A Nyström-like Approach to Integral Equations with Singular Kernels

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ABSTRACT

Traditional boundary element methods use panel-based discretization and exhibit low order convergence. In this paper, a new approach is proposed to discretize a singular integral equation. Global, numerically orthogonal bases are used to represent a solution, and mapping functions are used to represent the geometry. This method is capable of achieving spectral convergence, similar to the Nyström method for integral equations with non-singular kernels. In test case of a sphere, six digits of accuracy is achieved with 500 unknowns, which is about three orders of magnitude fewer than required by a panel method.

Keywords: Nyström method, singular integral, spectral convergence, boundary element method

1 INTRODUCTION

When boundary element methods [10, 11] are used to solve Laplace or Helmholtz problems associated with complicated three-dimensional geometries, the associated integral equation is typically discretized using a piecewise constant basis, and a system of equations is generated using either a Galerkin or a collocation scheme. The resulting matrix is then solved iteratively using acceleration [5,8,9,13,17,20, 22]. This approach has become the method of choice for exterior problems and enjoys success in applications such as interconnect extraction [26], MEMS and fluidic simulation [21, 25], as well as in calculating bimolecular solvation energy [3, 14]. However, piecewise-constant bases are low order, and therefore large numbers of unknowns are needed to achieve high accuracy. While acceleration techniques make it possible to solve such problems, memory is often a bottleneck. Therefore, there is much interest in developing higher order methods [6, 12, 15] that can achieve faster convergence and reduce problem size. In [7, 15], the use of a higher order basis based on B-splines resulted in faster *algebraic* convergence, while in [6, 12], the aim was to attain *spectral* convergence. In this paper, we propose a new kind of higher order basis and demonstrate spectral convergence (error decays exponentially with number of unknowns). Our method differs from [6, 12] in that we use an explicit high order basis in our approach.

It is well know that the Nyström method can attain spectral convergence for second kind integral equations with non-singular kernels by using collocation points as quadrature points [1]. However, the method breaks down for three-dimensional Laplace and Helmholtz problems, since the kernels are singular. Our approach can be applied to singular integrals and is able to achieve spectral convergence like the Nyström method. On the other hand, our method can have a different interpretation as an interpolation approach, similar to [6]. This interpretation allows an efficient implementation of matrix-vector multiplication that can be used in an iterative solution of the resultant matrix equation. With this implementation, the speed of our approach without acceleration may still be competitive with low-order accelerated methods for the same accuracy, with orders of magnitude lower memory use.

In the following section, we review the basics of boundary element method. In Section 3, we describe our proposed method. Numerical results are presented in Section 4 and finally in Section 5, we conclude with two interpretations of our approach.

2 BOUNDARY ELEMENT METHOD

The following integral equation will be used as our model problem:

$$\phi(\vec{r}) = \int_{\Omega} G(\vec{r}, \vec{r}')\sigma(\vec{r}')\, dS' \tag{1}$$

where $G(\vec{r}, \vec{r}')$ is Green's function $\left(\text{e.g. } \frac{1}{|\vec{r}-\vec{r}'|}, \frac{e^{k|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|}\right)$ and Ω is the surface boundary of a three-dimensional region of interest on which we would like to solve for the unknown quantity σ given an arbitrary ϕ.

2.1 Discretization

In order to numerically solve for σ, two representations are typically used: one for the surface geometry, and the other for the solution itself. A triangular mesh is commonly used to discretize the geometry, and a basis set, $\{B_i : i = 1, 2, \ldots, n\}$, is usually defined on the same mesh, with B_i's being non-zero only on a few triangles. The basis is used to discretize the unknown as in

$$\sigma(\vec{r}) = \sum_{i=1}^{n} a_i B_i(\vec{r}) \qquad \vec{r} \in \Omega^{mesh} \tag{2}$$

where Ω^{mesh} may be an exact or approximate geometry of the original domain Ω. In several widely used programs, the surface is approximated with flat panels, and the unknowns are assumed to be constant or vary linearly on these panels. Many engineering problems, however, have curvilinear boundaries, and discretization with flat panels introduces significant approximation in the geometry. While the mesh converges to the actual surface in the same manner as piecewise constant basis, in practice a large number of panels are

needed to achieve good accuracy. And the use of higher order basis alone will not improve convergence without adopting simultaneously a better representation of the curved surface. Higher order panels using B-splines [15] or Taylor series expansion of local surface curvature [23] have been used. While analytical expressions [11,18] of singular integrals are used in both cases, such formulae are not always possible for curved surfaces that cannot be described by polynomials. We take an alternative approach to represent the geometry exactly and numerically evaluate the integrals. This procedure can be generalized to any curvilinear surface if a mapping function can be found, as will be discussed in Section 3. The relative merit of precise or approximate surface representation depends mainly on the complexity of geometry since errors are introduced in both situations: quadrature is used to approximate integrals in the former case while polynomials are used to approximate the actual surface in the latter case.

