Iterative Solution of Dense Linear Systems

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Abstract

Integral equation methods have been used with great success in electromagnetic scattering calculations and in other problems involving unbounded computational domains. Their application is in many cases limited by the storage requirements of dense matrices and also by the rapidly increasing computational time. However, the use of iterative solvers and special methods for computing the matrix-vector products can greatly reduce both the CPU and memory requirements. In this work, the application of iterative solvers for three problems involving integral equations has been studied. For both the volume and the surface integral equation formulations of electromagnetic scattering the complex symmetric version of QMR is working efficiently. For the volume integral equation iterative solvers converge quickly even without preconditioning. We show how the eigenvalues of the coefficient matrix and the spectrum of the corresponding integral operator are related for a spherical scatterer. The matrix-vector products can be computed with a 3-dimensional FFT. For the surface integral equation of electromagnetic scattering we have applied the sparse approximate inverse preconditioner. For this problem, the fast multipole method can be employed for the calculation of the matrix-vector product. A third application is a surface integral formulation for an electrostatics problem, where the iterative solvers converge very quickly without preconditioning.

1 Introduction

Many problems in science and engineering can be cast either as partial differential equations (PDEs) or as integral equations (IEs). Each of these approaches have their benefits and limitations.

PDEs involve only local interactions and they thus give rise to systems of linear equations with sparse coefficient matrices. However, these sparse systems tend to be badly conditioned and the conditioning gets worse when the discretization is refined. The whole object has to be discretized, which can lead to large numbers of unknowns, especially for 3D problems. In computational electromagnetics the boundary conditions are in many cases given at infinity and thus also the space surrounding the object has to be discretized up to a suitable absorbing boundary condition.

IEs by contrast involve local and global interactions, thus giving rise to dense coefficient matrices. In many applications, these dense matrices are well conditioned, making them suitable for iterative solvers. IE methods in electromagnetism need no absorbing boundary conditions because the boundary conditions at infinity are automatically incorporated in the integral equation formalism. In many cases it is also possible to formulate the physical problem as a surface integral equation involving the unknown function only on the surface of the object, thereby reducing the number of unknowns.

The bottleneck for IEs is the solution of dense linear systems. The solution of dense systems with the state-of-the-art LAPACK library requires $\mathcal{O}(N^3)$ operations and $\mathcal{O}(N^2)$ units of storage, where N is the number of unknowns. In many cases the computational requirements, especially the huge memory space needed, severely limit the applicability of the IE method. In this paper we show how iterative solvers can reduce both the memory and CPU requirements.

2 Case studies

An efficient recipe for solving dense linear systems arising from integral equations is as follows:

- Choose an iterative solver
- Choose a preconditioner, if necessary
- Try to use a special method for computing the matrix-vector product without explicitly forming the whole matrix

In this work we have applied iterative solvers for dense matrices arising from three integral equation formalisms. The problems are

A: A volume integral equation for electromagnetic scattering [6]

B: A surface integral equation for electromagnetic scattering [1]

C: A surface integral equation for potential calculations in bioelectromagnetism [3]

Now we will discuss the application of iterative solvers for each of these cases.

2.1 Case A: volume integral equation for electromagnetic scattering

For inhomogeneous and anisotropic scatterers, the volume integral equation gives a flexible method for computing the electric field scattered by an arbitrary object. The whole volume of the particle must be discretized, which leads to many more discretatization points than in the surface integral formulation.

We have used piecewise constant basis functions in each cubic computational cell and a collocation approach for forming the coefficient matrix. The matrix is complex symmetric and thus non-Hermitian. We actually started with the so called discrete-dipole approximation, where each computational cube is replaced with an electric dipole [4]. Computationally this approach is very similar to the volume integral equation formalism.

