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

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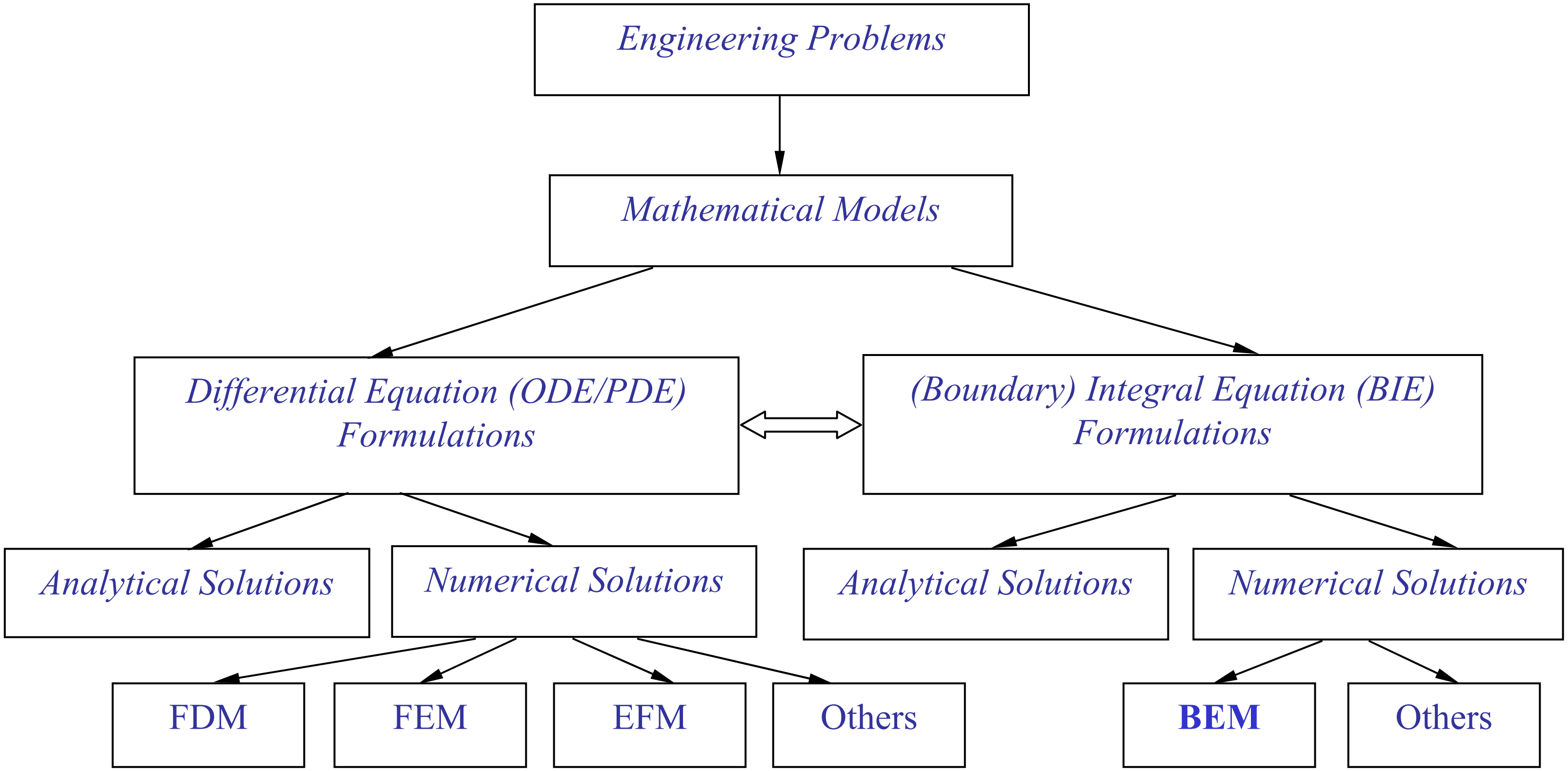
Outline

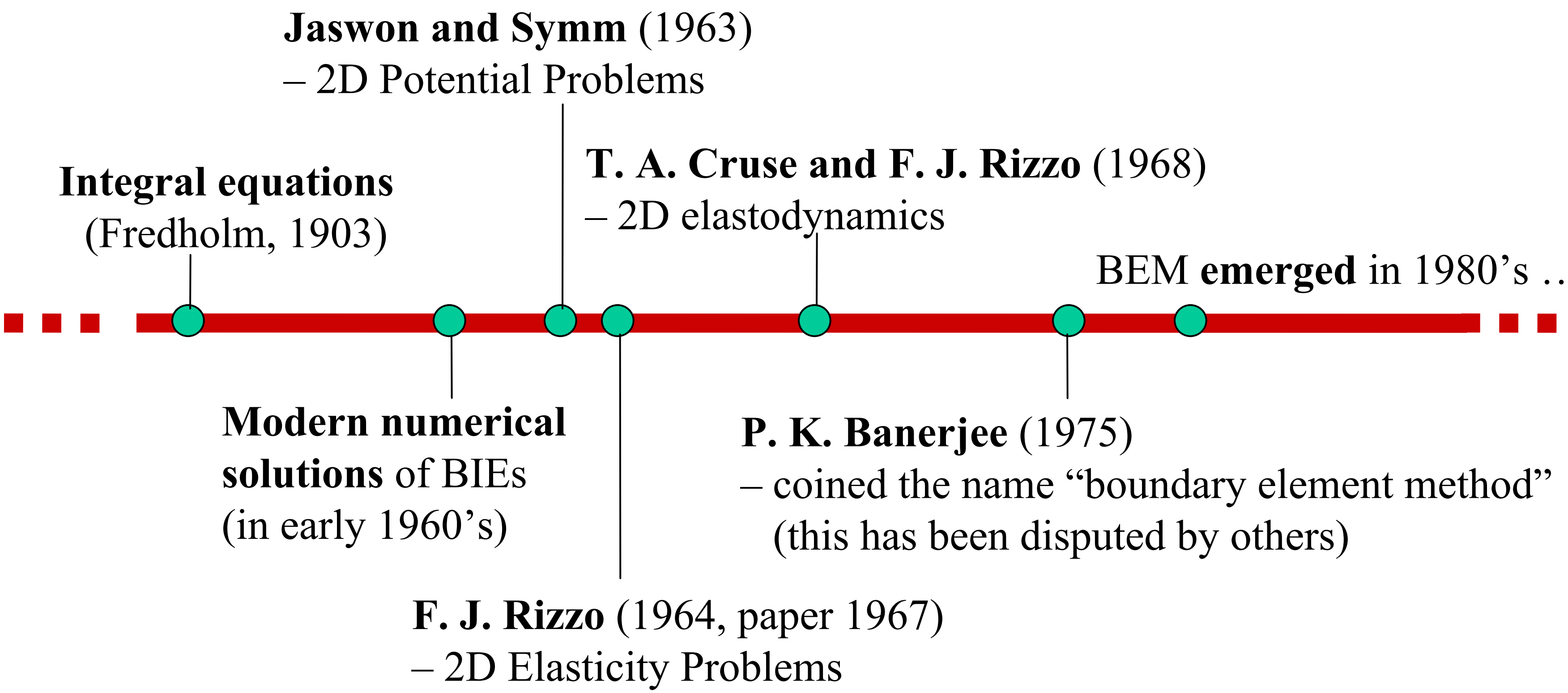
- An introduction to the Boundary Element Method (BEM)
- Applications of the BEM in solving engineering problems
- BEM in large-scale modeling of fiber-reinforced composites
- Discussions
- References
- Acknowledgements
- Further Information

An Introduction to the BEM

- Two Different Approaches in Computational Mechanics



A Brief History of the BEM



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 …

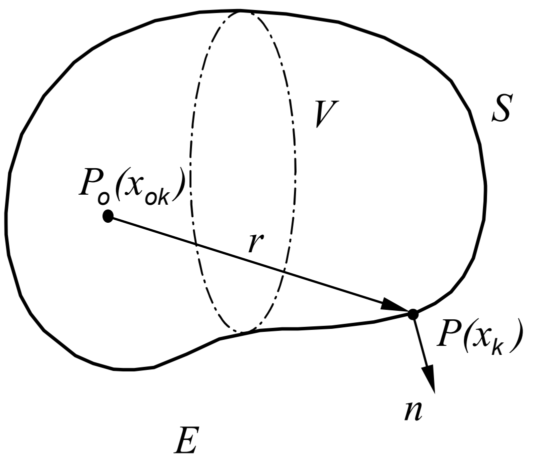
Mysteries:

- 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

$$\nabla^2 u(P) = 0, \qquad \forall P \in V.$$



- For 3D problems, the Green's function is

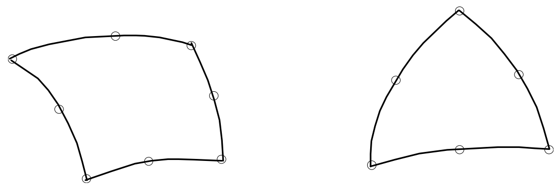
$$G(P, P_o) = \frac{1}{4\pi r}, \qquad r = |P_o P|.$$

- 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

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

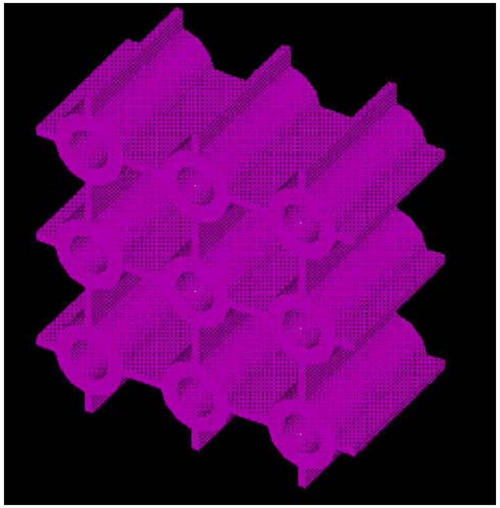
- Re-write the BIE to obtain the **weakly-singular form** of the BIE

$$\int_S \underbrace{\frac{\partial G}{\partial n}}_{O(1/r^2)} \underbrace{[u(P) - u(P_o)]}_{O(r)} dS = \int_S G\frac{\partial u}{\partial n} dS, \quad \forall P_o \in S.$$

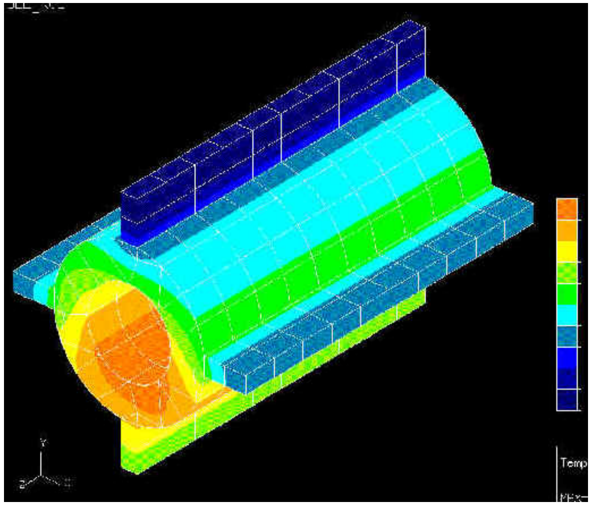
- Non-singular form also exists (Liu & Rudolphi, *EABE,* 1991 and *CM,* 1999)

