An Introduction to the Boundary Element Method (BEM) and Its Applications in Modeling Composite Materials

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Outline

• An introduction to the Boundary Element Method (BEM)
• Applications of the BEM in solving engineering problems
• BEM in large-scale modeling of fiber-reinforced composites
• Discussions
• References
• Acknowledgements
• Further Information
An Introduction to the BEM
- Two Different Approaches in Computational Mechanics

Engineering Problems

Mathematical Models

Differential Equation (ODE/PDE) Formulations

Analytical Solutions

FDM

Numerical Solutions

FEM

EFM

Others

(Boundary) Integral Equation (BIE) Formulations

Analytical Solutions

BEM

Numerical Solutions

Others
A Brief History of the BEM

**Integral equations** (Fredholm, 1903)
- 2D Potential Problems

**Jaswon and Symm** (1963)
- 2D Potential Problems

**Modern numerical solutions** of BIEs (in early 1960’s)

**T. A. Cruse and F. J. Rizzo** (1968)
- 2D elastodynamics

**P. K. Banerjee** (1975)
- coined the name “boundary element method”
  (this has been disputed by others)

**F. J. Rizzo** (1964, paper 1967)
- 2D Elasticity Problems

**BEM emerged in 1980’s …**
Advantages of the BEM and the Mysteries

Advantages:
• Accuracy – due to the semi-analytical nature and use of integrals
• More efficient in modeling stage due to the reduction of dimensions
• Good for stress concentration and infinite domain problems
• Good for modeling thin shell-like structures/materials
• Neat …

Mysteries:
• BIEs are singular which are difficult to deal with (wrong!)
• BEM is slow and thus inefficient (not necessarily!)
• FEM can solve everything. Who needs BEM? (not exactly true!)
Formulation: The Potential Problem

- **Governing Equation**

\[ \nabla^2 u(P) = 0, \quad \forall P \in V. \]

- **For 3D problems, the Green’s function is**

\[ G(P, P_o) = \frac{1}{4\pi r}, \quad r = |P_o P|. \]

- **BIE formulation**

\[ C(P_o)u(P_o) = \int_S \left[ G \frac{\partial u}{\partial n} - u \frac{\partial G}{\partial n} \right] dS, \quad \forall P_o \in S. \]

- **Discretization of the BIE using the boundary elements**

\[ [H]\{u\} = [G]\left\{ \frac{\partial u}{\partial n} \right\}, \quad \text{or} \quad [A]\{x\} = \{b\}. \]
Singular or Non-Singular?

- Re-examine the BIE

\[ C(P_o)u(P_o) = \int_S \left[ G \frac{\partial u}{\partial n} - u \frac{\partial G}{\partial n} \right] dS, \quad \forall P_o \in S. \]

The second integral in the BIE is singular and is considered as a CPV integral

- However, the constant in the free term is also a CPV integral

\[ C(P_o) = -\int_S \frac{\partial G(P, P_o)}{\partial n} dS(P). \]

- Re-write the BIE to obtain the **weakly-singular form** of the BIE

\[ \int_S \frac{\partial G}{\partial n} [u(P) - u(P_o)] dS = \int_S G \frac{\partial u}{\partial n} dS, \quad \forall P_o \in S. \]

\[ O \left( \frac{1}{r^2} \right) \quad O \left( r \right) \]

- Non-singular form also exists (Liu & Rudolphi, *EABE*, 1991 and *CM*, 1999)
Example: Results for Heat Transfer in a Fuel Cell

Predicted Temperature Distributions Using the BEM and FEM

(a) The fuel cell model  (b) BEM (max. temp. = 378.40 K)  (c) FEM (max. temp. = 378.31 K)
Example: Coupled Structural Acoustics Analysis

- Applications
  - Acoustic radiation/scattering from elastic structures submerged in fluids
  - Prediction of noises of an elastic structure in vibration
  - Dynamics of fluid-filled elastic piping system
  - Acoustic cavity analysis
The BIE Formulation for Structural Acoustics

