denotes the number of frequencies and N is the number of degrees of freedom by BEM discretization.
- After discretizing the resulting convolution equation $\check{A}(\xi) * \check{f}(\xi) = \check{g}(\xi)$ leads to the linear system

  $$\mathcal{A}\phi = \varrho\,,$$

  where $\mathcal{A} \in \mathbb{R}^{NM \times NM}$ and has a block circulant structure with M sparse blocks corresponding to the well known collocation matrices $\check{A}_k$.

Boris N. Khoromskij: On FE approximation to the Poincaré-Steklov operators on complicated (fractal) geometries

We discuss iterative methods of the linear-logarithmic complexity for efficient FE approximation to the Poincaré-Steklov operators associated with 2D elliptic equations on Lipschitz domains. The situation with more complicated (fractal) geometries is of a special interest.

The method is based on the *hp*-version of FEM using special geometric mesh by refinement towards the boundary [2]. The fast iterative solution process includes the construction of efficient, spectrally close (additive Schwarz type) preconditioner. Preconditioning to the Schur-complement matrix on the boundary (mixed or Neumann boundary conditions) can be based either on the diagonal scaling or on the $\mathcal{H}$-matrix approximation on graded meshes [1]. In the case of constant coefficients, we also discuss the h-version of the refined interface method [3]. The construction of stable extension operators in the above context is also considered.

Further applications to the data-sparse approximation of elliptic resolvent and heat semigroup will be addressed.

Finally, we present numerical results.

Part of this talk presents joint work with Markus Melenk, MPI Leipzig.

References

[1] W. Hackbusch and B.N. Khoromskij. *$\mathcal{H}$-Matrix Approximation on Graded Meshes.* The Mathematics of Finite Elements and Applications X, MAFELAP 1999, J.R. Whiteman (ed), Elsevier, Amsterdam, Chapter 19, 307-316, 2000.

[2] B.N. Khoromskij and J.M. Melenk. *Generalized Boundary Element Methods.* Preprint Nr. 45, MPI MIS Leipzig, 2001.

[3] B.N. Khoromskij. *On the fast computations with the inverse to harmonic potential operators via domain decomposition*, J. Numer. Lin. Alg. with Applications, v. 3(2), 91-111 (1996).

Steffen Börm: $\mathcal{H}^2$-Matrices

The talk gives a short introduction to subspaces of the set of $\mathcal{H}$-Matrices, namely *uniform $\mathcal{H}$-Matrices* and *$\mathcal{H}^2$-Matrices.*

Uniform $\mathcal{H}$-Matrices are defined by fixing spaces $\mathcal{V}_\tau$ for all clusters τ and requiring

$$M|_b \in \mathcal{V}_b := \operatorname{span}\{ac^T \mid a \in \mathcal{V}_\tau, c \in \mathcal{V}_\sigma\}$$

for all admissible blocks $b = \tau \times \sigma$. Only $\mathcal{O}(nk)$ units of storage are required to characterize an individual matrix in this space, but still $\mathcal{O}(nk \log n)$ units are required for the bases $\mathcal{V}_\tau$.

In order to achieve linear complexity, we require the spaces $\mathcal{V}_\tau$ to be nested, i.e., $\mathcal{V}_\tau|_{\tau'} \subseteq \mathcal{V}_{\tau'}$ for all sons τ' of a cluster τ. Storing only the transfer matrices between father and sons, the complexity for storage and matrix-vector multiplication is reduced to $\mathcal{O}(nk)$.

Eugene E. Tyrtyshnikov: BEM CAN BE 1000 TIMES FASTER THAN FEM

We consider a specific 2.5 dimensional problem described by the Maxwell equations in the media with piece-wise constant isotropic conductivity and compare two different solution approaches to the corresponding 2D problems arising in the course of evaluation of the Fourier integrals. First, we apply FEM on the coupled through the mortar polar (in the source region) and Cartesian meshes (outer region) with linear and bilinear elements. The meshes fit to the boundaries. The corresponding linear algebraic systems are solved by the GMRES with a separable preconditioner allowing for the iteration in a small subspace. Second, we apply BEM using the single-layer ansatz. We found that, for the y-dipole excitation, BEM can be more than 1000 times faster than FEM. Moreover, it is much more accurate (on the test with known analytical solution).

