Boundary-Integral Methods in Molecular Science and Engineering

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This course will present an introduction to the theory and practice of solving boundary-integral equations (BIE) using boundary-element methods (BEM)—a popular and computationally efficient alternative to finite-element methods (FEM) for the solution of partial-differential equations. The course will present these methods in the context of studying electrostatic interactions between biological molecules such as proteins.

Electrostatic effects play key roles in determining a biomolecule’s behavior, but are strongly influenced by the water molecules and dissolved ions. Atomistic theories such as molecular dynamics (MD) offer high resolution but are computationally expensive. Macroscopic continuum theory (e.g., the Poisson equation) is much faster to compute, and works remarkably well for many investigations.

Boundary-Integral Equations

Whereas the solution to a PDE is usually sought throughout a region of space, the solution of a BIE lies only on a surface in that space. This difference has substantial implications, and we will illustrate the advantages and disadvantages of these complementary but equivalent approaches. The course will provide a brief survey of application domains where BIE has been particularly successful, including not only biophysics but also electromagnetics, fluids, and elasticity. We will also describe the basic approaches for converting a suitable PDE problem to a BIE, emphasizing that the mathematics are quite accessible to students with basic PDE knowledge.

Boundary-Element Methods

Solving a BIE numerically is not like solving a PDE. We will present some of the key differences and describe how modern numerical techniques and computer architectures, as well as open-source software, make fast, large-scale calculations not only possible but actually quite straightforward.

For example, the system matrix for a finite-difference or finite-element calculation is sparse, reflecting the local nature of the differential operator. In contrast, a BIE leads to a dense matrix, whose computation grows quadratically with the number of unknowns. This course will describe how to use algorithms such as the fast multipole method (FMM) to solve BEM’s dense matrix problems using only linear time and memory.

The course’s conclusion will highlight recent research on BEM techniques for biomolecular electrostatics.