Title: Fast calculation of electro thermo static and elasticity fields in 3D-medium with isolated inclusions using application of Gaussian approximating functions

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Abstract: <span>The problem of calculation of electro and thermo static fields in an infinite homogeneous medium with a heterogeneous isolated inclusion (Kanaun et al) has shown to be reduced to the solution of integral equations for the fields inside the inclusion using Gaussian functions (V. Mazya) for the approximation of the unknown fields. Using this approach coefficients of the matrix of the discretized system will be obtained in closed analytical forms. Only information necessary to carry out the method is the coordinates of the centers of the Gaussian functions (nodes) in the region occupied by the inclusion ie. a mesh-free method. Using a regular grid of nodes the matrix of the discretized problem will have a Teoplitzs structure. Hence Fast Fourier Transform (FFT) technique can be used for the calculation of the matrix-vector products within an iterative solution of the system of linear algebraic equations of the discretized problem. The proposed algorithm is simple fast and does not require much computer memory. In practice this has led to over ten folds reduction in the required computational time and the allocated memory space and enabling consideration of very fine grids not possible with other tried solution methods. Comparisons of the numerical and exact solutions for electrostatic fields inside spherical inclusions with step changing properties are presented here. Second boundary value problem of elasticity for 3D-bodies with cracks is another problem where this approach has been applied successfully. References:S. Kanaun and S. Babaii A numerical method for the solution of thermo and electro static problems for a medium with isolated inclusions Journal of Computational Physics 192 471-493 (2003).V. Mazya Approximate approximation in The Mathematics of Finite Elements and Applications. highlights 1993 edited by J.R. Whitman 77 Wiley Chichester (1994).S. Kanaun A. Markov and S. Babaii An efficient numerical method for the solution of the second boundary value problem of elasticity for 3D- bodies with cracks Int J Fract DOI 10.1007/s10704-013-9885-5

Fast Calculation of Electro, Thermo Static and Elasticity Fields in 3D-medium with an Isolated Heterogeneous Inclusion using Gaussian Approximating Functions

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Heterogeneous Materials

- Matrix composites that consist of a homogeneous matrix and set of isolated inclusions.
  - Micro/Nano-composite polymers
  - Metal/Ceramic composites

- Cellular carbon/metallic/ceramic foam materials where each unit cell is an isolated inclusion in a homogeneous background medium (matrix).

- Human bones.
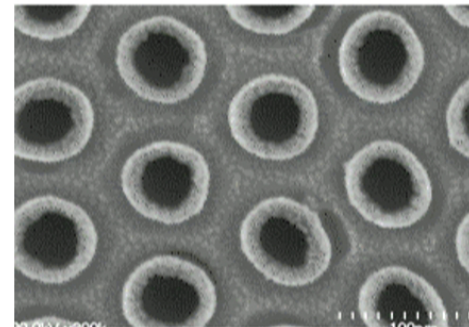
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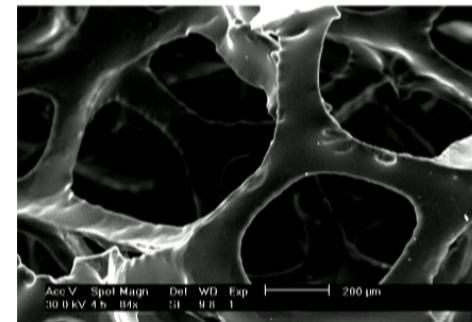
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Heterogeneous Materials

- 3D printed components of variety and mixed internal wall constructions, densities and sizes.

Image shows sample coupons, printed using extensive 3D printing facilities of CAMDT at Sheridan College, Davis Campus.

CAMDT: Center for Advanced Manufacturing and Design Technologies

The Challenge

- **Problem:**

  The problem of calculation of physical fields in heterogeneous materials has many engineering applications. An important class of such materials is matrix composites that consist of a homogeneous matrix and a set of isolated inclusions.

- **Challenge:**

  Traditional FEA requires tens of thousands if not millions of beam elements to model even a small sample of the foam material.
  Computational times are inhibitive if not impossible.

Quasicrystalline Approximation

- Heterogeneous cells are regarded as **isolated inclusions** subject to External Fields.

- Effective Field Method (EFM) is applied to reduce the problem to a **one particle problem.**

Google images

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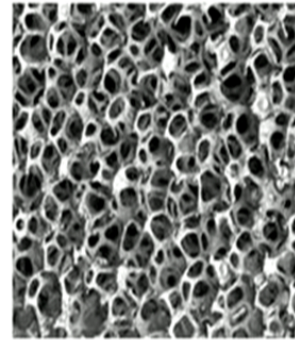
Modelling approach

$$\varphi(x) = \frac{1}{(\pi H)^{3/2}} \exp\left(-\frac{|x|^2}{Hh^2}\right)$$

Gaussian approximating functions (V. Maz'ya,1994) are proposed for the approximation of the fields inside the inclusions.