- **Governing Equations**
  - In elastic domain: \((c_1^2 - c_2^2)u_{k,ki}(P) + c_2^2u_{i,kk}(P) + \omega^2u_i(P) = 0, \quad \forall P \in V\)
  - In acoustic domain: \(\nabla^2\phi(P) + k^2\phi(P) = 0, \quad \forall P \in E\)

- **BIE Formulations**
  - In elastic domain: \(C_y(P_o)u_j(P_o) = \int_S U_y(P, P_o)t_j(P)dS(P) - \int_S T_y(P, P_o)u_j(P)dS(P)\)
  - In acoustic domain: \(C(P_o)\phi(P_o) = \int_S \left[ \frac{\partial G(P, P_o)}{\partial n} \phi(P) - G(P, P_o) \frac{\partial \phi(P)}{\partial n} \right] dS(P) + \phi'(P_o)\)

- **Interface Conditions**
  - Velocity continuity condition across the interface: \(\frac{\partial \phi}{\partial n} = \rho_f \omega^2 u_n\)
  - Stress equilibrium condition: \(t_i = -\phi n_i\)

- **Discretization of the BIE using boundary elements**
Results for A Structural Acoustics Analysis

Radiated Sound Pressure from Steel Spherical Shells with Different Thickness and Under an Internal Harmonic Pressure Load ($r = 5a, M = 112$)

![Graph showing radiated sound pressure for different thicknesses and methods (Analytical vs. BEM)]
Analysis of the Acoustic Fields of a Submarine

A simplified submarine model with BEM (Surface elements only)

Sound pressure in the exterior domain
BEM for Modeling Thin Layered Materials

**Advantages:**
- BEM is good for modeling thin shell-like materials/structures
- Much fewer elements are needed using the BEM than the FEM in the modeling (no element connectivity and aspect-ratio restrictions).
- *Accuracy.*

**Difficulties:** Treatment of the *nearly singular integrals* in the BIEs.
- 3D elasticity case (Liu, *IJNME*, 1998)
- 2D piezoelectricity case (Liu and Fan, *CMAME*, 2002)
Analysis of Fiber-Reinforced Composites with the Presence of the Interphases

A Unit Cell Model of Fiber-Reinforced Composites

Interphases in fiber-reinforced composites are modeled using the BEM and FEM to investigate their effects on the mechanical properties and interface failures of the material.
Analysis of Fiber-Reinforced Composites with the Presence of the Interphases (Cont.)

BEM (384 quadratic line elements)  FEM (10,188 quadratic area elements)
Analysis of Fiber-Reinforced Composites with the Presence of the Interphases (Cont.)

Stress distribution

Effective Young’s modulus

![Stress distribution](image1)

![Effective Young’s modulus](image2)
Analysis of Fiber-Reinforced Composites with the Presence of the Interphases (Cont.)

A Circular-Arc Crack Between the Interphase and the Matrix

Effects of the interphase materials on the stress intensity factor ($K_1 / \sigma_{\text{ave}} \sqrt{\pi R \alpha}$) for the circular-arc interface crack
BEM for Thin Piezoelectric Solids

Applications of Piezoelectric Materials
- Thin piezo films and coatings as sensors/actuators in smart materials
- Micro-electro-mechanical systems (MEMS)
- …

The mechanical and electrical coupling effect in piezoelectric materials
BEM for Thin Piezoelectric Solids (Cont.)

BIE for piezoelectricity (weakly-singular form):

\[
\int_S \mathbf{T}(P, P_0) [\mathbf{u}(P) - \mathbf{u}(P_0)]dS(P) = \int_S \mathbf{U}(P, P_0) \mathbf{t}(P)dS(P)
\]

\[+ \int_V \mathbf{U}(P, P_0) \mathbf{b}(P)dV(P), \quad \forall P_0 \in S,
\]

for a finite piezoelectric solid, in which (for 2D case):

\[
\mathbf{u} = \begin{cases} u_1 \\ u_2 \\ -\phi \end{cases}, \quad \mathbf{t} = \begin{cases} t_1 \\ t_2 \\ -\omega \end{cases}, \quad \mathbf{b} = \begin{cases} f_1 \\ f_2 \\ -q \end{cases},
\]