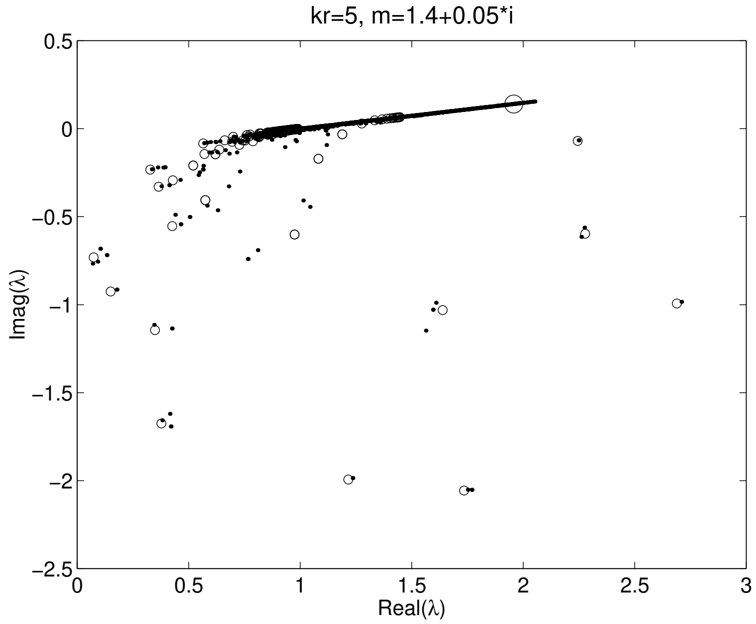

Figure 1: The eigenvalues of the coefficient matrix for case A are shown as small black dots. The points in the spectrum of the integral operator corresponding to off-line eigenvalues are shown as small circles. The properties of the integral operator predict that the line in the eigenvalue plot should extend from the point 1 to the point marked with a large circle.

We have tested various iterative methods in this setting [7] and after the test we chose the complex symmetric version of QMR [2] as the iterative method. For dielectric particles and particles with small refractive indices, the iterative methods converge quickly even without preconditioning. When the same particle is discretized with increasing resolution, the number of iterations stays practically constant.

We have also calculated the eigenvalues of the coefficient matrix and tried to relate these to the spectrum of the corresponding integral operator. Figure 1 shows the eigenvalues of the coefficient matrix and some points in the spectrum of the integral operator, when a sphere is discretized with 1064 computational elements. Most of the eigenvalues lie on a line in the complex plane. We can identify most of the eigenvalues below the line with points in the spectrum of the integral operator [5]. We can also predict the position of the line in the eigenvalue plots, but cannot yet give a water-proof physical or mathematical explanation for this.

For the volume integral equation we have used the fast Fourier transform (FFT) to compute the matrix-vector products. We assume that the computational cubes are at the gridpoints of a regular grid. We then use ghost cells to enlarge the computational grid to a cube. For a cube the matrix-vector product reduces to a convolution, which can be efficiently computed with a 3D FFT.

Using the complex symmetric version of QMR and the FFT for the matrix-vector products, we have solved the dense systems of linear equations arising from the volume integral equation with almost half a million unknowns [6].

2.2 Case B: A surface integral equation for electromagnetic scattering

The surface integral equation is the optimal formulation for electromagnetic scattering calculations in the sense that it minimizes the number of unknowns. For this case study we have used a Galerkin formulation [1] to compute the scattering by a perfectly conducting obstacle. The same formulation can be used for imperfectly conducting particles with the help of an impedance boundary condition. In the latter case, also the magnetic currents appear in the equations, but they are later eliminated in the assembly process.

The surface integral formulation leads to a dense system of linear equations with complex symmetric coefficient matrices. We have again used the complex symmetric version of QMR to solve these systems. This time, however, we need to use a preconditioner.

We have chosen to use the sparse approximate inverse preconditioner. We will determine the values of the preconditioner M by solving the problem

$$\min_{M} \|I - AM\|_F^2, \tag{1}$$

where $\|\cdot\|_F$ denotes the Frobenius norm. Note that this leads to independent least-squares problems for each column of M, *i.e.*

$$\min_{m_j} \|e_j - Am_j\|_F^2, \ j = 1, \ldots, N, \tag{2}$$

where m_j and e_j are the jth columns of M and I, respectively. For the construction of M we use two sparsity patterns. The first sparsity pattern specifies which elements in m_j will be nonzero. The second sparsity pattern determines which elements of A will be used in solving (2). The two sparsity patterns are determined either by proximity in the computational mesh or by the interaction strength in the coefficient matrix. Because M has to be symmetric, we construct the final preconditioner as $M' = (M + M^T)/2$.

In the left-hand part of Figure 2 we show the eigenvalues of the coefficient matrix for the surface integral equation in the case of a perfectly conducting sphere. The right-hand part of Figure 2 shows the eigenvalues of the preconditioned matrix AM. Figure 3 gives an example on how the convergence of QMR depends on the choice of sparsity patterns for the preconditioner.