Example: Results for Heat Transfer in a Fuel Cell

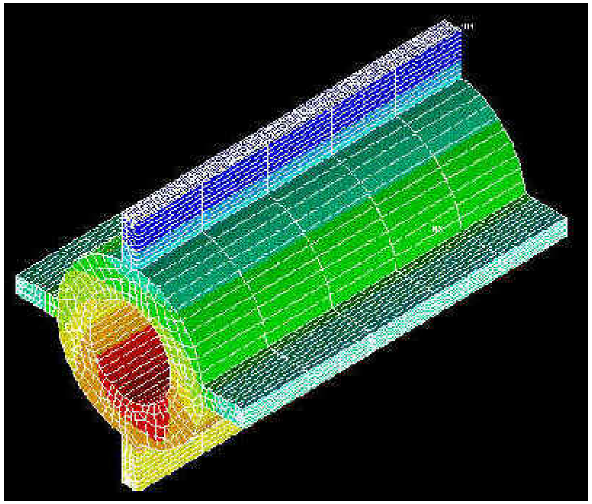
Predicted Temperature Distributions Using the BEM and FEM



(a) The fuel cell model



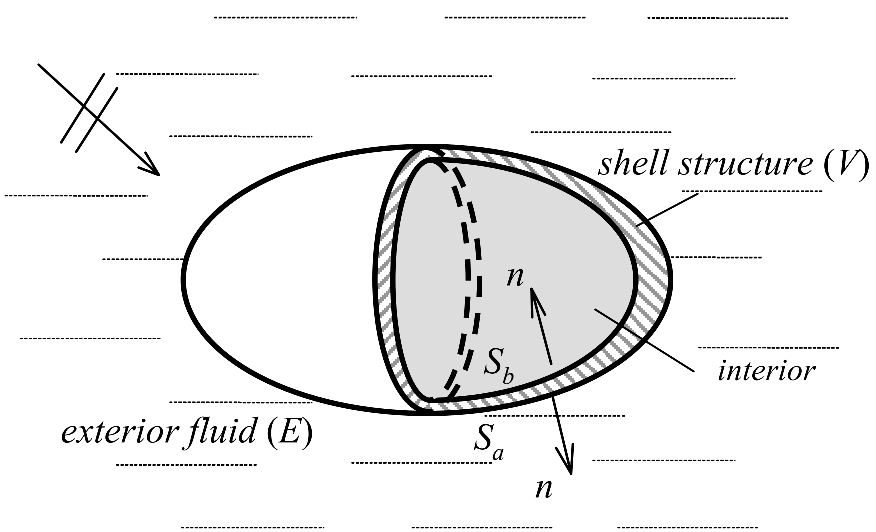
(b) BEM (max. temp. = 378.40 K)

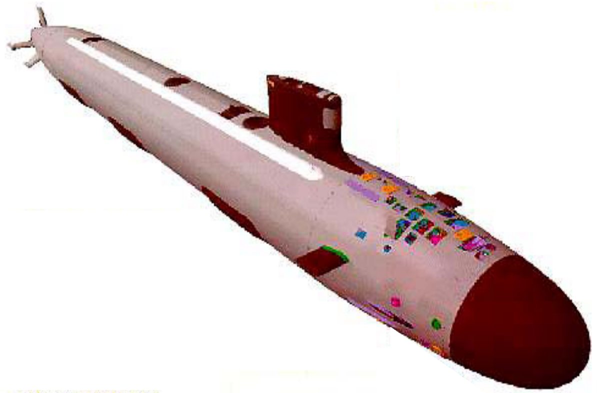


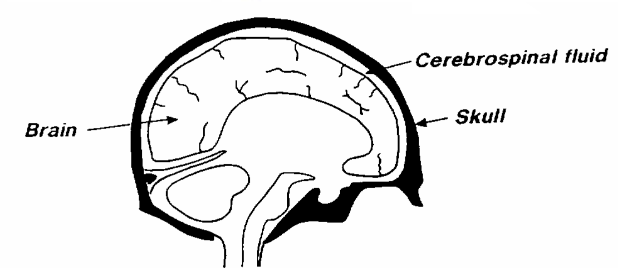
(c) FEM (max. temp. = 378.31 K)

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

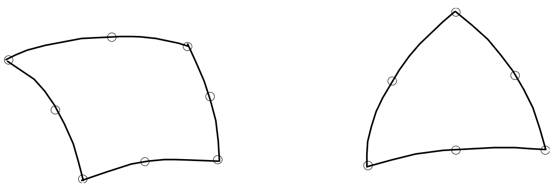






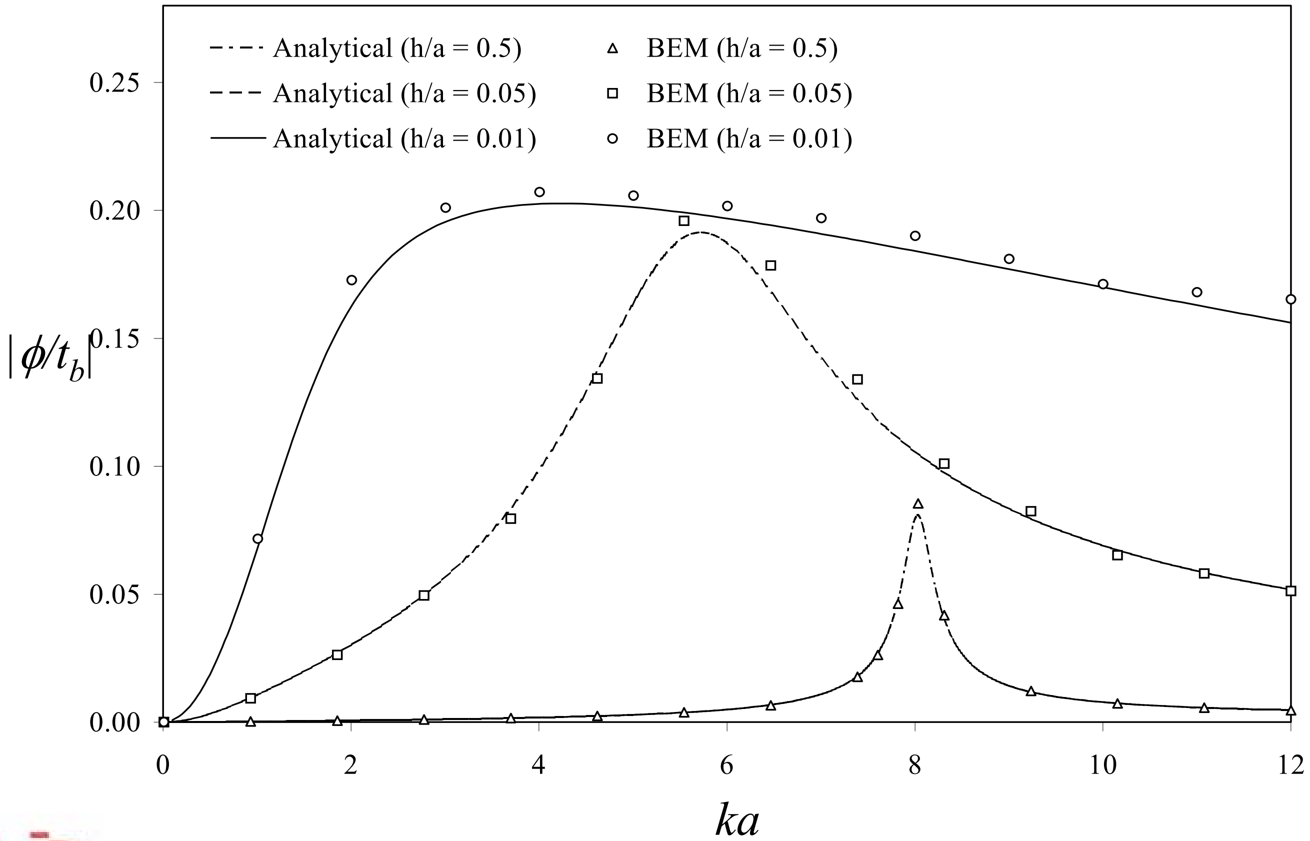
The BIE Formulation for Structural Acoustics

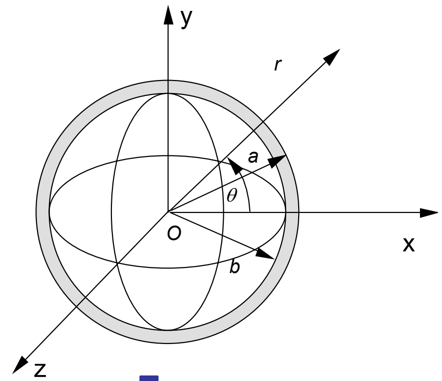
- Governing Equations
  - In elastic domain: $(c_1^2 - c_2^2)u_{k,ki}(P) + c_2^2 u_{i,kk}(P) + \omega^2 u_i(P) = 0, \quad \forall P \in V$
  - In acoustic domain: $\nabla^2 \phi(P) + k^2 \phi(P) = 0, \quad \forall P \in E$
- BIE Formulations
  - In elastic domain: $C_{ij}(P_o)\mathbf{u}_j(P_o) = \int_S \mathbf{U}_{ij}(P,P_o)\mathbf{t}_j(P)dS(P) - \int_S \mathbf{T}_{ij}(P,P_o)\mathbf{u}_j(P)dS(P)$
  - In acoustic domain: $C(P_o)\phi(P_o) = \int_{S_a}\left[\frac{\partial G(P,P_o)}{\partial n}\phi(P) - G(P,P_o)\frac{\partial \phi(P)}{\partial n}\right]dS(P) + \phi^I(P_o)$
- 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



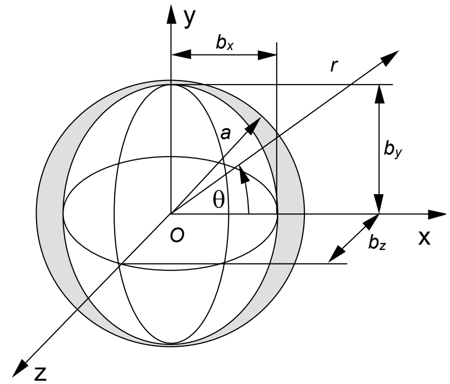
Results for A Structural Acoustics Analysis

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

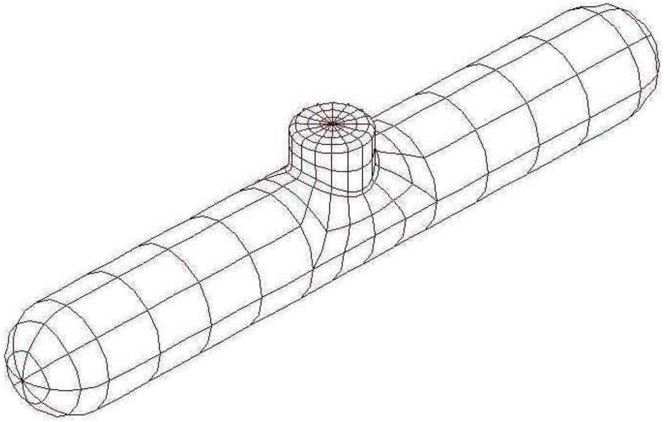




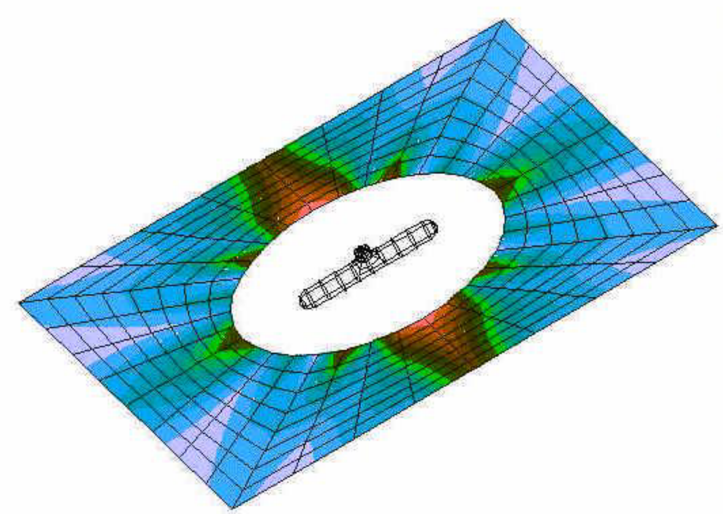
Difficult for FEM



Analysis of the Acoustic Fields of a Submarine



A simplified submarine model with BEM
(Surface elements only)

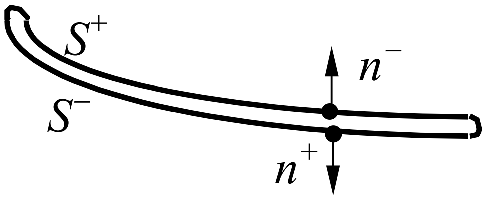


Sound pressure in the exterior domain

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*.

