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Preconditioning First and Second Kind Integral Formulations of the Capacitance Problem *

Johannes Tausch and Jacob White

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1 Introduction

Engineering programs which compute electrostatic capacitances for complicated arrangements of conductors commonly set up the electrostatic potential u as a superposition of surface carges σ

$$u(x) = \int_S G(x,y)\sigma(y)\,dS(y)\,.$$

where $G(x,y) = 1/4\pi|x-y|$ is the Green's function for the Laplacian in the three-space. For a specified potential on the conductor surface(s) S, this approach leads to an integral equation of the first kind on S for the charge density σ. The capacitance is the net-charge on the conductors and is given by the surface integral of σ.

It is standard to discretize this integral equation with a collocation scheme. The resulting linear system is dense and can be large for complex geometries of S. In the recent past, there has been a major progress to sparsify this system with the fast multipole method. As a result the matrix vector product can be carried out in $\mathcal{O}(N)$ operations and thus the solution of the linear system with an iterative scheme like GMRES is feasible [1, 3].

However, discretizations of the first kind integral formultation lead to matrices with condition numbers which increase as the mesh is refined. This behavior makes the iterative solution of the linear system more expensive and sometimes impossible without a good preconditioner. Furthermore, the numerical analysis of the discretization error as well as the design of adaptive mesh refinement stragies are more difficult for first kind formulations. Some of these issues are still unresolved for collocation schemes.

For smooth surfaces, the difficulties associated with the first kind formulation can be entirely avoided using a second kind integral formulations for the capacitance problem, and we investigate two different types. Typically, the arising

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operators are compact on smooth surfaces and thus the Riesz-Fredholm theory provides a framework for analyzing the second kind formulation. Of particular importance is the result that the condition number of a discretized second-kind formulation is bounded independent of discretization mesh, and so requires no preconditioning.

The issues are quite different when the surfaces contain edges and corners, as is quite common in engineering problems. The integral operators in the second kind formulations are no longer compact, and the discretizations generate somewhat more ill-conditioned matrices. In addition, for problems with corners, empirical evidence suggests that first kind formulations produce significantly more accurate results for a given discretization. Since the corners introduce localized nonsmoothness, we investigate local inversion preconditioners for first and second kind formulations for the nonsmooth case.

2 Second Kind Formulations

The first formulation we consider was suggested by Mikhlin [2] and is based on writing the electrostatic potential as a superposition of a surface dipole potential and the potential due to one point charge in each conductor

$$u(x) = K\mu + \sum_j q_j G(x, x_j) = \int_S \frac{\partial}{\partial n_y} G(x, y)\mu(y)\, dS(y) + \sum_j q_j G(x, x_j)\,.$$

The point charges in this approach are necessary to ensure that the potential decays like $1/r$. It turns out that the scalars q_j are the desired capacitances, if the net-dipole density for each conductor vanishes. Taking into account the jump relations of the dipole operator, we obtain the integral equation

$$\begin{aligned} (1/2 + K + P)\mu + \sum_j q_j G(x, x_j) &= f(x)\,, \quad x \in S \\ \int_{S_j} \mu &= 0\,, \quad j = 1, \ldots, n\,. \end{aligned}$$

The operator P is defined by

$$P\mu(x) = \sum_j \int_{S_j} \mu\, dS\, \chi_j(x)\,,$$

where χ_j denotes the characteristic function of conductor j.

Once the dipole density μ has been determined, the charge denstity σ can be calculated by an application of the hypersingular integral operator

$$\sigma(x) = -\int_S \frac{\partial^2}{\partial n_x \partial n_y} G(x, y)\mu(y)\, dS(y) - \sum_j q_j \frac{\partial}{\partial n_x} G(x, x_j)\,.$$

We also investigate an alternative approach which allows the direct calculation of the charge density without resorting to the dipole density. To obtain this

formulation we remark that in the capacitance problem the potential assumes a constant value p_i within each conductor. Thus the normal derivative of the potential on the conductor surfaces when approached from the inside vanishes. Taking into account the jump relation of the adjoint operator, we obtain

$$(1/2 + K^*)\sigma(x) = 1/2\,\sigma(x) + \int_S \frac{\partial}{\partial n_x} G(x,y)\sigma(y)\,dS(y) = 0\,, \quad x \in S\,.$$

The integral equation above is singular. This is because the orthogonal complement of the range of the operator $(1/2 + K^*)$ consists of the functions which are constant on each conductor surface. Thus the equation

$$(1/2 + K^* + P)\,\sigma - \sum_j q_j \chi_j = 0$$

has a unique solution for any choice of the scalars q_j. We can choose these scalars so that the potential of σ satisfies the given conductor potentials. This leads to the integral equation

$$\begin{aligned} (1/2 + K^* + P)\sigma + \sum_j q_j \chi_j &= 0\,, \quad x \in S \\ \int_{S_j} G(x_j, y)\sigma(y)\,dS(y) &= p_j\,, \quad j = 1, \ldots, n\,, \end{aligned}$$

Note that this integral equation is adjoint to Mikhlin's formulation.

3 Preconditoning

Since the eigenvalues of a compact operator can only accumulate in the origin, discretizations of second kind integral equations will require only a relatively small number of iterations to converge. This situation changes when corners and edges are present. In this case the operators are no longer compact and the iteration may be accelerated with a preconditioner.

