Boundary-Integral Methods in Molecular Science and Engineering

Lecture 2: There’s More Than One Way to Skin a Cat

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Outline for Lectures

✔ Biology is awesome. If you can solve Poisson, you can join in the fun!

• There’s more than one way to skin a cat. Sometimes PDEs can be advantageously reframed as integral equations.

• Numerical solution of integral equations presents different challenges than do PDEs.

• A diversity of unusual computational challenges will continue to drive biological simulation.
Deriving a Boundary Integral Equation

- Key Concept: Unknowns are on boundaries between regions

In homogeneous dielectric:

\[
\hat{\phi}(r) = \sum_i \frac{q_i}{4\pi \epsilon I |r - r_i|} + \int_\Omega \frac{\sigma_p(r')}{4\pi \epsilon I |r - r'|} dA'
\]

\[
\frac{\partial \hat{\phi}_I}{\partial n^+} - \frac{\partial \hat{\phi}_I}{\partial n^-} = \frac{\sigma_p(r)}{\epsilon I}
\]

Original boundary conditions

\[
\nabla^2 \varphi_I(r) = - \sum_{i=1}^{n_c} \frac{q_i \delta(r - r_i)}{\epsilon_I} I
\]

\[
\nabla^2 \varphi_{II}(r) = 0
\]

\[
\varphi_I(r_\Omega) = \varphi_{II}(r_\Omega)
\]

\[
\epsilon_I \frac{\partial \varphi_I}{\partial n}(r_\Omega) = \epsilon_{II} \frac{\partial \varphi_{II}}{\partial n}(r_\Omega)
\]

\[
\sigma_p(s) + \frac{\Delta \epsilon(s)}{4\pi \epsilon(s)} n(s) \cdot \int_\Omega \frac{s - s'}{|s - s'|^3} \sigma_p(s') ds' = -\frac{\Delta \epsilon(s)}{4\pi \epsilon(s)} n(s) \cdot \sum_k \frac{q_k}{\epsilon(r_k)} \frac{s - r_k}{|s - r_k|^3}
\]

This can be derived from any of several paths: variational principles, Gauss’s law, or Green’s theorem
Why Bother With Integral Equations?

Easy problem:
\[ \nabla^2 \phi = 0 \]
\[ \phi(r_\Gamma) = f(r_\Gamma) \]
\[ \frac{\partial \phi(r_\Gamma)}{\partial n} = g(r_\Gamma) \]

Medium problem:
\[ \nabla^2 \phi = 0 \]
\[ \phi(r_\Gamma) = f(r_\Gamma) \]
\[ \frac{\partial \phi(r_\Gamma)}{\partial n} = g(r_\Gamma) \]

Exterior problems? To infinity

Problems with mostly empty, uninteresting space
The Advantages of PDE Solvers

1. More general
   - nonlinear problems
   - continuously varying material properties
2. Easier to parallelize
3. Sometimes easier to write down
The Capacitance Problem

- Charge accumulates on surface of conductor when it is raised to a potential relative to ground:

\[ Q = CV \]

\[ V = \int_{\Gamma} \sigma(r') \frac{1}{|r - r'|} dA' \]

What about the singularity?

The singularity is integrable!

\[ \phi(r) = \int \frac{1}{|r - r'|} dA' \]

\[ = \int_{0}^{\alpha} \frac{1}{|r'|} \left[ 2\pi r' dr' \right] \]

\[ = 2\pi a \]
Similarity Between FEM and BEM

- Both weighted residual methods:

**FEM**

\[ \mathcal{L}^{\text{diff}} u = f \]

\[ \tilde{u}(r) = \sum_i u_i \chi_i(r) \]

Enforce
\[ < e, \chi_i >= 0 \]
(Galerkin method)

**BEM**

\[ \mathcal{L}^{\text{int}} u = f \]

\[ \tilde{u}(r) = \sum_i u_i \chi_i(r) \]

Enforce
\[ < e, w_i >= 0 \]

Galerkin:
\[ w_i(r) = \chi_i(r) \]
Differences Between BEM and FEM

1. Extra freedom in choosing test functions

   Collocation: test = delta functions
   \[ < e, \delta(r - r_i) > = 0 \]
   \[ \int_{\Omega} \delta(r - r_i) \cdot (L^{\text{int}} \tilde{u} - f) \, dA = 0 \]
   \[ e(r_i) = (L^{\text{int}} \tilde{u} - f)(r_i) = 0 \]

2. Matrix elements are harder to compute

   Galerkin FEM:
   \[ A_{ij} = \int_{\Omega} \nabla \chi_i(r) \cdot \nabla \chi_j(r) \, d\Omega \]
   Smooth integrand:
   Easily computed with quadrature!