Stefan A. Sauter: Alternative representations of classical boundary integral operators allowing cheap quadrature formulae and low order panel-clustering approximations

Alternative representation of boundary integral operators corresponding to elliptic boundary value problems are employed as a starting point for numerical approximations as, e.g., Galerkin boundary elements including numerical quadrature and panel-clustering. These representations have the advantage that the integrands of the integral operators have a reduced singular behaviour allowing to choose the order of the numerical approximations much lower as for the classical formulations.

Low order discretizations for the single layer integral equations as well as for the classical double layer potential and the hypersingular integral equation are considered. We will present fully discrete Galerkin boundary element methods where the storage amount and the CPU-time grows only linearly with respect to the number of unknowns.

Simon Chandler-Wilde: A Matrix Compression Technique for Scattering by Rough Surfaces

This is joint work with Anja Meier, Brunel. We consider a two-dimensional scattering problem in the perturbed half-plane $D = \{x = (x_1, x_2)|x_2 > f(x_1)\}$ for some $f \in C^{1,1}(\mathbb{R})$. The total field satisfies the Helmholtz equation $\Delta u + k^2 u = 0$ in D, $\partial u/\partial n = ik\beta u$ on ∂D, for some given coefficient $\beta \in L^\infty(\partial D)$, and an appropriate radiation condition on the scattered field component. The problem is a model of some problems of outdoor noise propagation over ground surfaces. We solve the problem numerically by reformulating it as a boundary integral equation, truncating the boundary, and applying a Nyström method, based on a uniform grid on ∂D, that is superalgebraically convergent if f and β are smooth. We compress the matrix by interpolating $g(u) := H_0^{(1)}(k\sqrt{(s-t)^2 + u})$, and similar terms, where $u = (f(s) - f(t))^2$, by an interpolating polynomial of degree $\leq L$. This leads to a representation of the matrix as a sum of products of diagonal and Toeplitz matrices. Exponential convergence as $L \to \infty$ can be shown, but $L > k(\sup f - \inf f)^2/|s-t|$ is needed before the convergence sets in. The cost of a matrix vector multiply is $O(L^2 N \log N) + O(L^3 N)$ and the storage requirement $O(LN)$, so that the method is effective if $k(\sup f - \inf f)$ is not too large.

Mario Bebendorf: Efficient numerical solution of pde's using low-rank matrices

In the last few years low-rank matrices have been successfully applied for the solution of linear systems arising from boundary element methods. This is done by approximating so called η-admissible blocks within the system matrix by low-rank matrices. For this purpose we present a new efficient algorithm that generates a partition of the systematrix into subblocks having this property. To find an approximant to a prescribed accuracy using only few entries from the original matrix is the second problem that will be addressed. Numerical examples show the correctness of the accuracy and complexity estimates.

The second part of the talk refers to low-rank approximation of FEM-inverses. Numerical results that compare compression rates for the Laplacian and the operator $\operatorname{div} c(x) \operatorname{grad}$ with a nonsmooth coefficient c indicate that smoothness of coefficients is not necessary for the fact that these matrices can be blockwise approximated by low-rank matrices. The current status of an attempt to give reasons for this observation is presented.

Iwan Gawriljuk: Discrete solution operators for partial differential equations

We consider the solving operators for parabolic (the operator exponential), elliptic (the normalized operator hyperbolic sine funktion) and hyperbolic (the operator cosine function) partial differential equations as operator valued functions with values in a Banach space. In order to get various discretizations of these functions we use two kinds of constructive representations of solutions of corresponding differential equations, namely representations based on the Cayley transform and on the Dunford-Cauchy integral. The last representation together with Sinc-quadratures allows to get discrete and parallel parabolic and elliptic solving operators with an exponential convergence rate. Together with the technique of H-matrices these discretizations lead to algorithms of low complexity.

For the hyperbolic solving operator we propose three various approaches which possess various stability, convergence and complexity properties.

H. Harbrecht, R. Schneider: Wavelet Based Fast Solution of BEM

Solving a boundary integral equation by the Galerkin scheme leads to a densely populated system matrix which is often ill conditioned. Thus, the computation of the solution requires at least $\mathcal{O}(N_J^2)$ operations, where N_J denotes the number of unknowns. This makes the boundary element method unattractive for the practical usage.