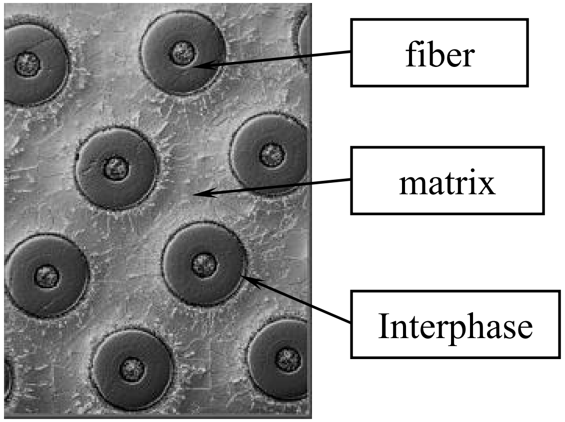


Difficulties: Treatment of the ***nearly singular integrals*** in the BIEs.

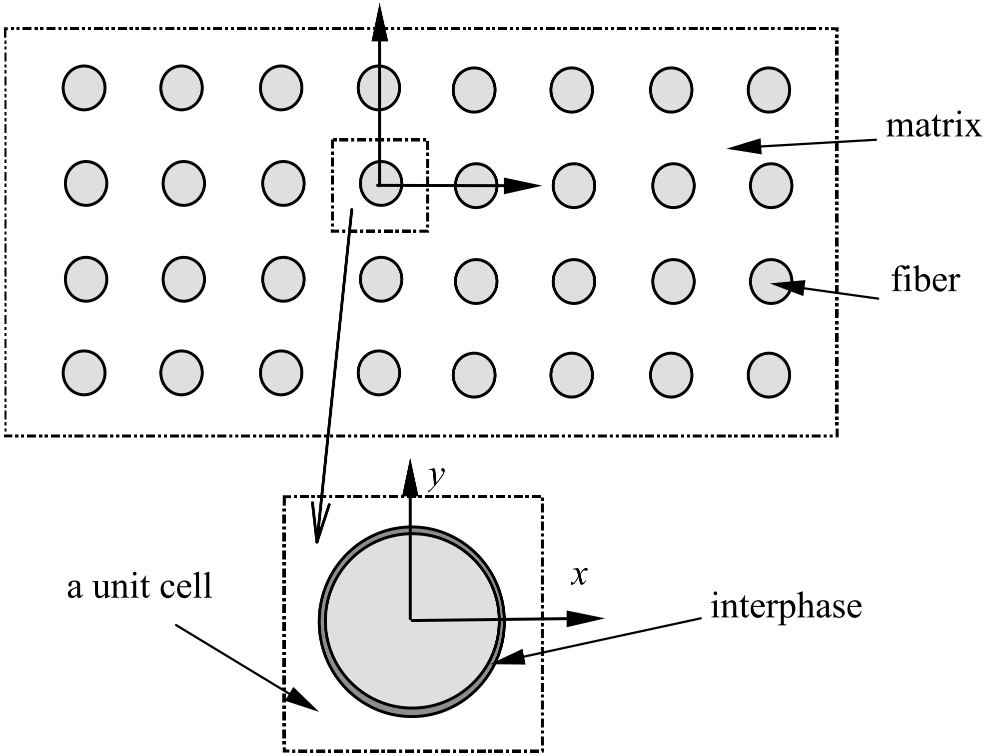
- 3D elasticity case (Liu, *IJNME*, 1998)
- 2D elasticity case (Luo, Liu and Berger, *CM*, 1998)
- 2D piezoelectricity case (Liu and Fan, *CMAME*, 2002)

Analysis of Fiber-Reinforced Composites with the Presence of the Interphases

A Unit Cell Model of Fiber-Reinforced Composites

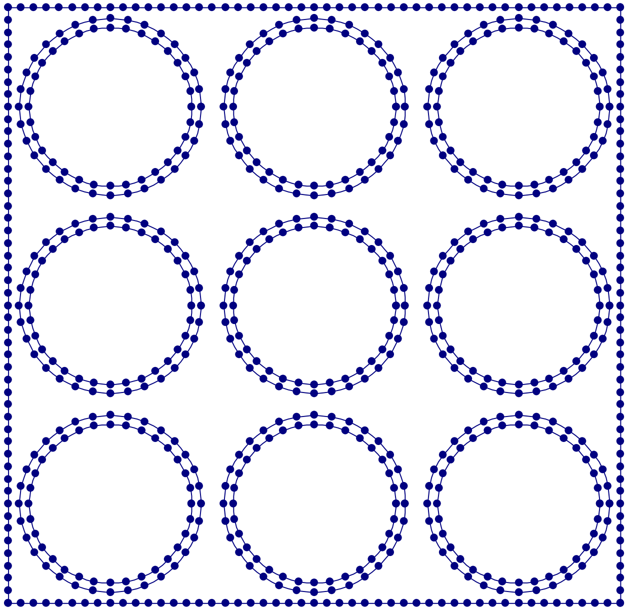


A fiber-reinforced composite

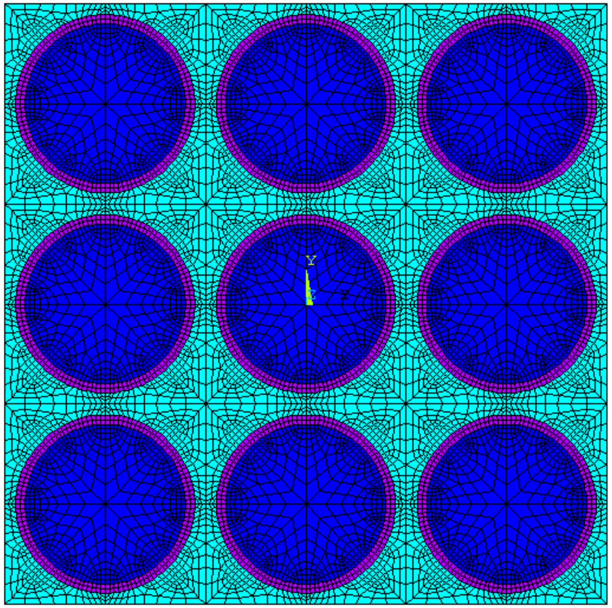


Interphases in fiber-reinforced composites are modeled using the BEM and FEM to investigate their effects on the mechanical properties and interface failures of the material.

Analysis of Fiber-Reinforced Composites with the Presence of the Interphases (Cont.)

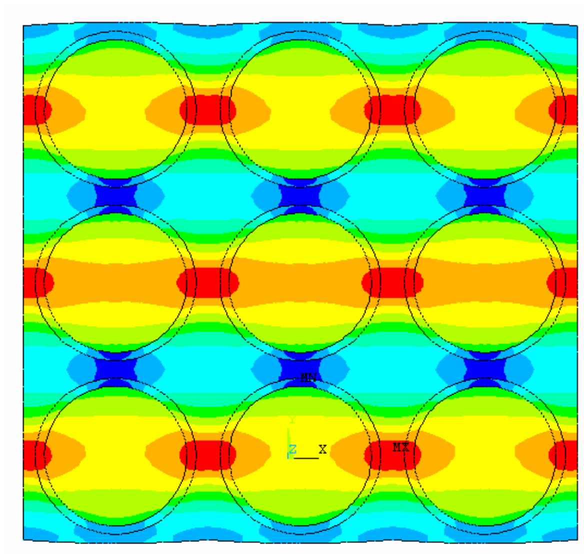


BEM (384 quadratic line elements)

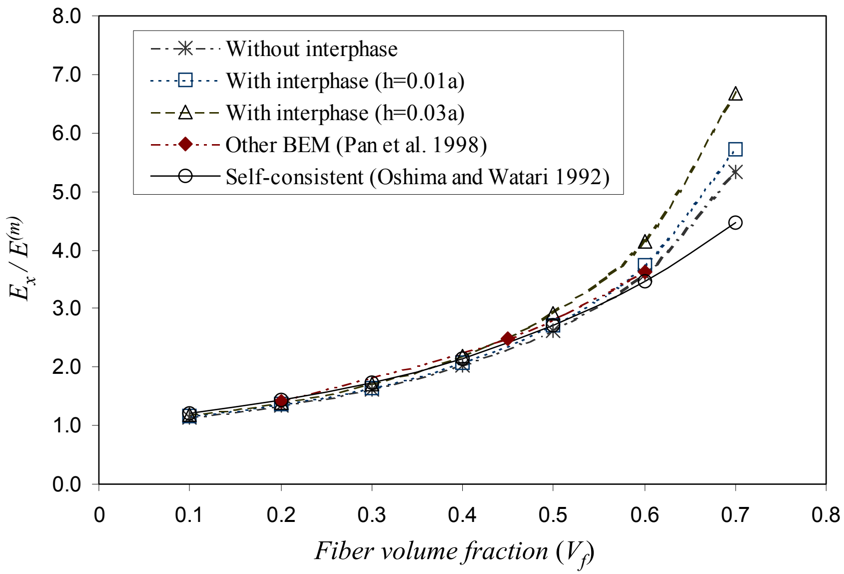


FEM (10,188 quadratic area elements)

Analysis of Fiber-Reinforced Composites with the Presence of the Interphases (Cont.)



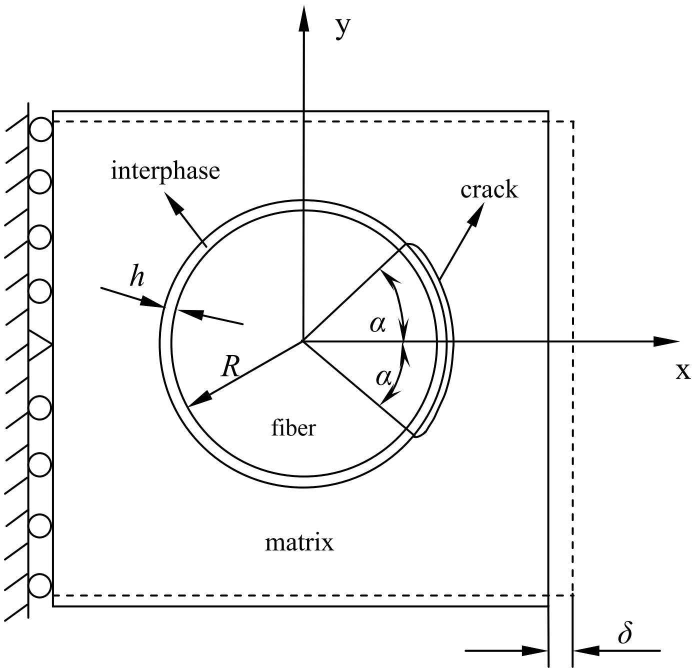
Stress distribution

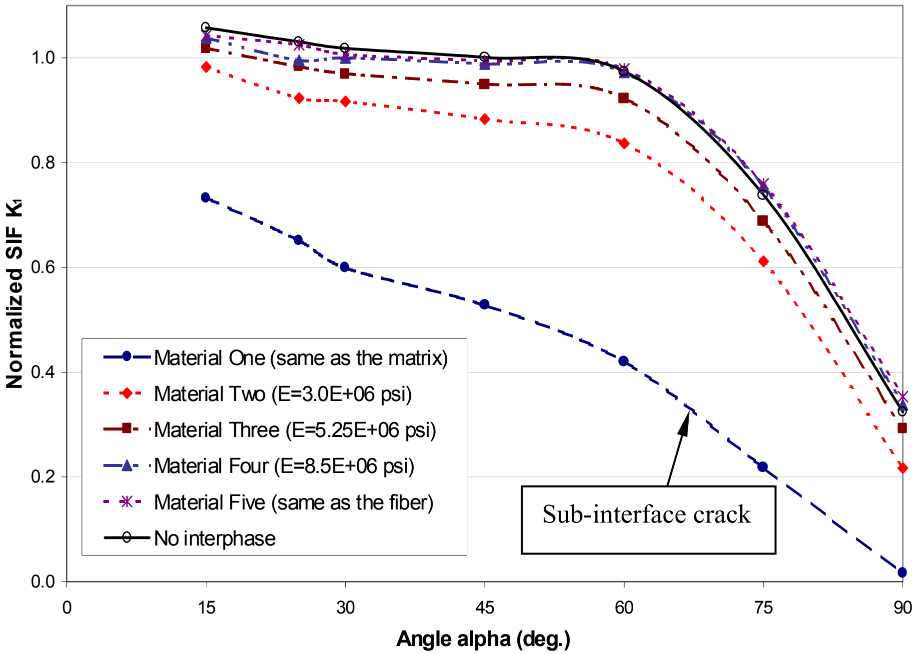


Effective Young's modulus

Analysis of Fiber-Reinforced Composites with the Presence of the Interphases (Cont.)