   Galerkin BEM:
   \[ < \chi_i, L^{\text{int}} \tilde{u} > = 0 = < \chi_i, f > \]
   \[ \int_{\Omega} \int_{\Omega} (r G(r) \delta) \left( \sum_j \chi_j(x) \chi_j'(x) \right) dA_d\Omega \]
   Double integral of a singular function!!
Using Quadrature to Compute Panel Integrals

- In 1D, N-point Gauss quadrature is exact for polynomials up to order \(2N-1\).

- What happens as the field point approaches the panel? (Here, the middle of the hypotenuse)

- Using Stroud’s rules

- [http://people.scs.fsu.edu/~burkardt/m_src/stroud.html](http://people.scs.fsu.edu/~burkardt/m_src/stroud.html)
Good News: Analytical Laplace Integrals

- For a planar element with polynomial charge distribution, we can analytically compute

\[
\varphi(r) = \int_{\text{element}} \frac{\sigma(r')}{|r - r'|} dA'
\]

Potential due to monopole distribution

\[
\frac{\partial \varphi(r)}{\partial n(r)} = n(r) \cdot \nabla \int_{\text{element}} \frac{\sigma(r')}{|r - r'|} dA'
\]

Normal field due to monopole

\[
\varphi(r) = \int_{\text{element}} n(r') \cdot \nabla \frac{\mu(r')}{|r - r'|} dA'
\]

Potential due to dipole distribution

- Many people fear BIE/BEM due to panel integrals when they don’t have to!

Hess+Smith, 1964; Newman, 1986
Green’s Representation Formula

• Well-known fact: a function harmonic in a region $D$ is completely specified by its boundary values
  
  Dirichlet: given $\phi(r_D) = f(r_D)$
  Neumann: given $\frac{\partial \phi}{\partial n}(r_D) = g(r_D)$

• Not so well known: if you know both, the potential anywhere in $D$ is given by

$$
\phi(r) = \int_S \phi(r') \frac{\partial}{\partial n(r')} \left( \frac{1}{|r - r'|} \right) dA' - \int_S \frac{\partial \phi(r')}{\partial n(r')} \left( \frac{1}{|r - r'|} \right) dA'
$$

Thus you can solve Laplace by finding the other boundary condition!
Another Formulation

Region I:
\[ \nabla^2 \varphi(r) = -\sum_{i=1}^{n_c} q_i \delta(r - r_i) \]

Region II:
\[ \nabla^2 \varphi(r) = \kappa^2 \varphi(r) \]

\[
\begin{bmatrix}
\frac{1}{2} I + D_{I,a}^a & -S_{I,a}^a \\
\frac{1}{2} I - D_{II,a}^a & \epsilon_{I,II} S_{II,a}^a
\end{bmatrix}
\begin{bmatrix}
\phi_a \\
\frac{\partial \phi_a}{\partial n}
\end{bmatrix}
= \begin{bmatrix}
\sum_i q_i G_{I,i}^a \\
0
\end{bmatrix}
\]

- Derivable using Green’s theorem in the interior and exterior regions
- Unknowns are potential and its normal derivative!
Fast Solvers For Integral Equations

• Consider the physical meaning of

\[
\phi(r) = \int_{\Omega} \sigma(r') \frac{1}{|r - r'|} dA'
\]

Computing the field at a number of surface points due to a distribution of sources!

• Adopt fast-summation methods like fast multipole, etc, with \textit{preconditioned Krylov methods} such as GMRES

\[x^k \in \{b, Ab, A^2b, \ldots, A^{k-1}b\}\]
The Fast-Multipole Method

- Optimal (linear-scaling) algorithm for the N-body problem

\[ f(\vec{x}_j) = \sum_{i=1}^{N} c_i K(\vec{x}_i - \vec{x}_j) \quad j \in [1 \ldots N] \]

Direct \( O(N^2) \) \quad FMM \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \quad \qua
The FMM in One Dimension

• “Natural” to combine computation with traversal

Greengard+Rokhlin (1987)
Modifications for BEM

- Fast multipole method, etc., are generally built around interacting “point” sources:

  - Easy: add a sparse “local correction” matrix
  - Pretty, but difficult: compute multipole coefficients directly from basis functions

Potentials at all points are accurately computed...

