Application of Domain Decomposition Methods in Micromechanics

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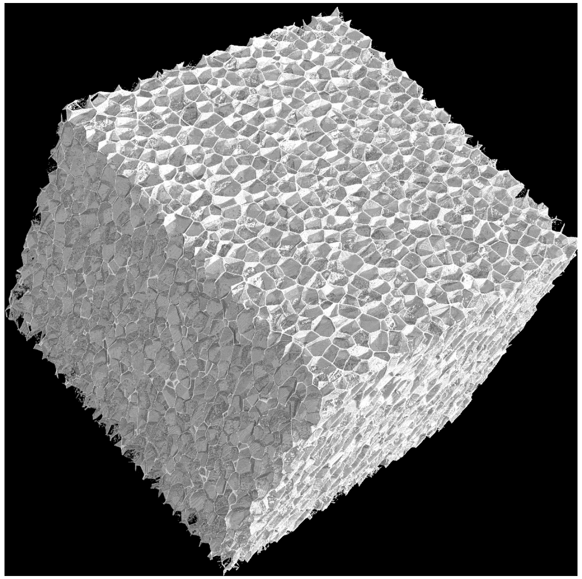
Overview

1. Introduction to Micromechanics and Virtual Material Design
2. Effective Thermal Conductivity of Composite Materials - Explicit Jump Immersed Interface Method (EJIIM)
3. Effective Elastic Behavior of Porous Media – DDFEM (parallel, hierarchical shape functions, variant of all-floating FETI)

1. Introduction: Classification of Inhomogeneous Materials

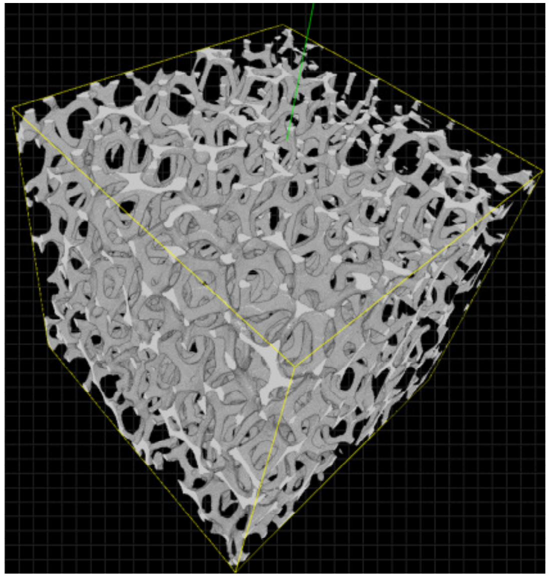
Matrix inclusion arrangements



Only matrix shows connected topology.

- Closed cell foams
- Nonwovens
- Most composite materials

Interwoven phase arrangements



The phases are not distinguishable topologically.

1. Open cell foams
2. Granular materials

Porous and cellular materials can be treated as inhomogeneous materials in which one constituent has zero stiffness or conductivity.

1. Introduction: Problem Formulation

Given:

1. Mechanical properties of the single phases of inhomogeneous materials
2. Geometrical microstructural parameters (pore size, porosity) of inhomogeneous materials

Find:

1. Macroscopic mechanical behaviour of the structures made of the inhomogeneous material
2. Relation, which describes the macroscopic material parameters as function of the given parameters of the phases and the geometry

Application:

Virtual material design and material optimization

1. Introduction: Virtual Material Design

Macroscopic Properties

- Effective thermal conductivity (Poisson)
- Permeability (Stokes)
- Tortuosity (Poisson)
- Effective elastic coeff. (Elasticity)
- Thermal characteristic length
- Viscous characteristic length

→

Application

- Thermal insulating materials
- Bending and compression stiffness
- Acoustic absorption and impedance
  (Biot Parameter)
- Filtration of particles

1. Introduction:
Micromechanically Based Multiscale Models

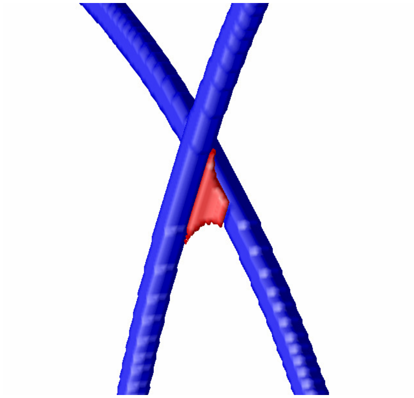
The full resolution of the microstructure in the whole macroscopic component is not possible.