A Circular-Arc Crack Between the Interphase and the Matrix



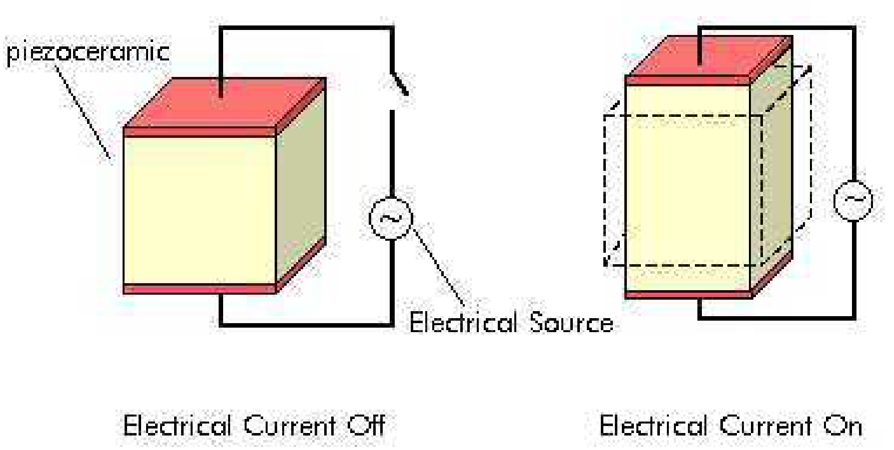


Effects of the interphase materials on the stress intensity factor ($K_1 / \sigma_{ave}\sqrt{\pi R \alpha}$) for the circular-arc interface crack

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):

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

$$+\int_V \mathbf{U}(P,P_0)\mathbf{b}(P)dV(P), \qquad \forall P_0 \in S,$$

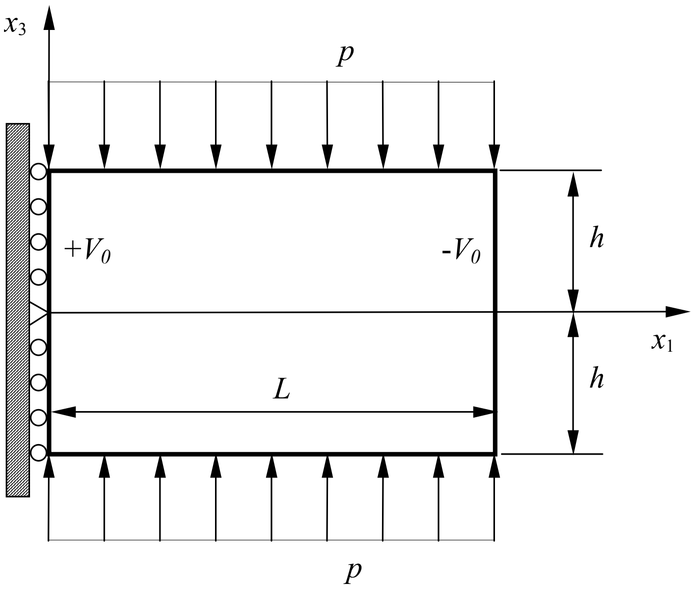
for a *finite* piezoelectric solid, in which (for 2D case):

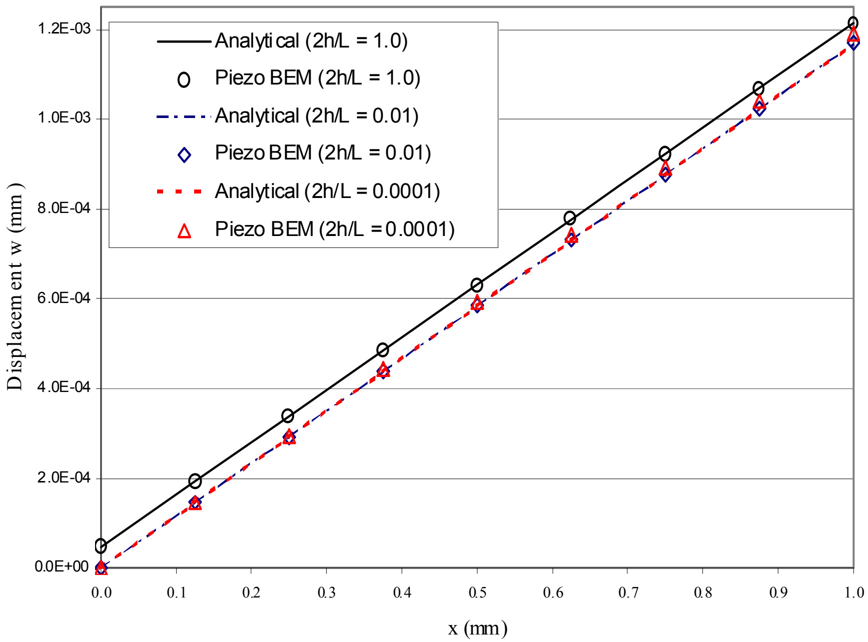
$$\mathbf{u} = \begin{Bmatrix} u_1 \\ u_2 \\ -\phi \end{Bmatrix}, \qquad \mathbf{t} = \begin{Bmatrix} t_1 \\ t_2 \\ -\omega \end{Bmatrix}, \qquad \mathbf{b} = \begin{Bmatrix} f_1 \\ f_2 \\ -q \end{Bmatrix},$$

$$\mathbf{U} = \begin{bmatrix} U_{11} & U_{12} & \Phi_1 \\ U_{21} & U_{22} & \Phi_2 \\ U_{31} & U_{32} & \Phi_3 \end{bmatrix}, \qquad \mathbf{T} = \begin{bmatrix} T_{11} & T_{12} & \Omega_1 \\ T_{21} & T_{22} & \Omega_2 \\ T_{31} & T_{32} & \Omega_3 \end{bmatrix}.$$

BEM for Thin Piezoelectric Solids (Cont.)

A PZT-5 Strip Subjected to Pressure Load *P* and Voltage V_0



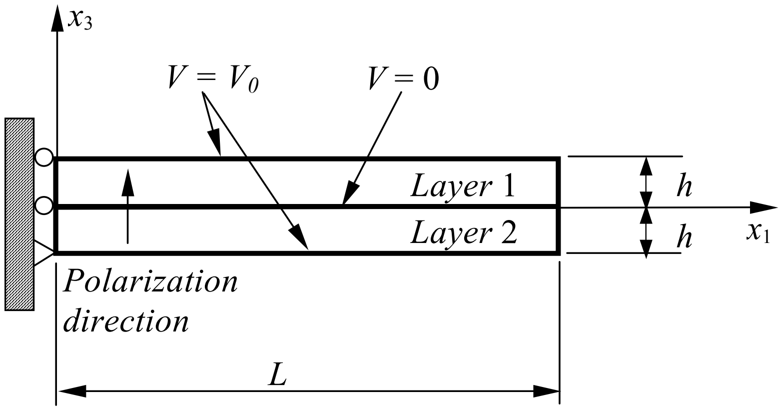


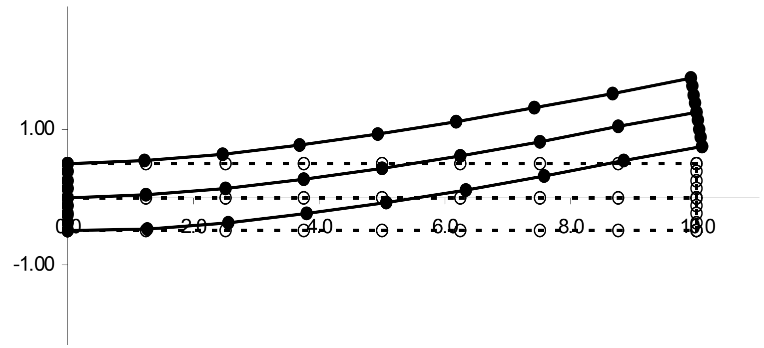
Displacement component *w* along the bottom edge of the strip ($M = 24$) for different thicknesses

BEM for Thin Piezoelectric Solids (Cont.)

Analysis of Piezoelectric Parallel Bimorph

(Bending deformation with applied voltage)





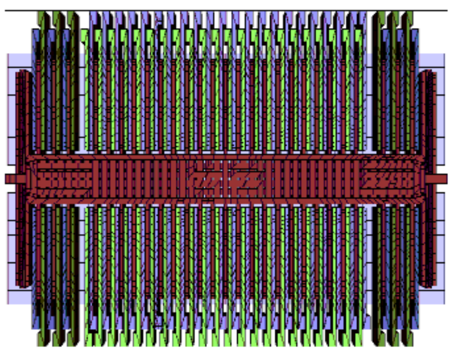
A parallel bimorph

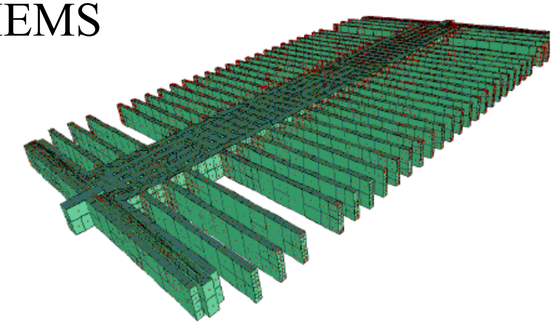
The deformed shape

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

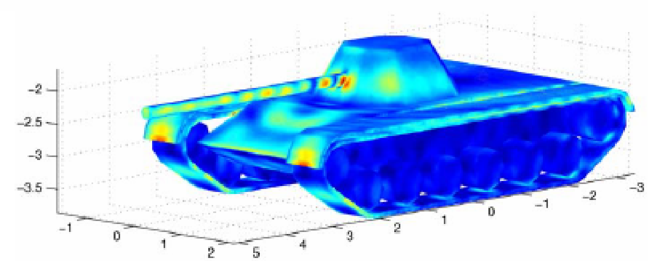
Current Status of the BEM Research

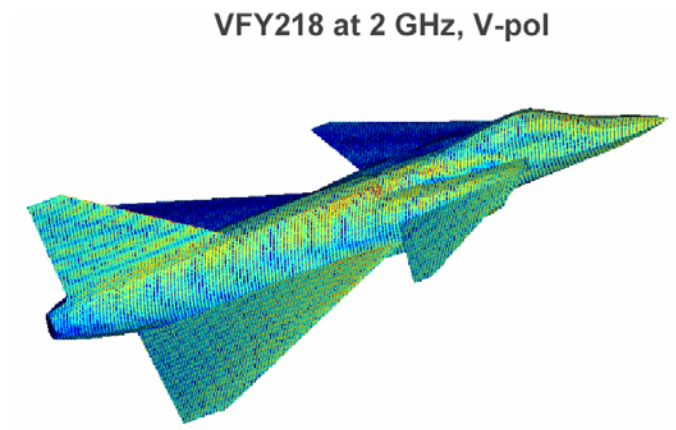
- Fast solvers that can solve problems beyond the reach of other methods
- Large-scale analyses with DOFs above 20M
- Multi-physics and multi-scales