The fast multipole algorithm decomposes the problem domain into a hierarchy of cubes, this decomposition can also be used to construct preconditioners [4, 3].

Denoting the intersection of the surface S with cube i by S_i, the part of the operator K from S_j to S_i is given by

$$K_{ij}\sigma_j(x) := \int_{S_j} \frac{\partial}{\partial n_y} G(x,y)\sigma(y)\,dS(y) \quad x \in S_i\,.$$

The idea of the (nonoverlapping) local inversion preconditioner is to solve the integral equation for each surface S_i neglecting the interaction of the other pieces. Thus the preconditioner factors the second kind integral equation $(1/2 + K)\sigma = f$ in the form

$$\tilde{\sigma}_i + \sum_{i \neq j} (1/2 + K_{ii})^{-1} K_{ij} \tilde{\sigma}_j = f_i$$

where

$$\tilde{\sigma}_i = (1/2 + K_{ii})\sigma_i \,.$$

This approach is conceivable for isolated corners like the tip of a cone, because in this case the operators K_{ij} are compact for $i \neq j$. Moreover, if the integral operator is weakly singular in the corner, then the size of the cubes can be made small enough such that the norm of the operators K_{ii} is less than $1/2$ and thus the operator $1/2 + K_{ii}$ has a continuous inverse. Hence the transformed system is of second kind with a compact operator.

In the case of edges, the operator K_{ij} is not compact if the cubes i and j are adjacent and intersect the same edge. Still, the integral equation can be transformed into the form "identity plus compact" by an overlapping preconditioner. Denoting all neighbors of cube i by $N(i)$ and the operator on the cube i and its neighbors by $K_{N(i)}$ we can factor the integral equation in the form

$$\tilde{\sigma}_i + \sum_{j \notin N(i)} (1/2 + K_{N(i)})^{-1} K_{ij} \tilde{\sigma}_j = f_i \,.$$

4 Preliminary Numerical Results

Numerical experiments were carried out for two different domains, namely the unit sphere and an L-shaped domain. The sphere gives rise to compact integral operators, whereas the L-block has corner and edge singularities. For the sphere the discretization is almost uniform, wereas the mesh of the L-block was refined towards the edges.

All equations were discretized with piecewise constant collocation, the arising linear systems were solved with multipole accelerated GMRES, where the expansion order in all experiments was set to three. Increasing this value did not result in significant changes.

The discretization errors of the capacitance and the numbers of iterations for the sphere are dispayed in Table 4. The results there suggest that the discretization errors for all three integral formulations decay like $\mathcal{O}(h^2)$. The number of GMRES iterations varies between the formulations, they remain constant for both second kind formulations, but grow for the first kind formulation without preconditioner as the mesh is refined. The increase can be avoided by preconditioning, but only if the same cube hierarchy is used for all mesh refinements. If the cubesize is reduced to avoid expensive preconditioners, then the number iterations grows as well.

Table 4 displays the iteration results for the L-block. The capacitances suggest that the first kind formulation converges faster to the true value than the second kind formulations. As expected, the number of iterations for the first kind formulation increases when refining the mesh and the increase can be slowed down by the use of the overlapping preconditioner. The second kind formulations require a comparatively small number of iterations to converge, even for small panel sizes. Preconditioners can further accelerate the iteration.

number Panels		192		768		3072	
First Kind	no PC	0.321	(4)	0.085	(9)	0.022	(11)
	OL 1		(6)		(6)		(6)
	OL 2		(5)		(7)		(9)
Dipole	no PC	0.286	(5)	0.074	(6)	0.019	(6)
Adjoint	no PC	0.382	(5)	0.100	(4)	0.025	(5)

Table 1: Comparison of the discretization errors and iterations obtained for the sphere. The number of iterations required to reduce the residual to 10^{-6} are shown in brackets. OL 1 refers to the overlapping preconditioner with constant cube size, OL 2 refers to the overlapping preconditioner with decreasing cube size

number Panels		350		1400		5600	
First Kind	no PC	12.626	(17)	12.658	(27)	12.663	(40)
	OL		(12)		(7)		(8)
	OL*		(12)		(18)		(24)
Dipole	no PC	12.467	(13)	12.602	(14)	12.648	(15)
	OL 1		(9)		(9)		(10)
	OL 2		(7)		(8)		(10)
Adjoint	no PC	12.310	(10)	12.485	(12)	12.582	(14)
	OL 1		(7)		(8)		(8)
	OL 2		(8)		(9)		(11)

Table 2: Comparison of the calculated capacitances and iterations obtained for the L-shaped domain. The number of iterations required to reduce the residual to 10^{-6} are shown in brackets.

5 Conclusion

For problems with smooth surfaces discretizations of the second kind formulations result in better conditioned linear systems than the first kind formulation by maintaining the accuracy of the approximation. In addition, the adjoint formulation directly produces surface densities which are more useful in subsequent application than the dipole layer.

The conditioning of all formulations worsens in the case of non-smooth domains, although the ill-conditioning appears to be milder for the second kind formulations. Local inversion preconditioners are effective at removing this ill-conditioning, though the spatial extent required for the preconditioner is still under investigation. Finally, the convergence of discretization error is slower for the second kind formulation, and this may be an artifact of the piecewise constant collocation used for the experiments. We will investigate higher order approximation schemes in our future research.

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