Modeling of complex material behavior can be simplified by introducing 2 or 3 scales:

Microscopic Level << Mesoscopic Level << Macroscopic Level

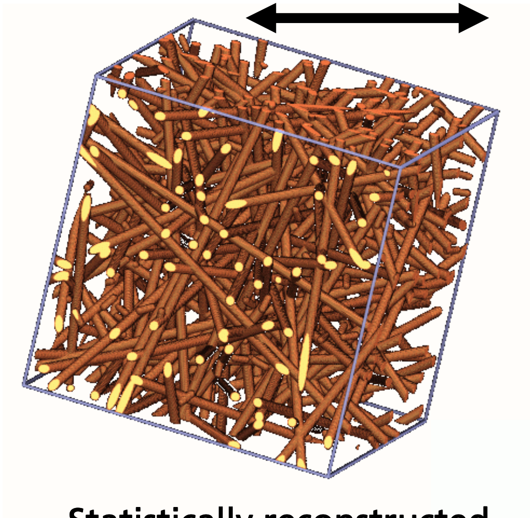
(Hashin, 1983)

10 µm



Detail of the binder distribution between two crossing fibres

1 mm



Statistically reconstructed microstructures

1 m

Glasswool plates

Micromechanically based constitutive models have a clear physical basis compared to semi-empirical models.

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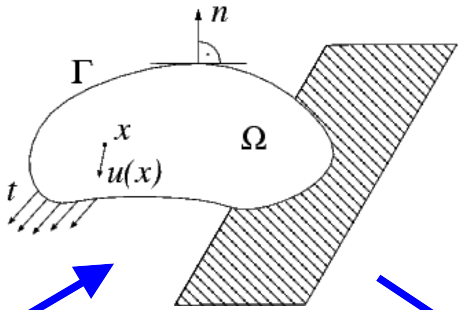
1. Introduction: Computational Homogenization

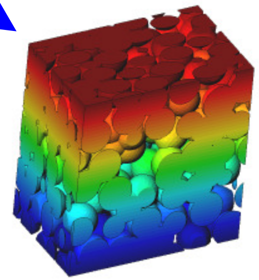
The (empirical) constitutive law for all points M is replaced by the following approach:

Standard FEM

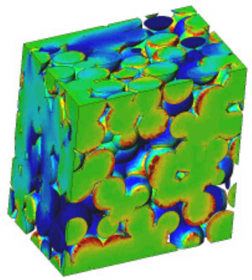


$\sigma(x), \mathbf{q}(x)$

$\varepsilon(\mathbf{x}), \nabla u(\mathbf{x})$



μFEM



Standard Homogenization:

global periodicity

Comp. Homogenization:

more realistic local periodicity

Nonlinear Case

- Fully coupled system
- Computationally expensive

Linear Case

- Computation of micro b.v.p. for all "basis functions" of discretized macro fields in advance

"M" macroscopic quantity

This technique does not require any constitutive assumption on the macrolevel.

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1. Introduction: Micromechanics - First-order Homogenization and Localization in Linear Elasticity

Microscale Variables:

$$\epsilon(\mathbf{x}) = \mathbf{A}(\mathbf{x})\langle\epsilon\rangle \quad \text{Strain}$$

$$\sigma(\mathbf{x}) = \mathbf{B}(\mathbf{x})\langle\sigma\rangle \quad \text{Stress}$$

Localization

Macroscopic Variables:

$$\langle\epsilon\rangle := \frac{1}{V}\int_{\mathbf{V}} \epsilon(\mathbf{x})\mathbf{dV} \quad \text{Strain}$$

$$\langle\sigma\rangle := \frac{1}{V}\int_{\mathbf{V}} \sigma(\mathbf{x})\mathbf{dV} \quad \text{Stress}$$