MEMS





Electromagnetic wave scatterings from targets

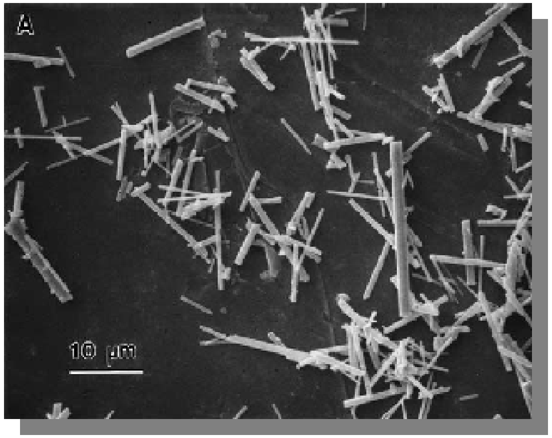
(Chew, et al., 2004)

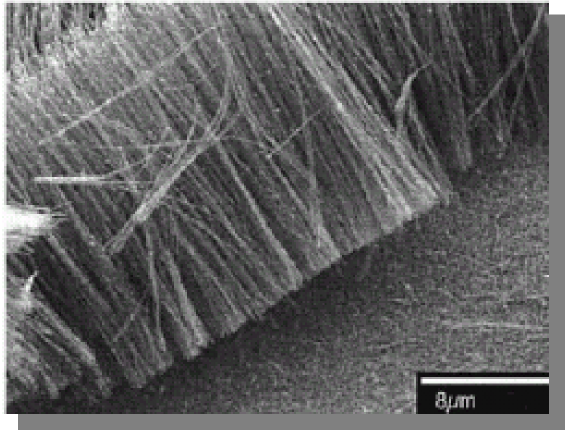
Large-Scale Modeling of Fiber-Reinforced Composites with a Fast Multipole Boundary Element Method

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:

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

with $S = \bigcup_{\alpha} S_\alpha$

For each rigid inclusion S_α:

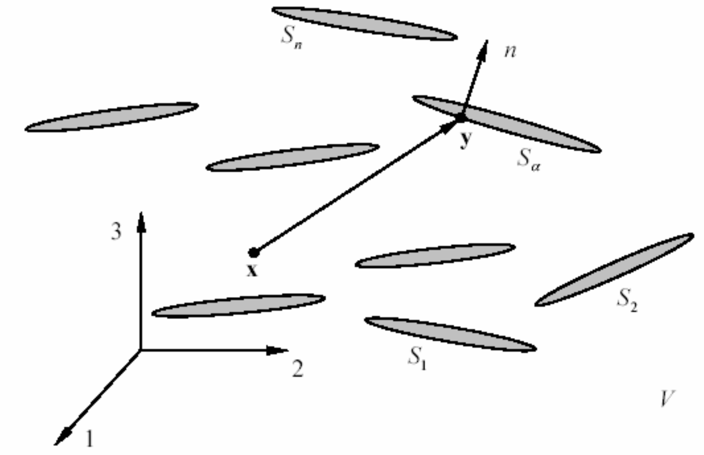
$$\mathbf{u}(\mathbf{y}) = \mathbf{d} + \boldsymbol{\omega} \times \mathbf{p}(\mathbf{y}) \qquad (2)$$

with **d** and **ω** being the rigid-body translation and rotation, respectively

It can be shown that:

$$\int_{S_\alpha} \mathbf{T}(\mathbf{x},\mathbf{y})\mathbf{u}(\mathbf{y}) dS(\mathbf{y}) = \mathbf{0} \qquad (3)$$

for each rigid inclusion S_α



Boundary Integral Equation Formulation (Cont.)

"Simplified" BIE formulation for rigid-inclusion problems:

$$\mathbf{u}(\mathbf{x}) = \int_S \mathbf{U}(\mathbf{x}, \mathbf{y})\mathbf{t}(\mathbf{y})dS(\mathbf{y}) + \mathbf{u}^{\infty}(\mathbf{x}), \qquad \forall \mathbf{x} \in S \qquad (4)$$

Both **u** and **t** are unknown. Need six more equations for each inclusion

Consider the equilibrium of each inclusion (6 equations):

$$\int_{S_\alpha} \mathbf{t}(\mathbf{y})dS(\mathbf{y}) = \mathbf{0}; \qquad (5)$$

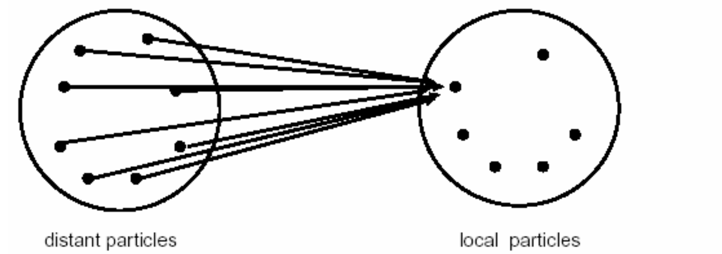
$$\int_{S_\alpha} \mathbf{p}(\mathbf{y}) \times \mathbf{t}(\mathbf{y})dS(\mathbf{y}) = \mathbf{0}; \qquad (6)$$

for $\alpha = 1, 2, \ldots, n$

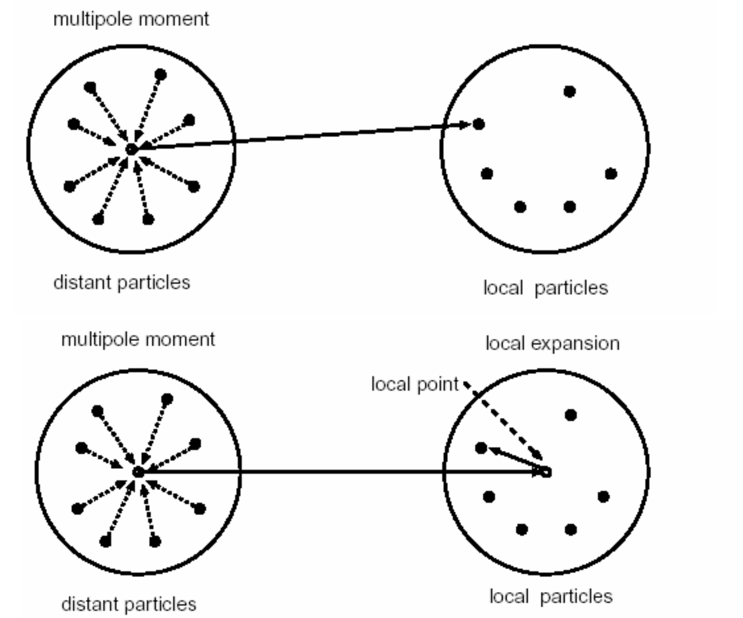
Eqs. (4-6) provide enough equations for solving the rigid-inclusion problem

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
- A review: **Nishimura**, *Applied Mechanics Review*, July 2002



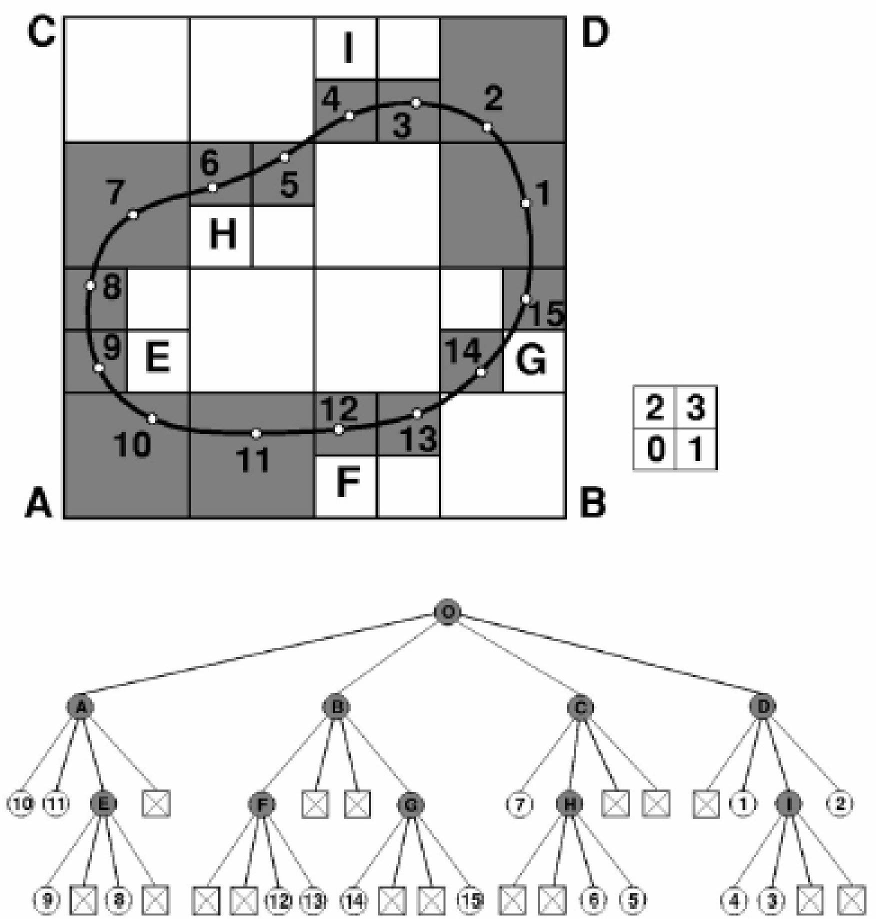
Conventional evaluation of contribution from distant particles: $O(N^2)$ algorithm



Evaluation with the multipole moment and the local expansion: $O(N)$ algorithm

(From **Yoshida, 2001**)

Fast Multipole Algorithm



(Nishimura, 2002)

- 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

Fast Multipole Expansions

Apply the following expansion:

$$\frac{1}{r(\mathbf{x},\mathbf{y})} = \sum_{n=0}^{\infty}\sum_{m=-n}^{n} S_{n,m}(\overrightarrow{\mathbf{Ox}})\overline{R_{n,m}}(\overrightarrow{\mathbf{Oy}}) \qquad (7)$$

where **O** represents a third point, $R_{n,m}$ and $S_{n,m}$ are solid harmonic functions

Displacement kernel is written as:

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

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

The FMM expansion:

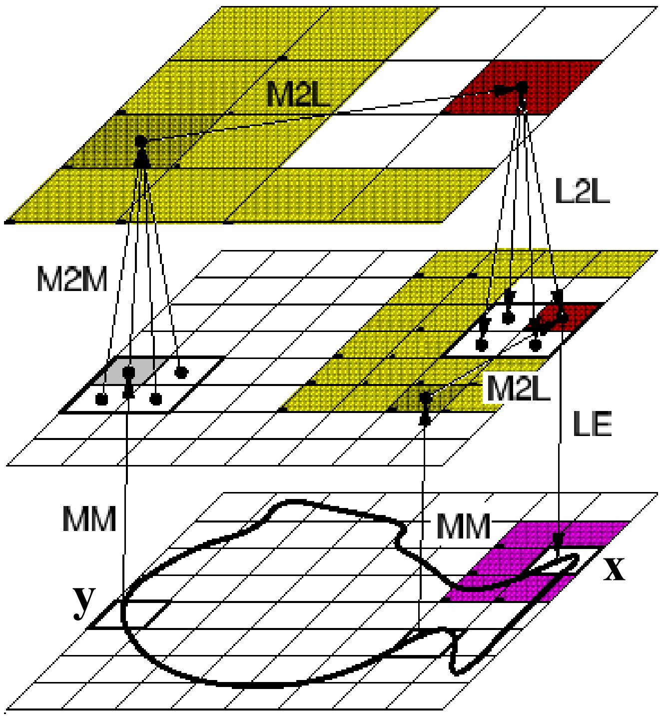
$$\int_{S_o} U_{ij}(\mathbf{x},\mathbf{y})t_j(\mathbf{y})dS(\mathbf{y}) = \frac{1}{8\pi\mu}\sum_{n=0}^{\infty}\sum_{m=-n}^{n}\left[F_{ij,n,m}(\overrightarrow{\mathbf{Ox}})\overline{M_{j,n,m}}(\mathbf{O}) + G_{i,n,m}(\overrightarrow{\mathbf{Ox}})\overline{M_{n,m}}(\mathbf{O})\right] \qquad (9)$$

where the four multipole moments are given by:

$$M_{j,n,m}(\mathbf{O}) = \int_{S_o} R_{n,m}(\overrightarrow{\mathbf{Oy}})t_j(\mathbf{y})dS(\mathbf{y}); \qquad M_{n,m}(\mathbf{O}) = \int_{S_o}(\overrightarrow{\mathbf{Oy}})_j R_{n,m}(\overrightarrow{\mathbf{Oy}})t_j(\mathbf{y})dS(\mathbf{y}) \qquad (10)$$

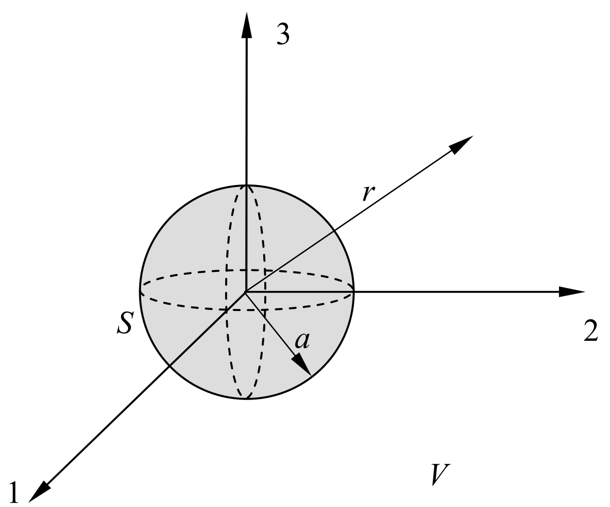
Fast Multipole Algorithm (Cont.)

upward and downward passes

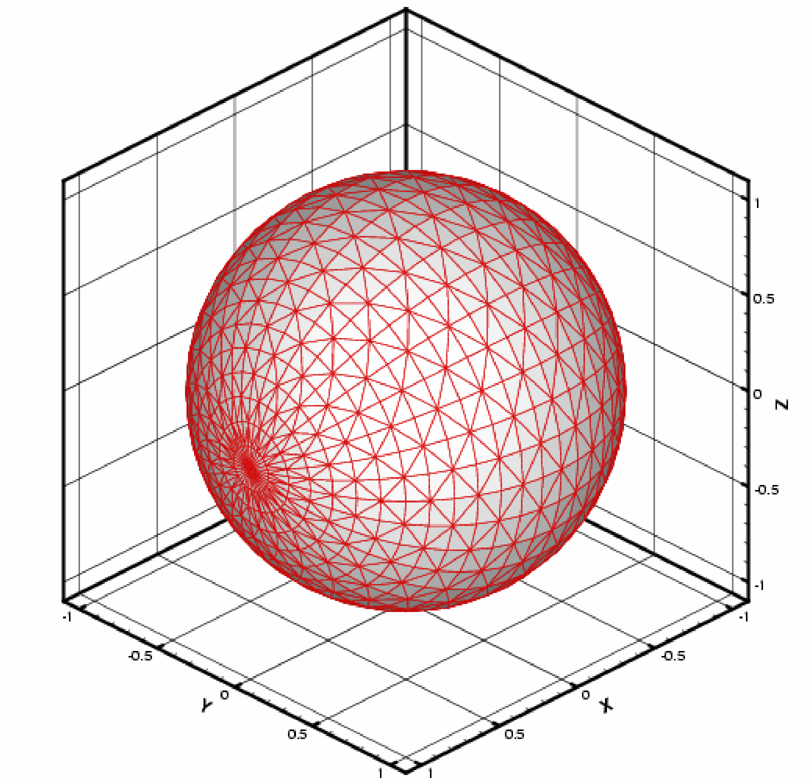


(Nishimura, 2004)

A Rigid Sphere in Elastic Medium

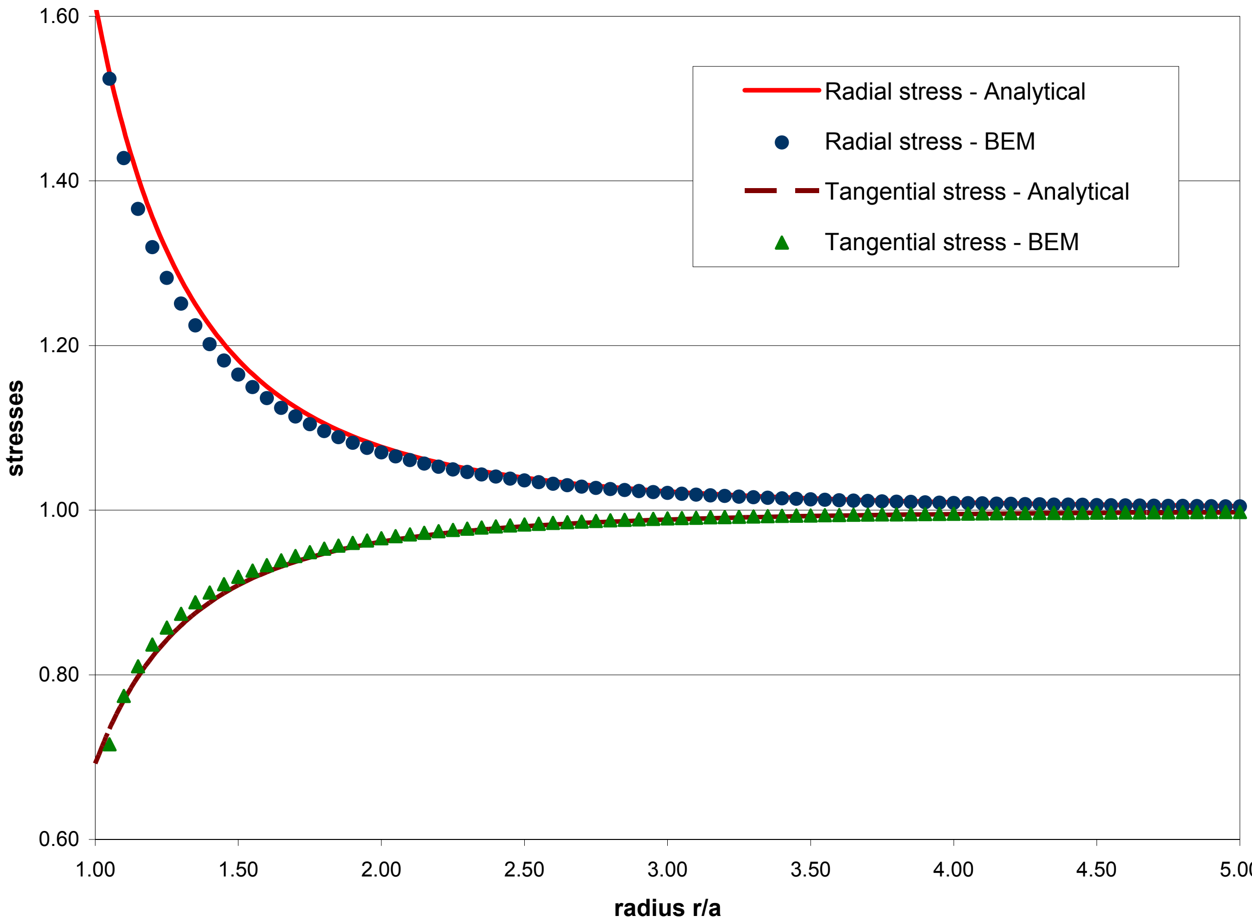


A sphere with tri-axial loading



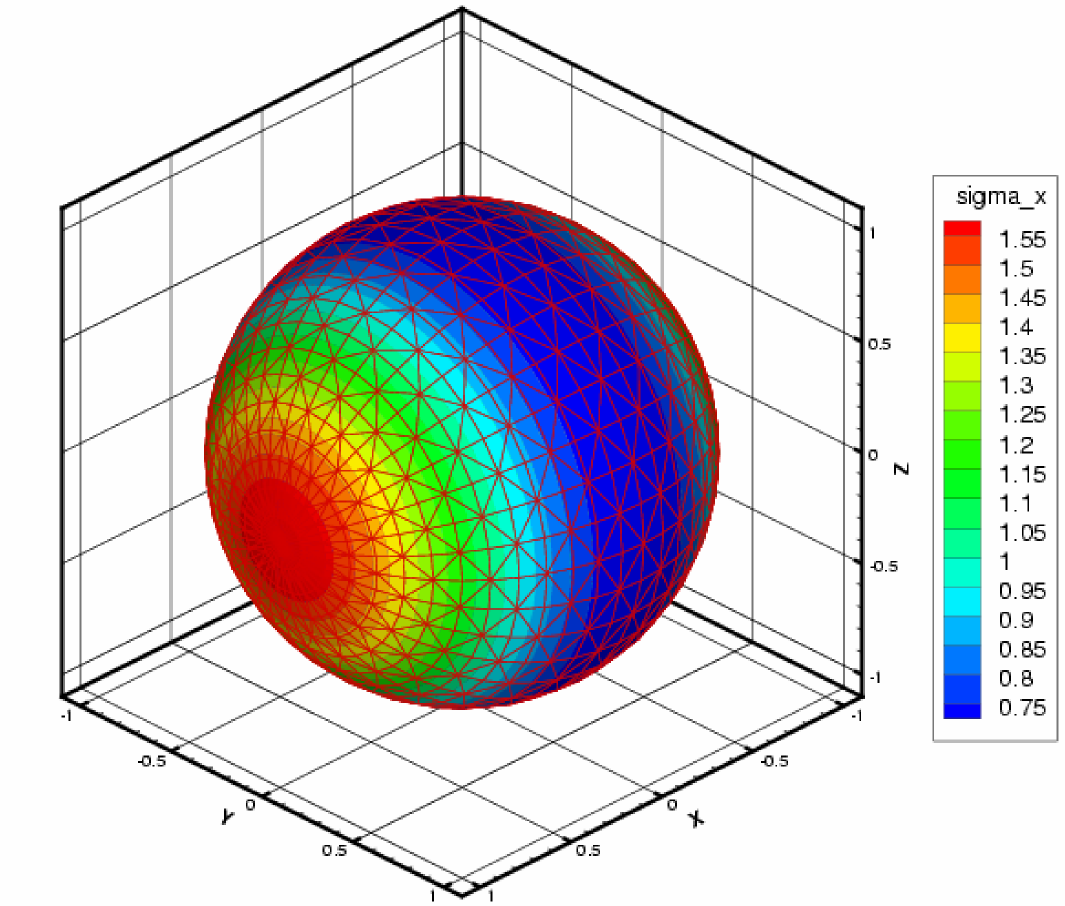
A BEM mesh with 1944 constant elements

A Rigid Sphere in Elastic Medium (Cont.)