Gaussian Approximating Function

1. The action of the integral operator of the problem on such functions has a simple analytical form.

2. The method is in fact **"mesh-free".** The initial information required for carrying out the method is only the coordinates of the nodes inside the region occupied by the inclusions.

3. The final matrix of the linear algebraic system of equations is non-sparse and high dimensions for 3D problems. **High Computational Costs!**

Solution Method

Fast matrix-vector product algorithms had to be implemented.

Fast Algorithms

Fourier Transform Technique

Using a regular grid of the nodes:

- The matrix of the discretized problem can be arranged to have the **Toeplitz** (Constant Diagonal) structure.

- Fast matrix-vector product algorithm is possible with **Fourier Transform** in Conjugate Gradient iterative solver .

Applications: Published Case Studies

1. **A numerical method for the solution of thermo- and electro-static problems for a medium with isolated inclusions**.

   (Direct LU decomposition solver),

   Journal of Computational Physics, 2003

2. **A numerical method for the solution of 3D-integral equations of electro-static theory based on Gaussian approximating functions.**

   (Iterative Conjugate Gradient solver with Multipole Expansion method for matrix-vector product),

   Applied Mathematics and Computation, 2006

Applications: Published Case Studies

3. **Effective conductive and dielectric properties of matrix composites with inclusions of arbitrary shapes.**

   (Toeplitz matrix using Fourier Transform Techniques for Matrix-vector product),

   I. J. Engineering Science, 2007

4. **Effective properties of matrix composites with non-ellipsoidal inclusions.**

   (Fourier Transform Techniques),

   Continuum Models and Discrete Systems (CMDS 11), 2007

Applications: Published Case Studies

5. **An efficient numerical method for the solution of the second boundary value problem of elasticity for 3D-bodies with cracks.**
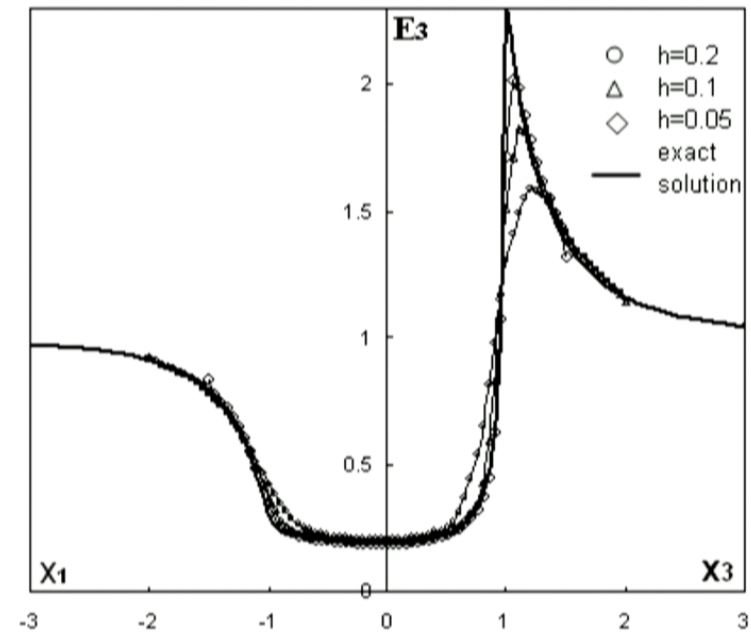
   (Toeplitz structure using Fourier Transform Techniques),

   I. J. Fracture, 20013

Results of Numerical Analysis

Unit radius spherical inclusion with
Parabolic distribution of dielectric properties along its radius.

- h=0.2 is achieved using direct methods (time = 1hr). Matrix size: 3'993 x 3'993

- h=0.1 is using FMM (time =45 min). Matrix size: 27'783 x 27'783

- h=0.05 is using FT method (time= 10 min). Matrix size: 206'763 x 206'763
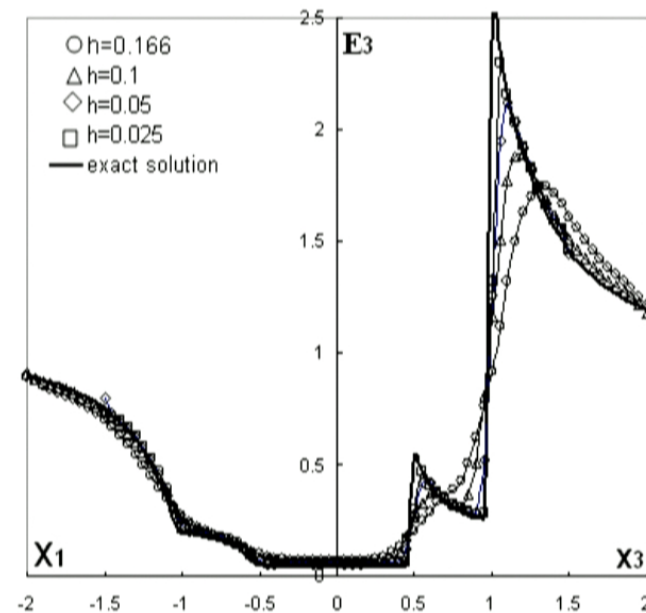

LU decomposition for Direct method.
FMM is implementation of the Multipole expansion method.
FT stands for Fourier Transform technique together with TOEPLITZ matrix.