2.2 Galerkin and Collocation Formulation

In order to solve for the set of coefficients a_i's in equation (2), a Galerkin or collocation scheme is commonly used. Galerkin methods enforce orthogonality between the residual and a chosen basis while the collocation scheme minimizes the residual at a set of points. In either case, unknown coefficients can be solved from a $n \times n$ matrix equation:

$$\sum_{i=1}^{n} a_i \underbrace{\int B_j(\vec{r}) \int G(\vec{r},\vec{r}')B_i(\vec{r}')\, dS' dS}_{A_{ji}^{Galerkin}} = \int B_j(\vec{r})\phi(\vec{r})\, dS \tag{3}$$

or

$$\sum_{i=1}^{n} a_i \underbrace{\int G(\vec{r}_j,\vec{r}')B_i(\vec{r}')\, dS'}_{A_{ji}^{Collocation}} = \phi(\vec{r}_j) \tag{4}$$

where $\vec{r}_j$'s are locations of collocation points. Each entry in the Galerkin matrix involves two integrations over the support of a basis: one for the source basis, and the other for the target basis. In contrast to the Galerkin approach, each entry in the collocation matrix involves only one integration over the support of a source basis. The outer integral of the Galerkin formulation is typically done with quadrature, therefore it is computationally more expensive. Although convergence theory is better developed for the Galerkin approach [2], in practice collocation is often used for its simplicity and efficiency.

3 SPECTRAL METHOD

An alternative basis for discretization is the set of numerically orthogonal polynomials defined on quadrature points. In contrast to a panel-based representation whereby orthogonality is only partially maintained by spatial separation of bases' supports, this approach ensures good orthogonality for arbitrarily high order bases, though their supports have significant overlap. The improvement in accuracy is significant: the method exhibits a spectral convergence rate. In this section, we will describe the basis, the techniques for integration over curved surfaces, and other features associated with this approach.

3.1 Numerically Orthogonal Basis

Consider a global surface Ω of coordinates (x, y, z) that can be partitioned into a few regions and each of which can be associated with a one-to-one mapping function:

$$P : \vec{r}_{flat}(u, v) \rightarrow \vec{r}_{curve}(x, y, z) \tag{5}$$

defined on a local patch of coordinates (u, v). In a complicated geometry where exact mapping is not possible, a high order approximation, consistent with the basis order, has to be used since convergence is limited by the lower accuracy of the two. A second requirement is the availability of good quadrature points associated with each patch. For example, in a rectangular patch a tensor product of one-dimensional Gauss-Lobatto quadrature points is used, and basis set can be similarly defined as polynomials that take on unit value at one of the grid points but zero at all other grid points. In one dimension, these are the Lagrangian interpolating polynomials [4] such that

$$\ell_i(u_k) = \delta_{ik} \qquad i, k = 1, \ldots, m \tag{6}$$

where u_k is coordinate of kth quadrature point. The bases on a rectangular patch can therefore be written as a product of two one-dimensional polynomials as in

$$B_{ij}(u, v) = \ell_i(u)\ell_j(v). \tag{7}$$

Therefore, if m quadrature points are used along each dimension, there will be m^2 basis functions. A good set of quadrature points ensures orthogonality as the inner product over a patch approximated by the same quadrature points is always zero by design. For the bases associated with a boundary node, the support will span across nearby patches so that computed solutions will be continuous along patch boundaries. The use of such a numerically orthogonal basis was proposed in the spectral element method [19] and is well known in the finite element community. However, to authors' knowledge, it has not yet been applied to the boundary element method, perhaps hindered by the difficulty of panel integration, the subject of the next section.

3.2 Integration over Curved Surfaces

Once the mapping function (5) and basis functions (7) have been defined on a patch, the integration over the actual surface can be performed using parametric coordinates (u, v). For an evaluation point at $\vec{r}(x, y, z)$:

$$\int_{(x,y,z)} G(\vec{r},\vec{r}')B(\vec{r}')\, dS' = \int_{(u,v)} G(\vec{r}, P(\vec{r}'))B(\vec{r}')|J(\vec{r}')|\, dS' \tag{8}$$

where $|J|$ is the Jacobian of the mapping function in (5). Note that the basis function, originally defined on the local patch, is also being used to represent the solution in the global surface through the mapping function:

$$B(\vec{r}'(x, y, z)) = B(P(\vec{r}'(u, v))) = B(\vec{r}'(u, v)). \tag{9}$$

An analytical expression for (8) is not generally available as the Jacobian can be very complicated, and straightforward quadrature in (u, v) coordinates is not sufficiently accurate

for evaluation points on or close to the source patch. It is shown in [6] that, however, the integral can be de-singularized in appropriately chosen polar coordinates. The key is to locate the origin of polar coordinates such that the radial coordinate ρ goes to zero at the singular point. The resultant integrand is smooth and Gauss quadrature points in (ρ, θ) coordinates can be used to evaluate the integral in equation (4):

$$A_{ji,patch}^{Colloc.} = \iint_{patch} G(\vec{r}_j, P(\vec{r}'(\rho,\theta)))B_i(\rho,\theta)|J(\rho,\theta)|\,\rho\,d\rho\,d\theta \tag{10}$$

where i and j, unlike in equation (7), are global indices of all nodes defined on all patches and $\vec{r}_j$'s are coordinates of collocation points defined by mapping all grid points onto global surface. The inner integral in (10) is evaluated by one-dimensional Gauss quadrature in ρ-coordinate, which in term is used to evaluate the outer integral, again by using one-dimensional Gauss quadrature in θ-coordinate. If a basis' support spans across a few patches, then its contribution to a matrix entry has to be summed up patch-wise, because separate polar coordinates have to be used on each patch.