\[
\mathbf{U} = \begin{bmatrix} U_{11} & U_{12} & \Phi_1 \\ U_{21} & U_{22} & \Phi_2 \\ U_{31} & U_{32} & \Phi_3 \end{bmatrix}, \quad \mathbf{T} = \begin{bmatrix} T_{11} & T_{12} & \Omega_1 \\ T_{21} & T_{22} & \Omega_2 \\ T_{31} & T_{32} & \Omega_3 \end{bmatrix}.
\]
A PZT-5 Strip Subjected to Pressure Load $P$ and Voltage $V_0$

Displacement component $w$ along the bottom edge of the strip ($M = 24$) for different thicknesses
Analysis of Piezoelectric Parallel Bimorph
(Bending deformation with applied voltage)

A parallel bimorph

The deformed shape

(Note that the thickness of the layers can be made arbitrarily small without the need to use smaller and smaller elements in the BEM)
Current Status of the BEM Research

- Fast solvers that can solve problems beyond the reach of other methods
- Large-scale analyses with DOFs above 20M
- Multi-physics and multi-scales

Electromagnetic wave scatterings from targets

(Chew, et al., 2004)
Large-Scale Modeling of Fiber-Reinforced Composites with a Fast Multipole Boundary Element Method

In collaboration with:
Professor Naoshi Nishimura at Kyoto University
The Approach

- A model with elastic matrix and rigid inclusions for fiber-reinforced composites is adopted (the **rigid-inclusion model**)
- This model is likely to be valid for short fibers or long fibers with much higher stiffness than that of matrix
- This approach is the first step towards more general elastic matrix/elastic fiber models
- The fast-multipole method is used to solve the large-scale BEM equations for this problem
Boundary Integral Equation Formulation

Representation integral:

\[ u(x) = \int_S \left[ U(x, y) t(y) - T(x, y) u(y) \right] dS(y) + u^\infty(x), \quad \forall x \in V \quad (1) \]

with \( S = \bigcup \alpha S_\alpha \)

For each rigid inclusion \( S_\alpha \):

\[ u(y) = d + \omega \times p(y) \quad (2) \]

with \( d \) and \( \omega \) being the rigid-body translation and rotation, respectively.

It can be shown that:

\[ \int_{S_\alpha} T(x, y) u(y) dS(y) = 0 \quad (3) \]

for each rigid inclusion \( S_\alpha \).
“Simplified” BIE formulation for rigid-inclusion problems:

\[ u(x) = \int_{S} U(x, y)t(y)\,dS(y) + u_{\infty}(x), \quad \forall x \in S \]  \hspace{1cm} (4)

Both \( u \) and \( t \) are unknown. Need six more equations for each inclusion.

Consider the equilibrium of each inclusion (6 equations):

\[ \int_{S_{\alpha}} t(y)\,dS(y) = 0; \]  \hspace{1cm} (5)

\[ \int_{S_{\alpha}} p(y) \times t(y)\,dS(y) = 0; \]  \hspace{1cm} (6)

for \( \alpha = 1, 2, \ldots, n \)

Eqs. (4-6) provide enough equations for solving the rigid-inclusion problem.
Fast Multipole Method (FMM)

- Ranked among the top ten algorithms of the 20th century (with FFT, QR, …)
- Developed by Rokhlin and Greengard (mid of 1980’s)
- For 3-D elasticity: Peirce and Napier (1995); Rodin, et al. (1997); Popov and Power (2001), and many others
- More research (more large-scale applications)
- Education or re-education
Fast Multipole Algorithm

- The entire boundary is divided into multi-level cells
- Each boundary element is placed in a cell, which contains a specified number of elements
- A tree structure of the boundary elements is obtained
- Interactions (integrations) of element-to-element is replaced by those of cell-to-cell
- Expansions are employed to accelerate the evaluations of these interactions

(Nishimura, 2002)
Fast Multipole Expansions

Apply the following expansion:

\[
\frac{1}{r(x, y)} = \sum_{n=0}^{\infty} \sum_{m=-n}^{n} S_{n,m}(\overrightarrow{Ox}) \overrightarrow{R}_{n,m}(\overrightarrow{Oy})
\]

(7)

where \( \overrightarrow{O} \) represents a third point, \( R_{n,m} \) and \( S_{n,m} \) are solid harmonic functions.