We have used the multilevel fast multipole method for the computation of the matrix-vector products. This work is still under development, but the first results are promising. The iterative solver in conjunction with the fast multipole method becomes faster than LAPACK for less than a thousand unknowns on a Silicon Graphics workstation. The time to compute a single matrix-vector product with the fast multipole method was about 80 seconds for a matrix with 100 000 rows, and this required about 500 Megabytes of memory.

2.3 Case C: Surface integral equation from electrostatics

The third case study is a surface integral equation from electrostatics. The motivation for this study is the bioelectric inverse problem. In magnetoencephalography (MEG) one wants to determine the location of the brain activity from measurements of the weak magnetic currents caused by electric currents in the brain. To solve this inverse problem, a series of direct problems

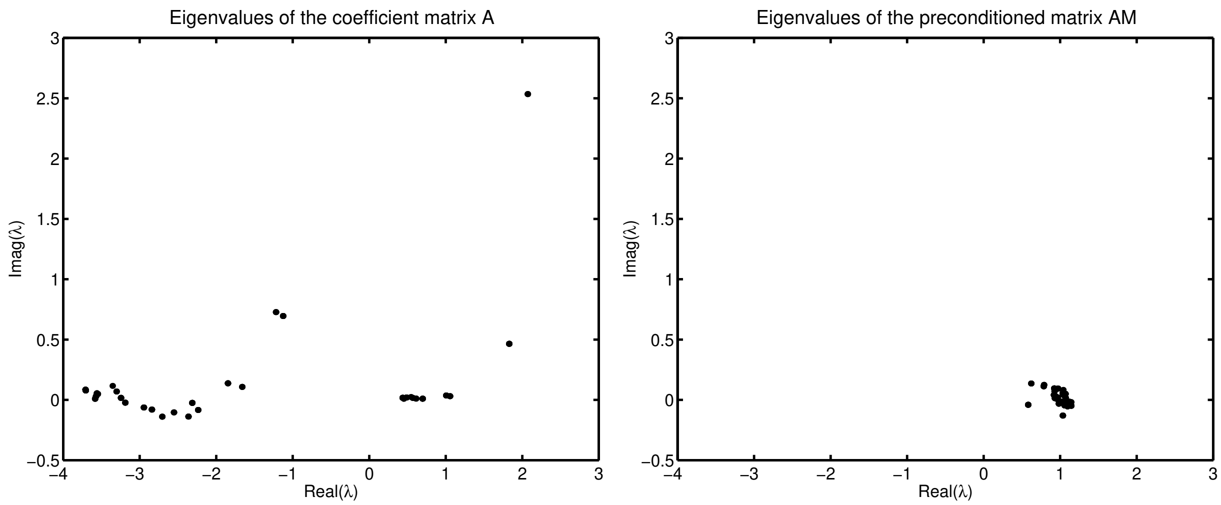

Figure 2: The left figure shows the eigenvalues of the coefficient matrix for case B. The right figure shows the eigenvalues of the preconditioned matrix.

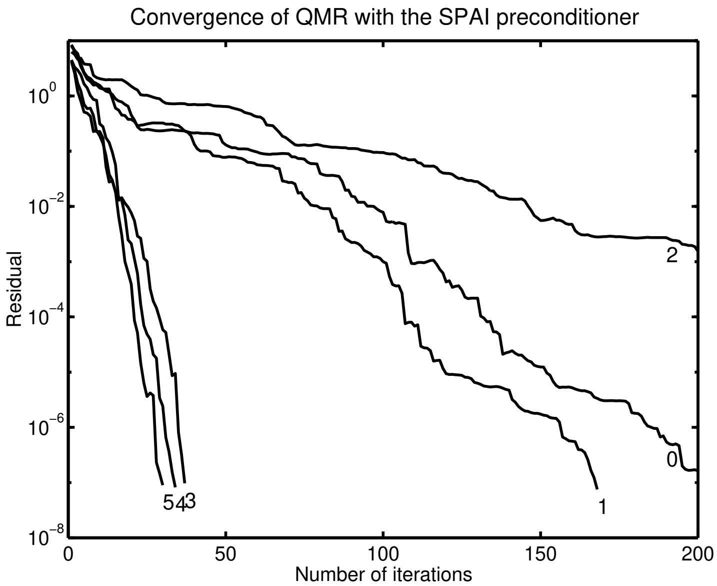

Figure 3: Convergence of QMR with the SPAI preconditioner for case B. The numbers below the curves indicate the level of preconditioner used, with 0 denoting unpreconditioned QMR and higher levels meaning larger sparsity sets.