Homogenization

Effective stiffness tensor:

$$\langle\mathbf{E}(\mathbf{x}) : \epsilon(\mathbf{x})\rangle = \langle\sigma\rangle = \mathbf{E}^* : \langle\epsilon\rangle$$

Hooke

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1. Introduction: First-order Homogenization and Representative Volume Element (RVE)

A volume V which fulfills the following so-called Hill condition (under general boundary conditions) is called RVE

Microscopic Stored-Strain Energy W = Macroscopic Stored-Strain Energy

$$W = \frac{1}{2}\langle \epsilon(\mathbf{x}) : \mathbf{E}(\mathbf{x}) : \epsilon(\mathbf{x}) \rangle \overset{!}{=} \frac{1}{2}\langle \epsilon \rangle : \mathbf{E}^* : \langle \epsilon \rangle$$

i.e.

$$\langle \sigma(\mathbf{x}) : \epsilon(\mathbf{x}) \rangle \overset{!}{=} \langle \sigma \rangle : \langle \epsilon \rangle$$

Zero-averaged microstructural fluctuations:

$$\tilde{\sigma}(\mathbf{x}) := \sigma(\mathbf{x}) - \langle \sigma \rangle \qquad \tilde{\epsilon}(\mathbf{x}) = \epsilon(\mathbf{x}) - \langle \epsilon \rangle$$

$$\langle \tilde{\sigma} : \tilde{\epsilon} \rangle = 0$$

The Hill condition is used to compute the effective material tensor.

1. Introduction: First-Order Homogenization in Heat Conductivity

Homogenization

Macroscopic Variables:

$$\langle \nabla u \rangle := \frac{1}{V} \int_V \nabla u(\mathbf{x}) \mathbf{dV}$$ Temperature Gradient

$$\langle \mathbf{q} \rangle := \frac{1}{V} \int_{\mathbf{V}} \mathbf{q}(\mathbf{x}) \mathbf{dV}$$ Heat Flux

Effective heat conductivity tensor:

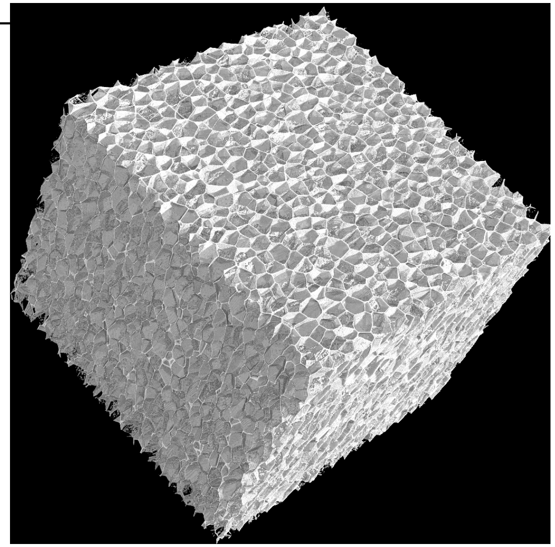
$$\langle \mathbf{q} \rangle = -\beta^* \langle \nabla u \rangle$$ Fourier Law

Hill Condition:

$$\langle \nabla u(\mathbf{x}) \cdot \beta(\mathbf{x}) \cdot \nabla u(\mathbf{x}) \rangle \stackrel{!}{=} \langle \nabla u \rangle \cdot \beta^* \cdot \langle \nabla u \rangle$$

The Hill condition is used to compute the effective material tensor.