Displacement kernel is written as:

\[
U_{ij}(x, y) = \frac{1}{8\pi\mu} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left[ F_{ij,n,m}(\overrightarrow{Ox}) \overrightarrow{R}_{n,m}(\overrightarrow{Oy}) + G_{i,n,m}(\overrightarrow{Ox})(\overrightarrow{Oy}) \overrightarrow{R}_{n,m}(\overrightarrow{Oy}) \right]
\]

(8)

which is in the form: \( U \sim k_n^{(1)}(\overrightarrow{Ox})k_n^{(2)}(\overrightarrow{Oy}) \)

The FMM expansion:

\[
\int_{S_o} U_{ij}(x, y)t_j(y)dS(y) = \frac{1}{8\pi\mu} \sum_{n=0}^{\infty} \sum_{m=-n}^{n} \left[ F_{ij,n,m}(\overrightarrow{Ox}) M_{j,n,m}(\overrightarrow{O}) + G_{i,n,m}(\overrightarrow{Ox}) M_{n,m}(\overrightarrow{O}) \right]
\]

(9)

where the four multipole moments are given by:

\[
M_{j,n,m}(\overrightarrow{O}) = \int_{S_o} R_{n,m}(\overrightarrow{Oy})t_j(y)dS(y); \quad M_{n,m}(\overrightarrow{O}) = \int_{S_o} (\overrightarrow{Oy})_j R_{n,m}(\overrightarrow{Oy})t_j(y)dS(y)
\]

(10)
upward and downward passes

(Nishimura, 2004)
A Rigid Sphere in Elastic Medium

A sphere with tri-axial loading

A BEM mesh with 1944 constant elements
A Rigid Sphere in Elastic Medium (Cont.)

Radial and tangential stresses obtained by a BEM model with 120 elements
A Rigid Sphere in Elastic Medium (Cont.)

Contour plot for stress on the surface of the sphere
Study of Fiber-Reinforced Composites: The Representative Volume Element (RVE)
A BEM Mesh

A BEM mesh used for the short fiber inclusion (with 456 constant elements)
Load Transfer Studies

A model with 216 “randomly” distributed and oriented short fibers
Efficiency of the Fast Multipole BEM

CPU time used for solving the BEM models for the short-fiber cases
A small RVE containing 2,000 CNT fibers with the total DOF = 3,612,000 (CNT length = 50 nm, volume fraction = 10.48%). A larger model with 16,000 CNT fibers and 28.9M DOFs was solved successfully on a FUJITSU HPC2500 supercomputer (at the Kyoto University) within 34 hours.
Modeling of CNT-Based Composites (Cont.)

Computed effective moduli of CNT/polymer composites using three RVEs and compared with NASA’s multi-scale results.
Discussions

• BEM is a very efficient numerical tool for many problems in engineering
• Computational mechanics can play a significant role in the development of composite materials
• Multi-scale, multiphysics and large-scale approaches are urgently needed for the development of new materials
• There are plenty of opportunities for the computational mechanics (FEM/BEM/BNM/Meshfree methods) in material modeling, bio-engineering and many other fields
A Bigger Picture of Computational Solid Mechanics

**FEM**: Large-scale structural, nonlinear, and transient problems

**BEM**: Large-scale continuum, linear, and steady state (wave) problems

**Meshfree**: Large deformation, fracture and moving boundary problems

“If the only tool you have is a hammer, then every problem you can solve looks like a nail!”
Future of Computational Mechanics

Large scale, multiscale, instant and visual!

An Example:
Virtual Reality (VR) with large scale MD simulations of a fractured ceramic nanocomposite (Spheres with different colors represent atoms of different materials in the nanocomposite)

(A. Nakano, et al., 2001)
References
(on BIE/BEM)


References
(on composites/nanocomposites and their modeling)

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