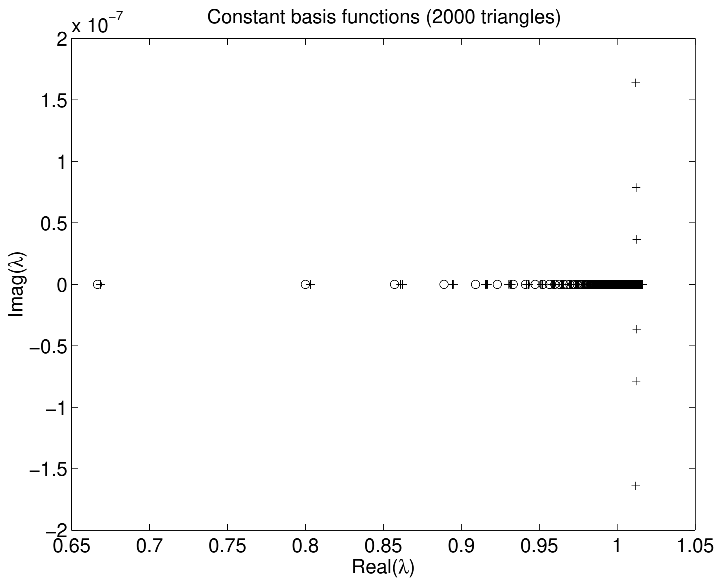

Figure 4: Eigenvalues of the scattering integral operator (circles) of case C for a sphere and the eigenvalues of the coefficient matrix (pluses), when the sphere was discretized with 2000 triangles. Piecewise constant basis functions and the collocation method were employed. Note the different scale for the imaginary parts.

have to be solved. The direct problem involves the calculation of the electric potential on the surface of the head starting from a dipolar source. The magnetic field outside the head can be recovered from the potential [3].

We are currently studying the solution of linear systems arising from three different discretization schemes: the collocation technique applied to constant and piecewise linear basis functions on triangles together with the Galerkin technique for piecewise linear basis functions. All of these coefficient matrices are slightly nonsymmetric.

For a spherical conductor model we can analytically compute the eigenvalues of the integral operator. Figure 4 shows these eigenvalue together with the eigenvalues of a coefficient matrix obtained from a discretization of the sphere with 2000 triangles.

The eigenvalue distribution suggests that iterative solvers should work very well for this linear system. We used the conjugate gradient method for solving the linear system, although the systems are slightly nonsymmetric. Indeed, the unpreconditioned conjugate gradient method reduced in initial residual by a factor of 10^{-8} in just 7 iterations independently of the number of unknowns. We tested this for three spheres discretized with 80, 720 and 2000 triangles. In the future we intend to utilize the fast multipole method for this application.

3 Conclusion

We have described three case studies where iterative solvers have been used to solve large dense systems of linear equations. For two of the problems, iterative solvers converge quickly even without preconditioning and for a given physical problem, the number of iterations is independent of the discretization. For the third problem a version of the sparse approximate inverse preconditioner was used.

For the volume integral equation of scattering we can use the fast Fourier transform for computing the matrix-vector product if the scatterer is discretized with cubic cells on a regular grid. For the surface integral equation of scattering the fast multipole method has been used and the same method will later be studied for the surface integral equation in electrostatics.

With iterative solvers and special method for computing matrix-vector products one can solve dense systems of linear equations with hundreds of thousands of unknowns. These techniques greatly reduce the need for CPU cycles and the memory consumption, because the matrices are not formed explicitly.

Acknowledgments: I would like to thank Kari Lumme for introducing me to the problem of electromagnetic scattering, Abderrahmane Bendali and M'Barek Fares for providing me with the surface integral code of electromagnetic scattering, Luc Giraud for discussions on the sparse approximate inverse preconditioners, and Satu Tissari for the collaboration in the electrostatic problem.

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