1. Introduction:
RVEs from 3D images – "Real structure" models

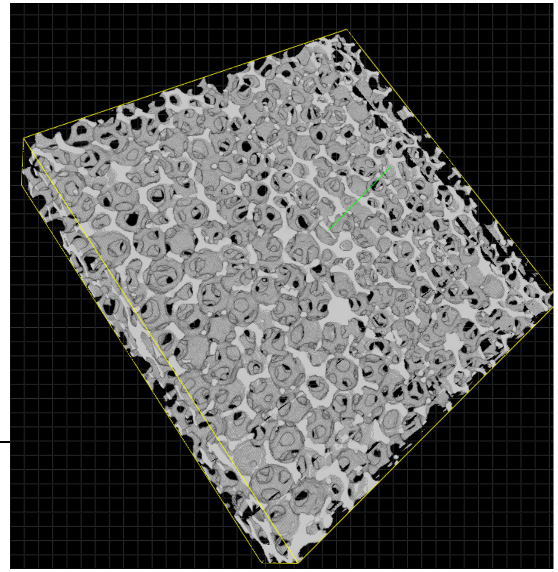


1. Selection of a sufficient large part of the 3D image (CT image)

2. Application of image processing techniques

3. Computation of 6 standard mechanical load cases (3 thermal load cases) to obtain the 4th order elastic stiffness tensor (the 2nd order heat conductivity tensor)

Repeat steps 1., 2., and 3. for further parts of the 3D image



Problems:

1. Errors in the 3D images lead to errors in the computed material constants.

2. Decomposition of different materials.

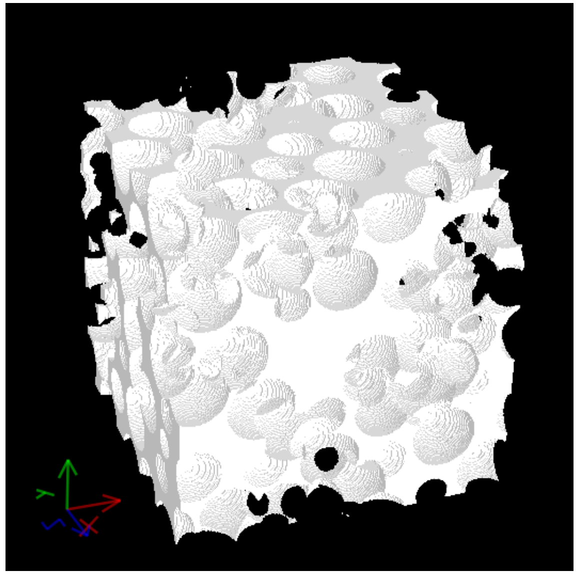
1. Introduction: Computer generated stochastic RVEs – Statistically reconstructed microstructures

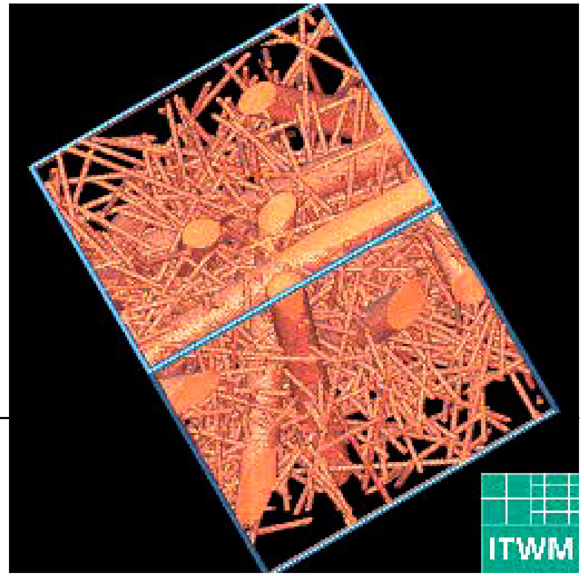
1. Determination of geometrical and statistical parameters of micro structure
   (fiber diameter, fiber cross section, fiber distribution)

2. Generation of the RVE in the computer by taking these parameters

3. Computation of 6 standard mechanical load cases (3 thermal load cases) to obtain the 4th order elastic stiffness tensor (the 2nd order heat conductivity tensor)

   Repeat steps 1., 2., and 3. for further computer generated stochastic RVEs





1. Introduction: Computer generated stochastic RVEs – reconstructed microstructures

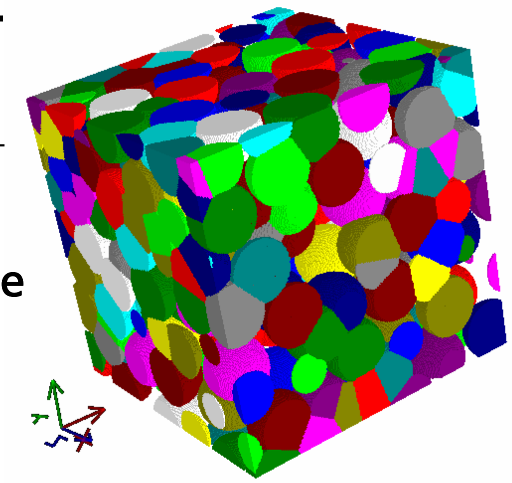
1. Determination of geometrical and statistical parameters of micro structure (fiber diameter, fiber cross section, fiber distribution)