Results of Numerical Analysis

Unit radius spherical inclusion with
Stepwise distribution of dielectric properties along its radius.

- h=0.166 is achieved using direct method (time = 1hr). Matrix size: 6'591 x 6'591

- h=0.1 is achieved using FMM (time =45 min). Matrix size: 27'783 x 27'783

- h=0.05 , h=0.025 is using FTT method (time= 10-15 min).
  Matrix size: 206'763 x 206'763
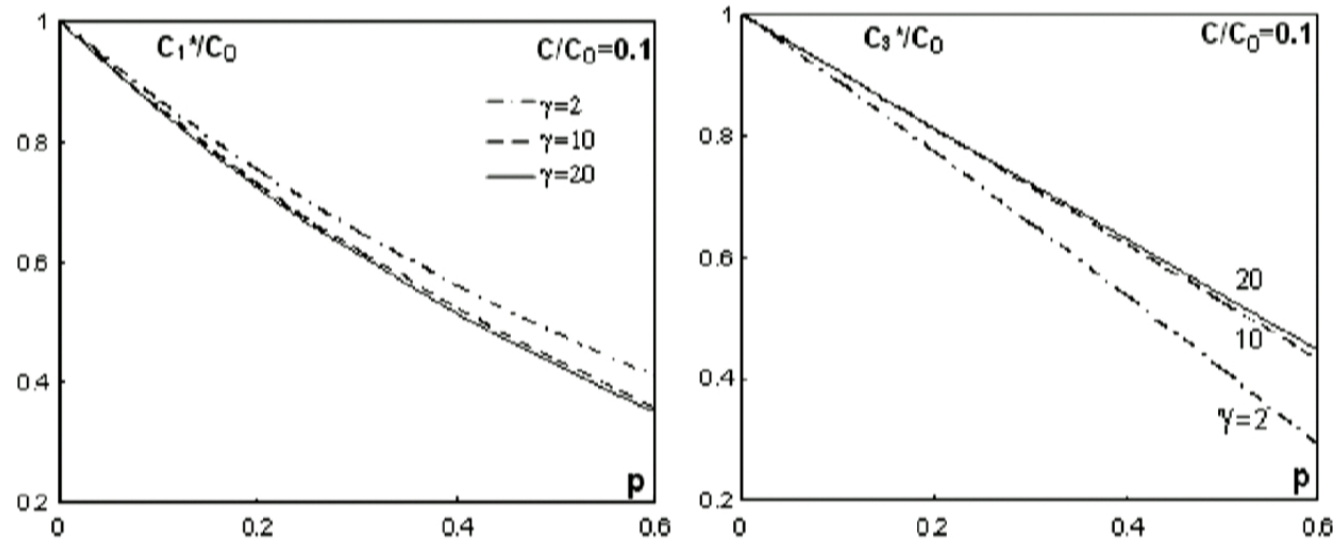 Matrix size: 531'441 x 531'443

