# 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

*Are finite-element methods the only way to solve elliptic partial differential equations? How can the Poisson equation help us understand how proteins interact, or help us design new drugs?*

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.

**Not Just Proteins:**
*Right*: Other important applications of boundary-integral methods

*Far right*: Electrostatic interactions play central roles in biology: (a) guiding a protein (blue and red) along a stretch of DNA (yellow); (b) positive electrostatic potential inside the ring (blue) attracts the negatively charged DNA

### Circuits



Layout

3D problem

### Fluids



Image: D. J. Willis et al., 2007


a

### Scattering



### Elasticity



Location of maximum stress


b

Image: Argiriadi et al., BMC Struct. Biol. (2006)