Fast Algorithms for 3-D Simulation

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ABSTRACT

One difficulty associated with computer simulation of micromachined devices is that the devices are typically geometrically complicated and innately three-dimensional. For this reason, attempts to exploit existing finite-element based tools for micromachined device simulation has proved difficult. Instead, micromachine device designers have been early adopters of the recently developed accelerated boundary-element methods. In this short paper the author will describe a little of the history of these methods, primarily to point the interested reader to the relevant literature.

Keywords: Integral Equations, Fast Solvers

1 Introduction

Simulating a micromachined device, like the electromechanical resonator in Figure (1), is extremely computationally challenging. One issue that makes simulation difficult is that the resonator's behavior is governed by the coupling between electrostatic, elastic and fluidic forces. The second issue is the computational expensive of calculating the domain-specific forces in such a geometrically complicated example. Forces that require resolution of the geometry's exterior, such as electrostatic or fluidic forces, are particularly expensive to compute.

When the equations that describe the exterior problem are linear and space invariant, as is typically the case for electrostatic and magnetic forces and can be the case for fluidic forces, an integral formulation of the problem will exist. Such formulations use Greens functions to eliminate the problem's exterior and typically involve only quantities of the problem surface. Such a formulation seems ideal when computing traction forces or electrostatic pressures on surfaces, but the integral formulation generates a particular numerical difficulty. Discretized integral equations generate dense matrices which are expensive to form and solve.

For example, consider the first-kind electrostatics problem,

$$\psi(x) = \int_{surfaces} \sigma(x') \frac{1}{4\pi\epsilon\|x - x'\|} da', \tag{1}$$

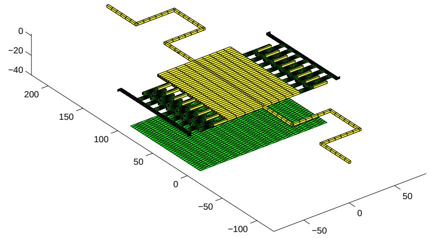

Figure 1: A Comb Resonator Example

where x is a point on the surface, $\psi(x)$ is the known conductor surface potential. The simplest discretization of (1) is to divide the surfaces into n flat panels over which the charge density is assumed constant. If the collocation points, the x_i's, are selected at the centroids of each panel, then the discretized system is

$$Pq = \Psi \tag{2}$$

where q is the n-length vector of panel charges, Ψ is the n-length vector of known centroid potentials, and $P_{i,j} = \int_{panel_j} \frac{1}{4\pi\epsilon\|x_i - x'\|} da'$.

2 The Fast Solver Approach

If direct factorization is used to solve (2), then the memory required to store the matrix will grow like n^2 and the matrix solve time will increase like n^3. If instead, a preconditioned Krylov-subspace method like GMRES [1] is used to solve (2), then it is possible to reduce the solve time to order n^2 but the memory requirement will not decrease.

In order to develop algorithms that use memory and time that grows more slowly with problem size, it is essential *not* to form the matrix explicitly. Instead, one can exploit the fact that Krylov-subspace methods for solving systems of equations only require matrix-vector products and not an explicit representation of the matrix. For example, note that for P in (2), computing Pq is equivalent to computing n potentials due to n sources and this can be accomplished in nearly order n operations [2], [4], [3]. Several researcher simultaneously observed the powerful combination of BEM, Krylov-subspace methods, and fast matrix-vector products [5]–[7]. Such methods are now referred to as accelerated BEM or, more pejoratively, as fast solvers.

Perhaps the first practical use of accelerated BEM was based on combining fast multipole algorithms for charged particle computations with low-order BEM to compute 3-D capacitance and electrostatic forces [8], [9]. Currently, almost all the programs for electrostatic force computation for microsensors use accelerated boundary-element methods. Extensions have appeared, such as computing inductance [13] or fluid drag [14], as well as algorithm improvements such as better adaptivity, higher-order elements and improved efficiency for high accuracy [11], [10].

3 General Green's functions

Most of the mature accelerated BEM codes are for $\frac{1}{r}$ kernels and use multipole expansions, because they were derived from the idea that computing Pq is equivalent to computing potentials from charges. Instead, it is possible to develop techniques which are Greens function independent, and there have been a variety of such approaches. There is the panel clustering idea [6], a multigrid style method [15], a technique based on the singular-value decomposition [17], and approaches based on using wavelet-like methods [16], [18], [19].

For problems with oscillatory kernels, such as acoustic or electromagnetic scattering, the above approaches fail because they all exploit multiresolution. That is, they all count on using less information to represent distant interactions. For the oscillatory kernel case, one can not count on multiresolution. The difficulty is, roughly, that phase information must be maintained no matter how distant the interactions. For very high frequency applications, there are specialized multipole algorithms [20]–[22], but these techniques collapse numerically at low frequencies. The only techniques that work for general kernels are based on projecting to a uniform grid and using the FFT [4], [23], [24]. FFT-based techniques, unfortunately, have efficiency problems for inhomogenous geometries.

4 Conclusions

In this brief paper the author described some of the history of fast methods for solving integral equations. The author would like to thank the many students who have developed codes using fast solvers including Keith Nabors, Joel Phillips, Matt Kamon, Michael Chou, Narayan Aluru, Wenjing Ye, Joe Kanapka and Xin Wang. This work was supported by the DARPA composite CAD program, the DARPA muri program, and grants from the Semiconductor Research Corporation.

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