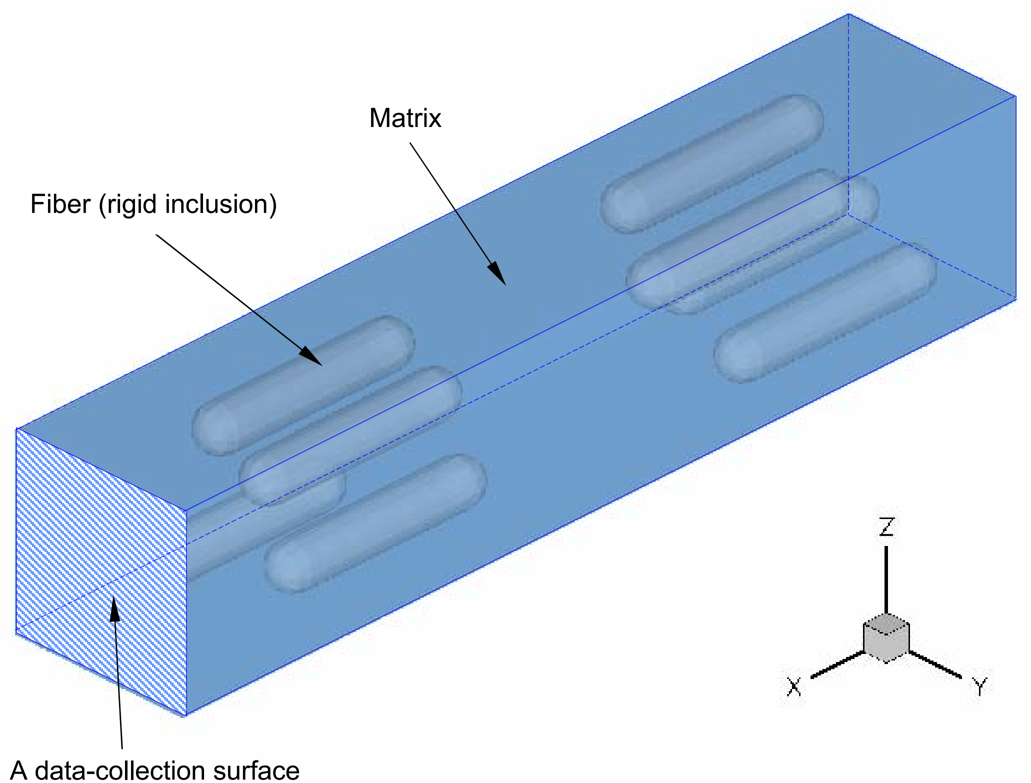
Radial and tangential stresses obtained by a BEM model with 120 elements

A Rigid Sphere in Elastic Medium (Cont.)

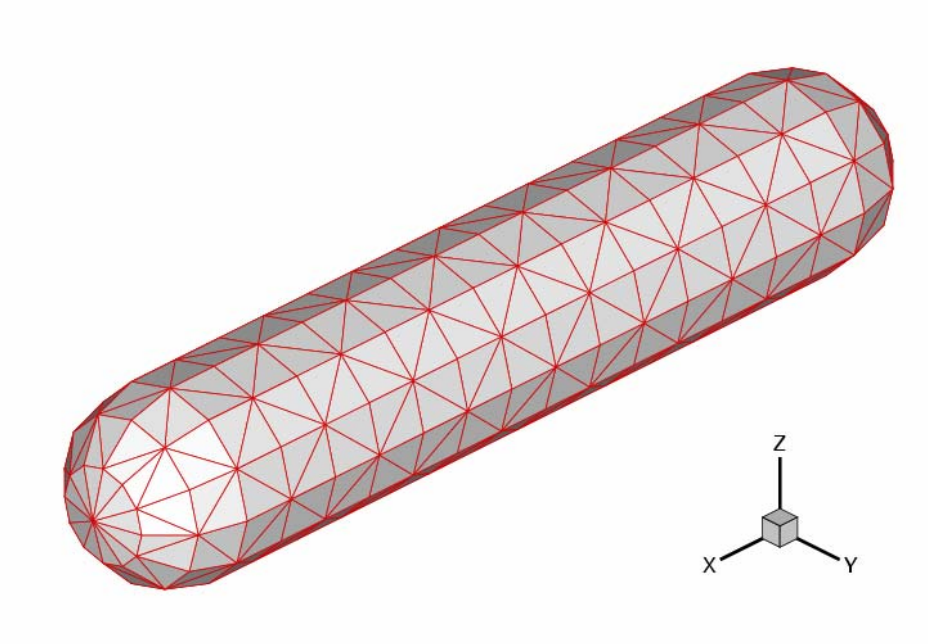


Contour plot for stress on the surface of the sphere

Study of Fiber-Reinforced Composites: The Representative Volume Element (RVE)

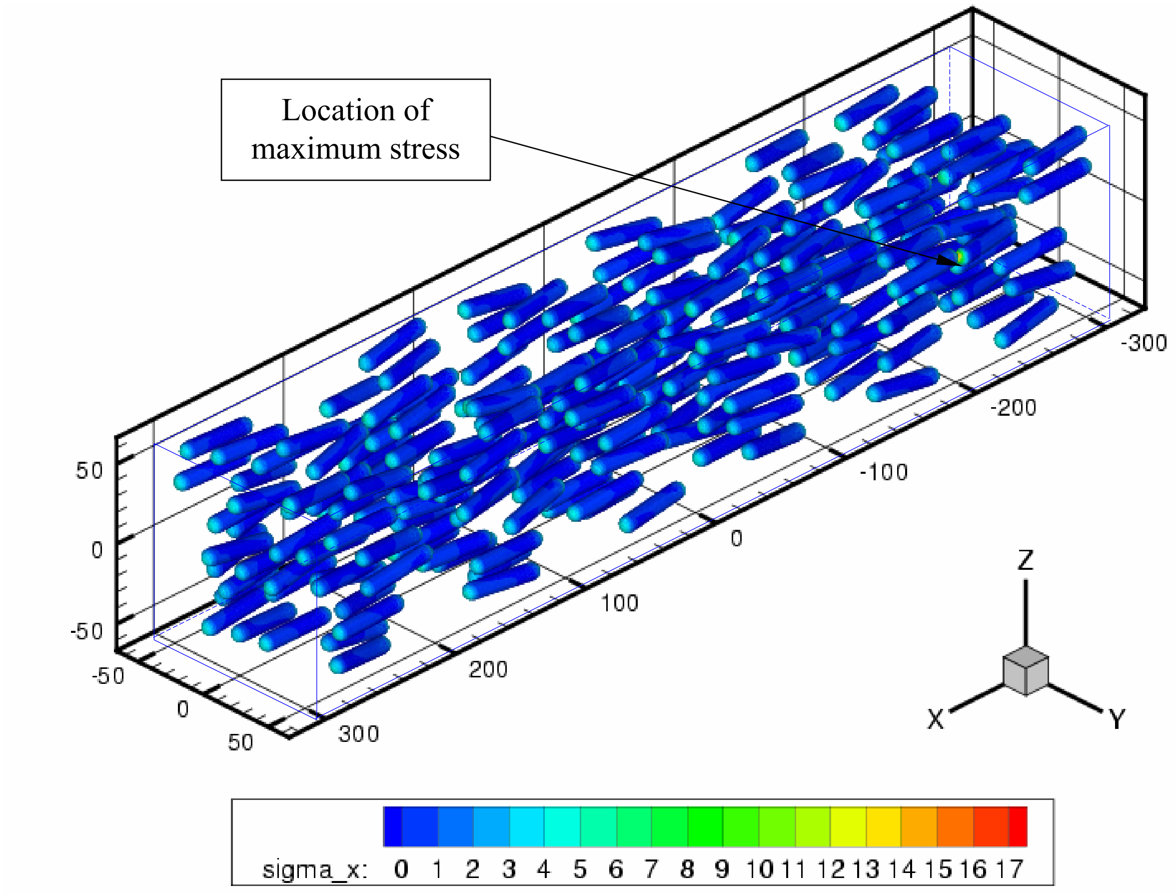


A BEM Mesh



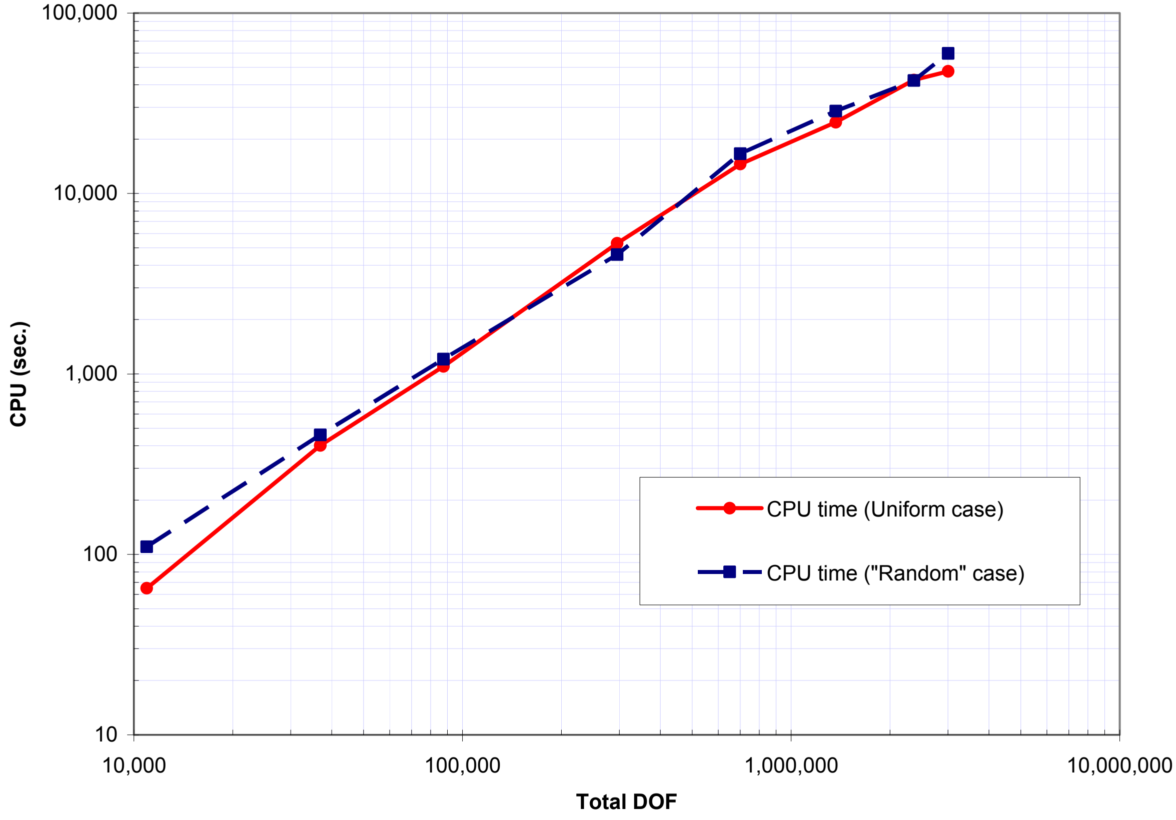
A BEM mesh used for the short fiber inclusion (with 456 constant elements)