In the last years fast algorithms, like the Fast Multipole Method and the Panel Clustering, have been developed to reduce the complextity considerably. Another fast method is the wavelet Galerkin scheme: one employs biorthogonal wavelet bases with vanishing moments for the discretization of the given boundary integral equation. The resulting system matrix is quasi sparse and can be compressed without loss of accuracy to only $\mathcal{O}(N_J)$ nonzero entries.

In this talk we present the principles as well as new developments of the wavelet Galerkin scheme for boundary integral equations. We consider the construction of suitable wavelet bases on manifolds. Besides the known a-priori compression we introduce an a-posteriori compression. It reduces the required memory for storing the system matrix by a factor 2–4.

Within the wavelet Galerkin scheme, the numerical integration of the matrix coefficients is an important and difficult task. The coefficients which correspond to wavelets with large supports have to be calculated with a high precision. Moreover, the most integrals are singular or nearly singular. We propose a hp-quadrature scheme which scales linearly with the number of unknowns.

Based on the well known norm equivalences, wavelet bases offer a simple diagonal preconditioning of the system matrix. But numerical experiments suggest that this naive preconditioning is not satisfactory for the matrices arising from boundary integral operators. We provide an improved preconditioner which is nearly that simple to perform.

Numerical experiments are performed which corroborate the theory. The matrix compression does not compromise the accuracy of the Galerkin scheme. However, we save a factor of storage 100–1000 and accelerate the computing time up to a factor 65.

Ronald Kriemann: Parallel Algorithms for $\mathcal{H}$-matrices

Although the complexity of the arithmetics of hierarchical matrices ($\mathcal{H}$-matrices) is linear up to logarithmic factors, in practice one has to deal with large constants. Therefore parallel algorithms for the arithmetics are of special interest.

At first load-balancing algorithms are introduced which are based on data or computations. Secondly parallel algorithms are shown for the matrix-vector- and matrix-matrix-multiplication and matrix-inversion. For the matrix-matrix-multiplication numerical results are presented which show the nearly perfect scaling one expects when working on shared-memory-architectures.

Markus Melenk: Panel clustering in the modelling of ferromagnetic materials

The magnetic response of a ferromagnetic material can be assessed from minimizers of suitable energy functionals. In the so-called "no-exchange energy" model, the energy functional consists of the anisotropy energy, the energy due to an applied magnetic field, and the magnetostatic energy. Computationally, this magnetostatic contribution $B(m, m)$ of a magnetization m to the total energy is the most expensive part as it represents long-range interactions. For an efficient evaluation of $B(m, m)$ in numerical schemes, we apply the panel-clustering technique by splitting the bilinear form B into a near-field part B_{near} and a far-field part B_{far}. For standard discretizations, e.g., by piecewise constant magnetizations m, the near-field part B_{near} corresponds to a sparse matrix; we show that the entries of the near field matrix can be computed with standard techniques from boundary element methods. The far-field part B_{far} is approximated by suitable low-rank matrices, and we give error estimates for these approximations. This panel clustering technique allows for the evaluation of $B(m, m)$ with almost linear complexity.

The results presented are from joint work with W. Hackbusch.

Maike Löhndorf: A short introduction in libbem

libbem is an object oriented designed liobrary for solving problems arising in boundary element methods. The talk gives an overview of the fundamental class concept, which is closely related to the mathematical structure of the discretization process, and the capabilities of the library. That are the Galerkin- and Collocationmethod on 2D surfaces of 3D domains with piecewise linear and piecewise constant ansatz functions on flat triangles for arbitrary kernels an panel clustering for the Laplace- and the Helmholtzkernel using taylor expansion.

Future work is concentrated on $\mathcal{H}^2$ matrices and the discretization of Maxwells equations by standard elements.

Some comparisons to the concepts library (Schwab Group, Zuerich) are made, which has the same roots as libbem, but has developed in different directions.

Lars Grasedyck: Solving the Algebraic Matrix Riccati Equation by use of $\mathcal{H}$-Matrix-Arithmetics

$\mathcal{H}$-matrices offer the new opportunity to represent the inverse matrices to some discretized elliptic partial differential operators in a data sparse format. The inversion as well as most other matrix-operations can be performed in almost linear complexity. For a simple linear quadratic control problem we use the matrix-sign function in order to solve the resulting algebraic matrix Riccati equation within the set of $\mathcal{H}$-matrices. This simple approach allows to solve the control problem with complexity $O(n\log(n)^3)$ compared to the quadratic complexity of multigrid approaches or cubic complexity of the classical methods of dense matrices.

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