BUT as we have seen, the representation of source distributions as point charges is NOT accurate!

- Different ways to address this:
  - Easy: add a sparse “local correction” matrix
  - Pretty, but difficult: compute multipole coefficients directly from basis functions
PetFMM: Open-source GPU FMM

- **Separate** tree traversal and computation

  - Use a data-aware queuing system
    - Can handle dependencies if necessary
    - Non-FMM tasks can also be queued

http://barbagroup.bu.edu/Barba_group/PetFMM.html
PetFMM: Open-source GPU FMM

- **Queuing** improves memory access efficiency

**Bottleneck:** small, separated data transfers for M2Ls

**Solution:** Batch all M2Ls associated with a given “target”

- Main memory
- Buffer (temp.)

> 20X as many M2Ls as other operations

Queue splits tasks to fit on thread blocks

GPU: Can give 10X speedup on downward pass!

CPU: Less important but still advantageous

[http://barbagroup.bu.edu/Barba_group/PetFMM.html](http://barbagroup.bu.edu/Barba_group/PetFMM.html)
PetFMM Performance: CPU and GPU

Cross-over for GPU: ~ 10X cross-over for CPU

Direct: $T_{CPU} > 200 T_{GPU}$

FMM: $T_{CPU} \sim 20-30 T_{GPU}$
Parallelization: Graph Partitioning

- Provably good partitioning by ParMETIS
- Partitioning is fast: < 1% of total cost on CPU
- Complete re-use of serial code!

Cruz, Knepley, Barba arXiv:0905.2637
PetFMM Scales to Hundreds of GPUs

- 760-node GPU cluster (T. Hamada, Nagasaki)

Cost of cluster: ~ US $420,000
Sustained: 34.6 Tflops
Performance/price: 80 Mflops/$

\[ \frac{T(512 \text{GPU})}{T(8 \text{GPU})} \approx 20 \]

In 20 sec:
8 GPU $\rightarrow N \approx 1 \times 10^8$
512 GPU $\rightarrow N \approx 3 \times 10^9$
**PetFMM Scaling on Modest GPU Clusters**

- 100 million point charges, uniformly distributed

- Near perfect scaling up to 64 GPUs!
- Further optimizations are in progress
Pre-corrected FFT Algorithm

- Inspired by particle-particle particle-mesh (P³M)
- $O(N \log N)$ but competitive in speed with fast multipole
- Algorithm is \textit{KERNEL INDEPENDENT} Laplace, Helmholtz, others...

1. Project charges to grid
2. FFT convolution of kernel with grid sources
3. Interpolate grid potentials
4. “Pre-correct” so that local interactions are accurate

Phillips and White (1997)
Applications of pFFT

Proteins

Circuit Simulation

Each region has frequency dependent permittivity and permeability.

FastAero: coupled pFFT/tree code

Willis, Peraire, White

EEG and MEG modeling

Fig. 1. Cross section of a nine-layer technology process ($\ell = 1, \ldots, L$; $L = 9$) featuring six metal layers ("NS", "Rx", "M1", "MT", "LY", and "M4") and four via layers ("CA", "V1", "VV", "AV"). The total surface enclosing the interconnect volume at each metal/via layer is denoted $S_p$, $p = 1, \ldots, P$; $P = 10$.

Cadence Design Systems
Summary:

- Many problems in potential theory can be rewritten from PDE form to BIE form

- BIEs tend to be most advantageous for exterior problems or problems with highly irregular boundaries

- Boundary-integral operators map surface source distributions to surface potentials and fields
References:


2. Atkinson and Han. “Theoretical Numerical Analysis.” Covers BEM in much less detail but it also introduces the theoretical background in good detail and also analyzes FDM and FEM.

3. McLean, W. “Strongly Elliptic Systems and Boundary Integral Equations.” First chapter has a nice historical account of integral equations and offers a more general framework than Atkinson.


   http://scidok.sulb.uni-saarland.de/volltexte/2007/1400/