Load Transfer Studies



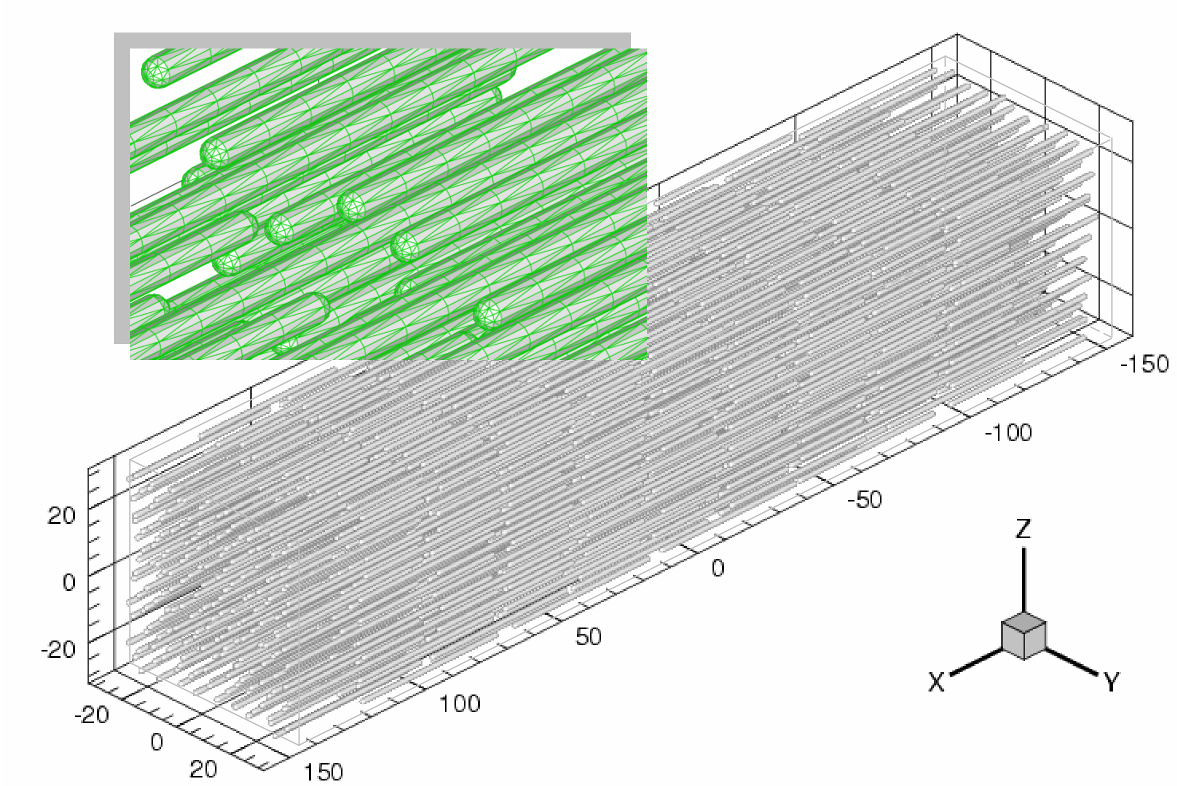
A model with 216 “randomly” distributed and oriented short fibers

Efficiency of the Fast Multipole BEM



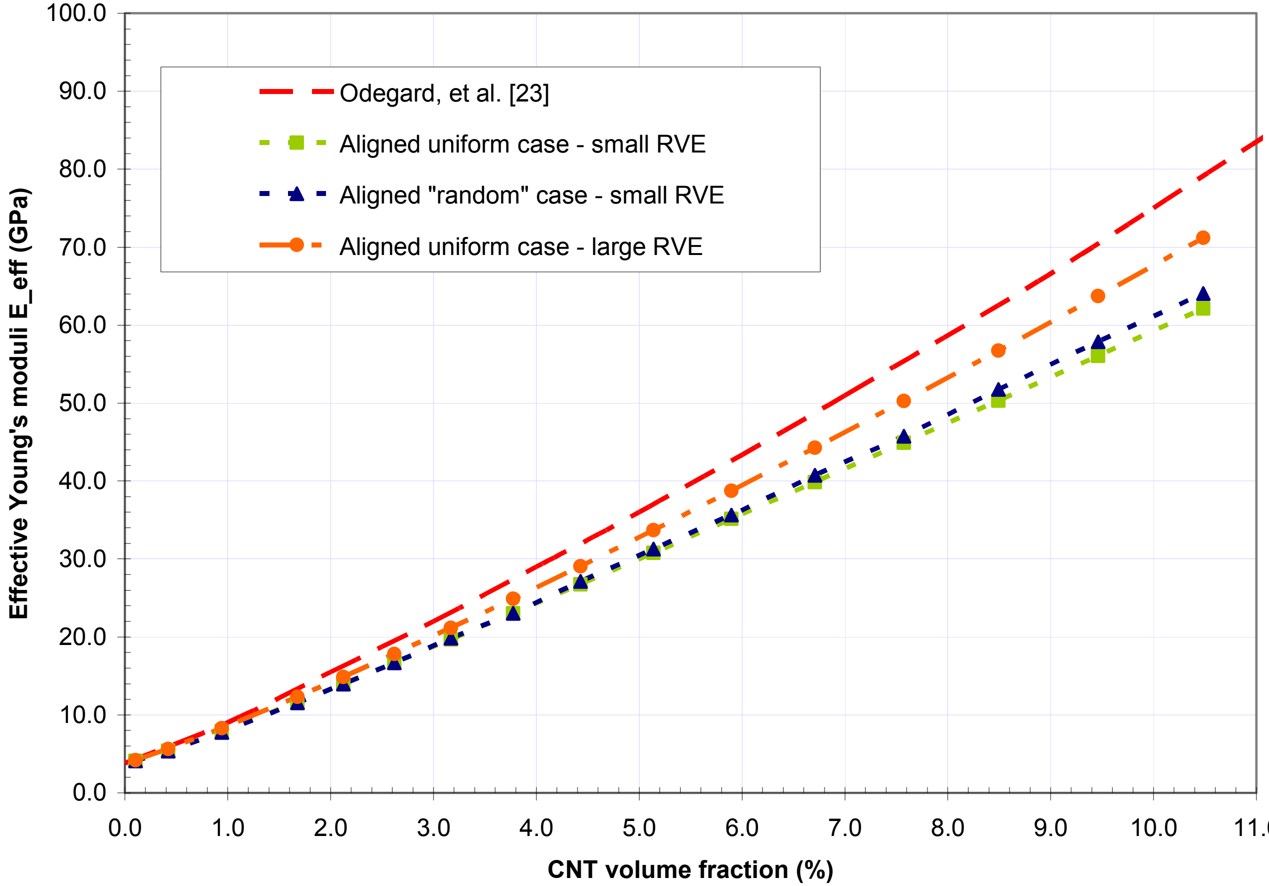
CPU time used for solving the BEM models for the short-fiber cases

Modeling of CNT-Based Composites (Cont.)



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.)



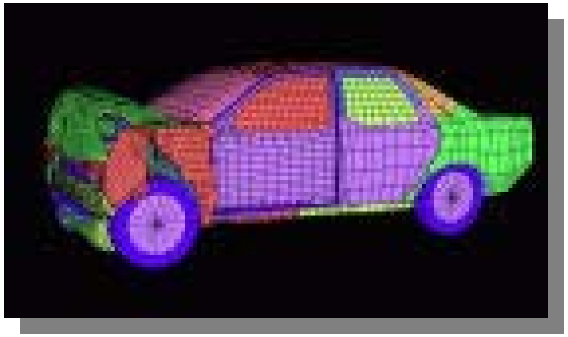
Computed effective moduli of CNT/polymer composites using three RVEs and compared with NASA's multi-scale results

Discussions

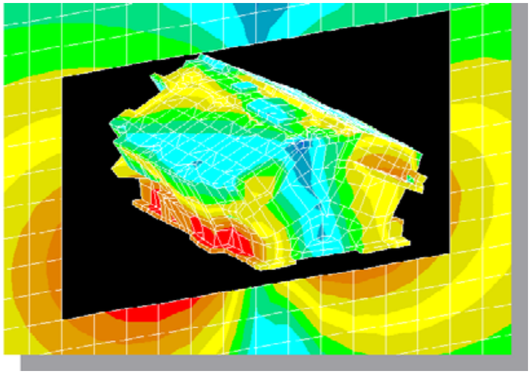
- BEM is a very efficient numerical tool for many problems in engineering
- Computational mechanics can play a significant role in the development of composite materials
- Multi-scale, multiphysics and large-scale approaches are urgently needed for the development of new materials
- There are plenty 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

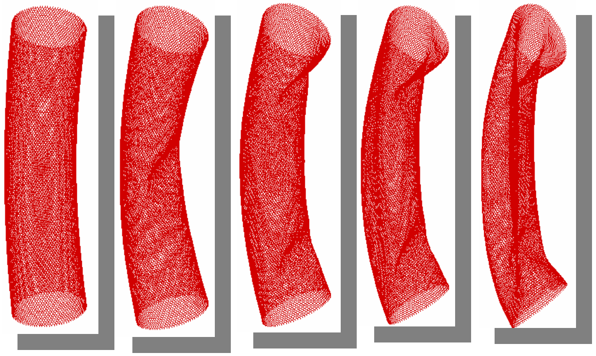
FEM: Large-scale structural, nonlinear, and transient problems



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



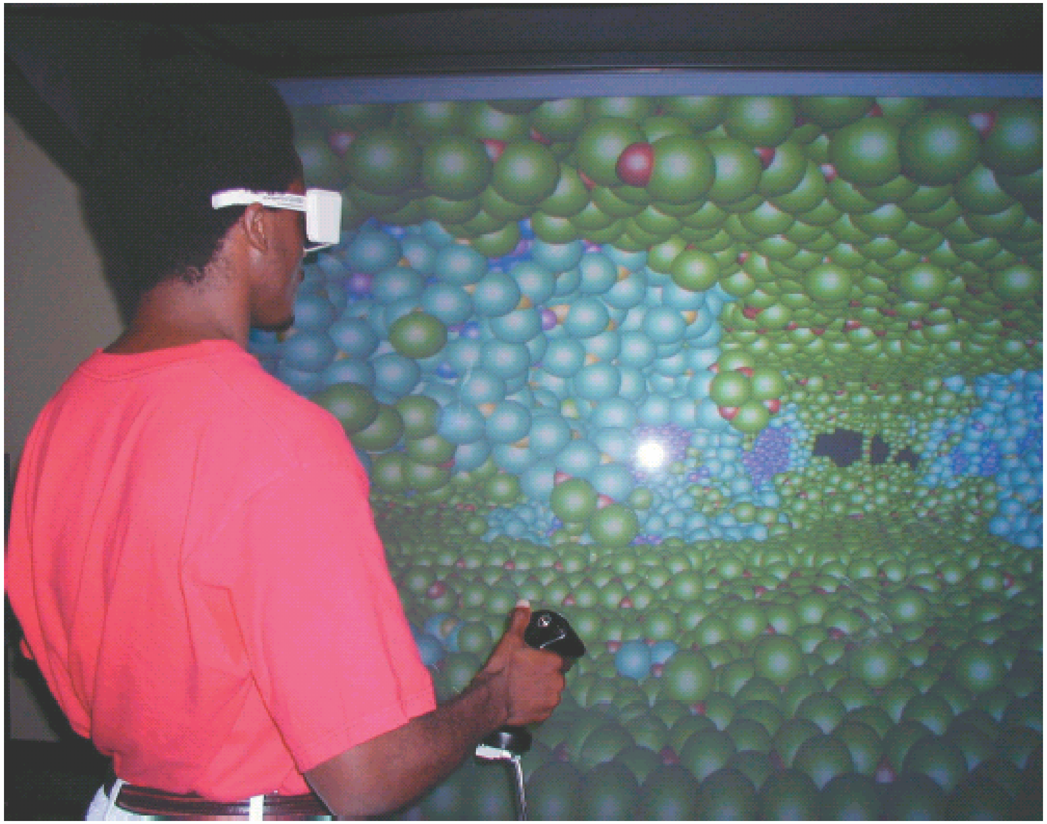
Meshfree: Large deformation, fracture and moving boundary problems



"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)

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(on BIE/BEM)

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