LU decomposition for Direct method.
FMM is implementation of the Multipole expansion method.
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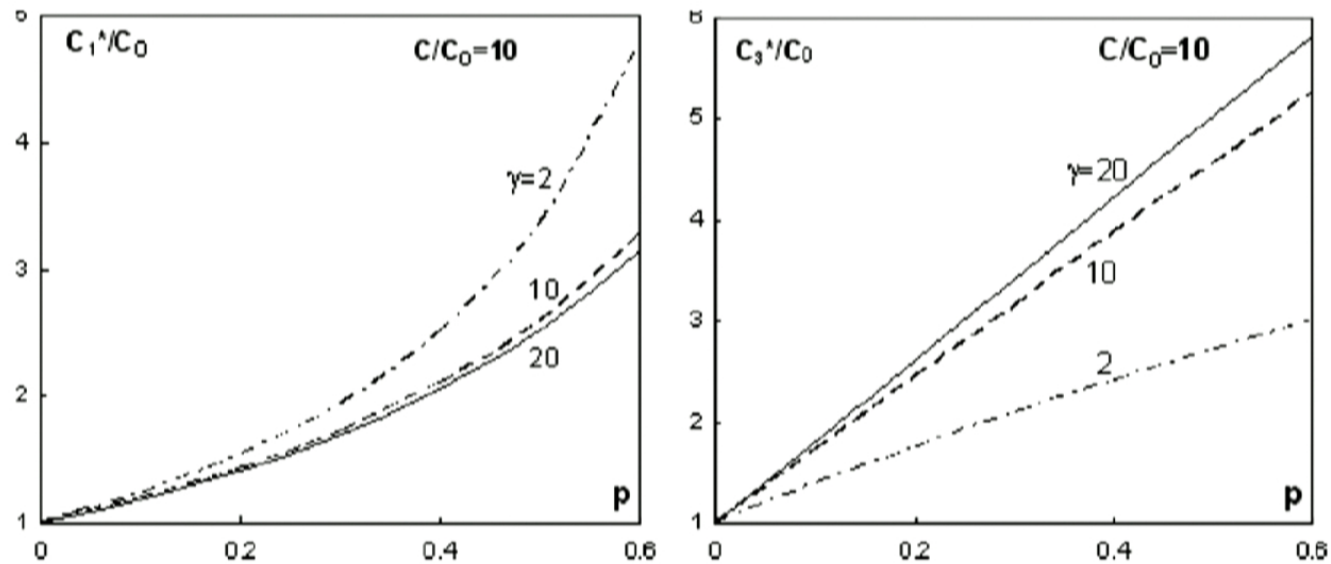
Results of Numerical Analysis

Cylindrical inclusions with property c in background medium c_0 with same orientation.

The graphs of the coefficients $c_1^*(p, \gamma)$ and $c_3^*(p, \gamma)$, where (p, γ) are inclusion volume fraction and cylinder aspect ratio respectively.

Results of Numerical Analysis

Cylindrical inclusions with property c in background medium c_0 with same orientation.
The graphs of the coefficients $c_1^*(p,\gamma)$ and $c_3^*(p,\gamma)$, where (p,γ) are inclusion volume fraction and cylinder aspect ratio respectively.

Results of Numerical Analysis

The graphs of the coefficients $c^*(p, \gamma)$ of heterogeneous cylindrical inclusions randomly but uniformly distributed over the orientations, the composite material is macro-isotropic. p and γ have their usual meanings.
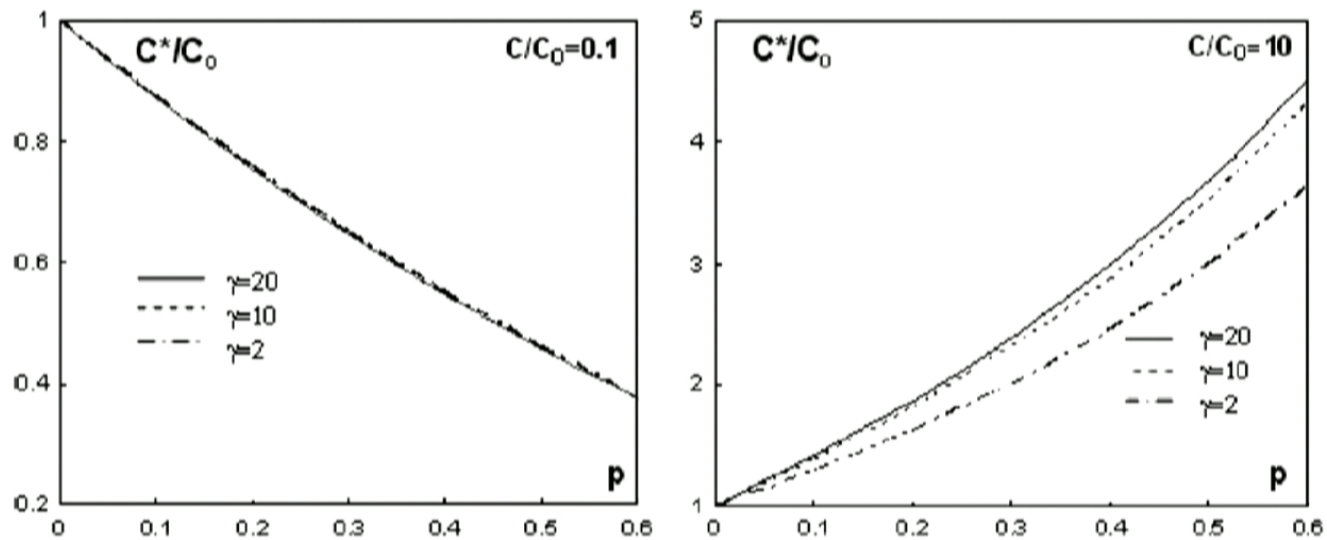
Outlook

1. Application to Elastic, Elasto-Plastic and viscoelastic problems.

2. Reliable approximation of material properties of 3D printed structures with mixed through thickness structures.

3. Reliable bone models for better assessment of the extent of human injuries in crash computational simulation models.

THANK YOU