Available online at www.sciencedirect.com
ScienceDirect
Journal of Computational Physics 219 (2006) 247–275
JOURNAL OF COMPUTATIONAL PHYSICS
www.elsevier.com/locate/jcp

# A high-order 3D boundary integral equation solver for elliptic PDEs in smooth domains

Lexing Ying [a,*], George Biros [b,c], Denis Zorin [d]

[a] Applied and Computational Mathematics, California Institute of Technology, CA 91125, United States
[b] Department of Mechanical Engineering, University of Pennsylvania, PA 19104, United States
[c] Department of Computer and Information Science, University of Pennsylvania, PA 19104, United States
[d] Courant Institute of Mathematical Sciences, New York University, NY 10012, United States

Received 29 September 2005; received in revised form 6 March 2006; accepted 20 March 2006
Available online 11 May 2006

**Abstract**

We present a high-order boundary integral equation solver for 3D elliptic boundary value problems on domains with smooth boundaries. We use Nyström's method for discretization, and combine it with special quadrature rules for the singular kernels that appear in the boundary integrals. The overall asymptotic complexity of our method is $O(N^{3/2})$, where $N$ is the number of discretization points on the boundary of the domain, and corresponds to linear complexity in the number of uniformly sampled evaluation points. A kernel-independent fast summation algorithm is used to accelerate the evaluation of the discretized integral operators. We describe a high-order accurate method for evaluating the solution at arbitrary points inside the domain, including points close to the domain boundary. We demonstrate how our solver, combined with a regular-grid spectral solver, can be applied to problems with distributed sources. We present numerical results for the Stokes, Navier, and Poisson problems.


*Keywords:* Boundary integral equations; Nyström discretization; Singular integrals; Nearly singular integrals; Fast solvers; Laplace equation; Stokes equation; Navier equation; Fast multipole method; Fast Fourier transform

## 1. Introduction

Potential theory has played a paramount role in both analysis and computation for boundary value problems for elliptic partial differential equations. Numerous applications can be found in fracture mechanics, fluid mechanics, elastodynamics, electromagnetics, and acoustics. Results from potential theory allow us to represent boundary value problems in integral equation form. For problems with known Green's functions, an integral equation formulation leads to powerful numerical approximation schemes. The advantages of such schemes are well known: (1) there is no need for volume mesh generation; (2) in many cases they result in operators with bounded condition number; (3) for exterior problems, they satisfy far-field boundary conditions

* Corresponding author. Tel.: +1 626 395 5760.
*E-mail addresses:* lexing@acm.caltech.edu (L. Ying), biros@seas.upenn.edu (G. Biros), dzorin@cs.nyu.edu (D. Zorin).

0021-9991/$ - see front matter 
doi:10.1016/j.jcp.2006.03.021

exactly; and (4) they typically exhibit high convergence rates when the domain boundary and boundary condition are sufficiently smooth.

Despite their advantages, numerical approximations to integral equations are plagued by several mathematical and implementational difficulties, especially if the goal is to obtain an algorithm that is asymptotically optimal, accurate, and fast enough to be useful in practical settings. Indeed, in order to get such an algorithm, for domains with smooth boundaries,[1] one has to address five main problems:

- *Fast summation.* The discretized operators are dense and the corresponding linear systems are prohibitively expensive to solve. Direct solvers are not applicable; iterative methods like GMRES can help, but still result in suboptimal complexity.
- *Fast and accurate quadratures.* One needs to use suitable quadrature rules to discretize the integral operators; the kernels are often singular or hypersingular, and the choice of the quadrature rule is important to obtain high-order convergence. This is a difficult problem that is made worst by the need to guarantee optimal complexity.
- *Domain boundary representation.* High-accuracy rules often require smooth approximations to the domain boundary. In two dimensions this is a relatively easy problem, but it is more complicated in the case of three dimensions.
- *Solution evaluation.* The solution is typically evaluated on a dense grid of points inside the domain. Such grids can include points arbitrarily close to the boundary, in which case nearly-singular integrals need to be evaluated. Again, the goal is to guarantee high accuracy at optimal complexity.
- *Volume potentials.* For problems with possibly highly non-uniform distributed forces, one has to devise efficient schemes for the computation of volume integrals, especially in the case where the support of the function coincides with a volumed domain that has a complex boundary.

In this paper, we present a method that addresses each in turn, save the last.

For two-dimensional boundary value problems in smooth domains, a number of highly efficient boundary integral solvers has been developed [5,21,23,33]. Most implementations are based on indirect formulations that result in integral equations with double layer potentials. In 2D, these kernels are often non-singular and the domain boundary can be easily parameterized; the boundary integrals can then be evaluated using standard quadrature rules, and superalgebraic convergence rates can be obtained. Such discretization combined with fast summation methods result in optimal algorithms. In three dimensions, however, the situation is radically different (we review the related work in the following section).

We present a 3D boundary integral solver for elliptic PDEs, for domains with smooth ($C^\infty$ or $C^k$-continuous for sufficiently large $k$, but not necessarily analytic) boundaries, which achieves high-order convergence with linear complexity with respect to the number of evaluation points. The distinctive features of our solver are: (1) fast kernel-independent summation; (2) arbitrary smooth boundaries and high-order convergence; (3) distributed forces that are uniformly defined in a box that encloses the target domain; and (4) high-accurate direct evaluation of the solution in a non-uniform distribution of points.

The operators are sparsified by our kernel-independent fast multipole method (FMM) [49], which makes it possible to accelerate the solution of the dense linear system for many elliptic PDEs of which the kernels have explicit expressions. We use Nyström's method to discretize the boundary integral equations. There are two reasons to prefer Nyström's method to Galerkin or collocation approaches: simpler implementation for superalgebraic convergence and, based on existing literature, lower constants [12].

Although the kernels of various PDEs are different, the behavior of their singularities are similar. We address the second problem (quadrature construction) by extending the local quadrature methods of [11] to integrate the singularities of various types. A key component of the solver is the ability to have high-order representations for arbitrary geometries with (relatively) minimal algorithmic and implementational complexity. Such a representation is described in detail in [51]. To compute the near-singular integrals for points close to the boundary, we adopt a high-order scheme to interpolate the solution from the values at points suffi-

[1] Domains with edges and corners present additional challenges that we do not discuss in this particle.