3.3 Equivalence between Galerkin and Collocation Formulation

In the Galerkin formulation in (3), the outer integral with the target basis is smooth and is typically approximated by quadrature. Since the supports of basis functions in (7) have been defined on patches associated with quadrature points, one can use the same points to approximate the outer integral. Since each basis is chosen to be non-zero at only one quadrature point, each row of the Galerkin matrix in (3) reduces to the corresponding row of the collocation matrix in (10) scaled by some constant. The right hand side in (3) is also equal to the corresponding right hand side in (4) scaled by the same constant. As a result, the Galerkin formulation for the particular choice of basis in (7) is equivalent to the collocation formulation. One can simultaneously take advantage of Galerkin scheme's convergence property and collocation scheme's computational efficiency.

4 COMPUTATIONAL RESULTS ON SPHERE

A unit sphere in an infinite fluid potential flow problem, which has an analytical solution [16, 20] is used to validate the proposed approach. In order to describe the spherical geometry, local patches on six faces of a cube centered at the origin is used, and a mapping function is defined by radially projecting any point on the cube to sphere. A $m \times m$ Gauss-Lobatto grid is set up on each patch, a set of m^2 basis is defined on the grid and $2m \times 2m$ quadrature points in polar coordinates are used to evaluate the integral. Both direct and iterative solvers are used to obtain a numerical solution. As opposed to an direct solver whereby integration over patches is done for individual basis functions in (10), at each iteration step, a weighted sum of all bases is integrated instead. This is equivalent to first interpolating on each patch via a set of Gauss-Lobatto points, then integrating the interpolated function over the corresponding global surface.

order	4	5	6	7	8	9	10
# unknowns	56	98	152	218	296	386	488
condition #	57	92	136	189	254	327	408
# iterations	6	8	8	7	7	5	4

Table 1: Matrix condition of direct and iterative solver.

Accuracy is assessed in terms of integrated error, which is the sum of errors at collocation points, normalized by area. Figure 1 shows the spectral convergence results and a comparison to the standard panel method. The improvement over

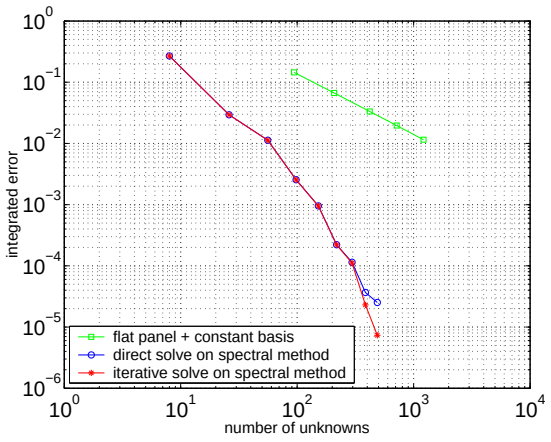

Figure 1: Accuracy comparison between the standard and spectral method.

the traditional approach is clear: not only is the accuracy better for the same degrees of freedom, or fewer unknowns needed for the same accuracy, but the method's advantage grows with increasing problem size or more stringent error tolerance. For the sphere problem, the spectral method is able to achieve six digits of accuracy with about 500 unknowns, which in our MATLAB® implementation, takes less than ten minutes in a 3GHz Intel® Xeon machine. By extrapolating the straight line in Figure 1, one can estimate that at least a million panels are needed for the standard method to achieve the same accuracy.

Table 1 shows matrix condition number and the number of iterations required to converge to 10^{-6} tolerance using GMRES [24], without any pre-conditioner. Note that the condition number and number of iterations are growing slowly with problem size.

5 CONCLUSIONS AND ACKNOWLEDGEMENT

As the title of the paper suggests, our approach is similar to the Nyström method in that it is also capable of achieving spectral convergence. For an integral equation with non-singular kernels, the Nyström approach uses quadrature points as collocation points and reduces to a set of algebraic equations. For singular kernels, however, our approach shows that the same spectral convergence can be obtained if explicit Lagrangian basis functions defined on quadrature points can be integrated sufficiently accurate. And the basis functions we use are the same as those in the spectral element method [19].

Alternatively, our approach can be seen as a more global interpolation of the underlying function, and carrying out the integration on patches. This is in contrast to the standard approach where accuracy and convergence is limited by panel-wise or local approximation. We also demonstrated that good accuracy and a well-conditioned matrix equation can be achieved by using a set of good interpolation points defined on patches. In this view, our method is similar to [6] although in that approach, uniform grids are used and a set of partition-of-unity weighting functions are introduced to make the underlying representation periodic.

The authors acknowledge the support of the MIT-SMA BioMEMS program, the NIH ICBP project, and the National Science Foundation.

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