2. Generation of the RVE in the computer by taking these parameters

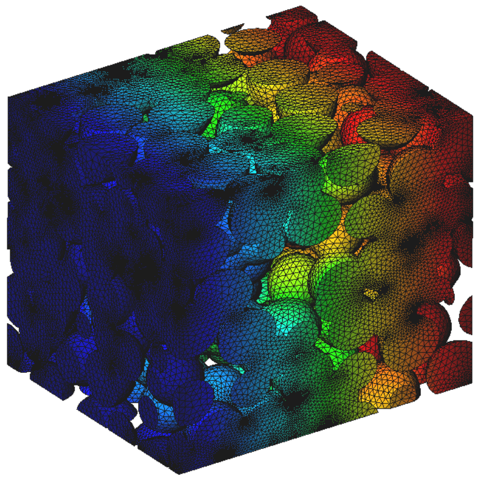
3. **Computation of 6 standard mechanical load cases (3 thermal load cases) to obtain the 4th order elastic stiffness tensor (the 2nd order heat conductivity tensor)**

   Repeat steps 1., 2., and 3. for further computer generated stochastic RVEs

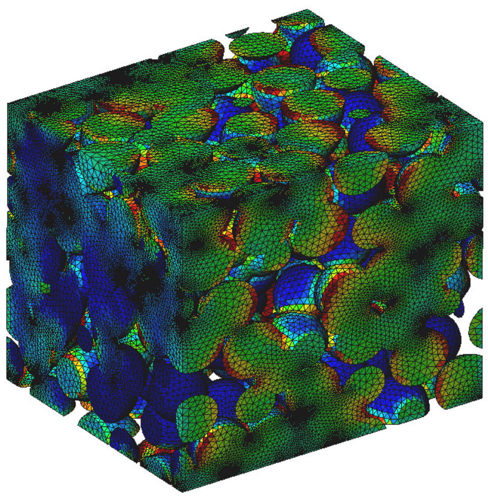
Stochastic Microstructure



Load



Stress



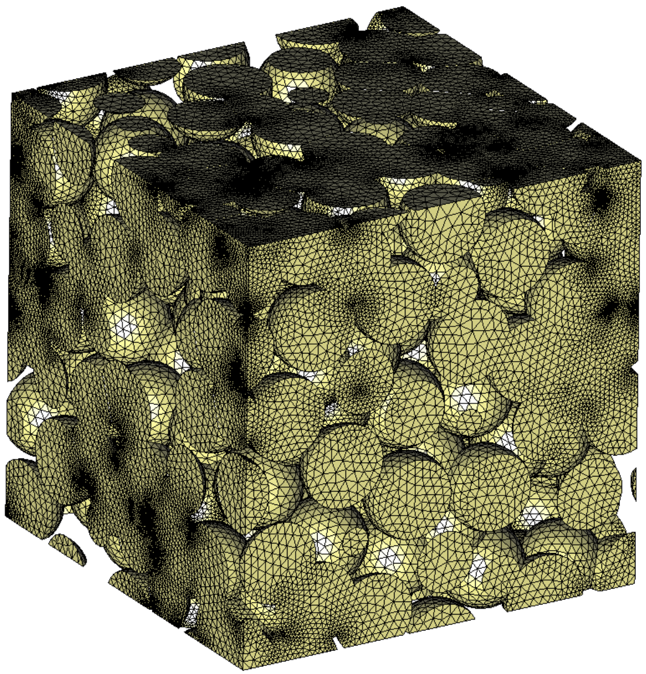
1. Introduction: FEM/FDM Approaches in Micromechanics

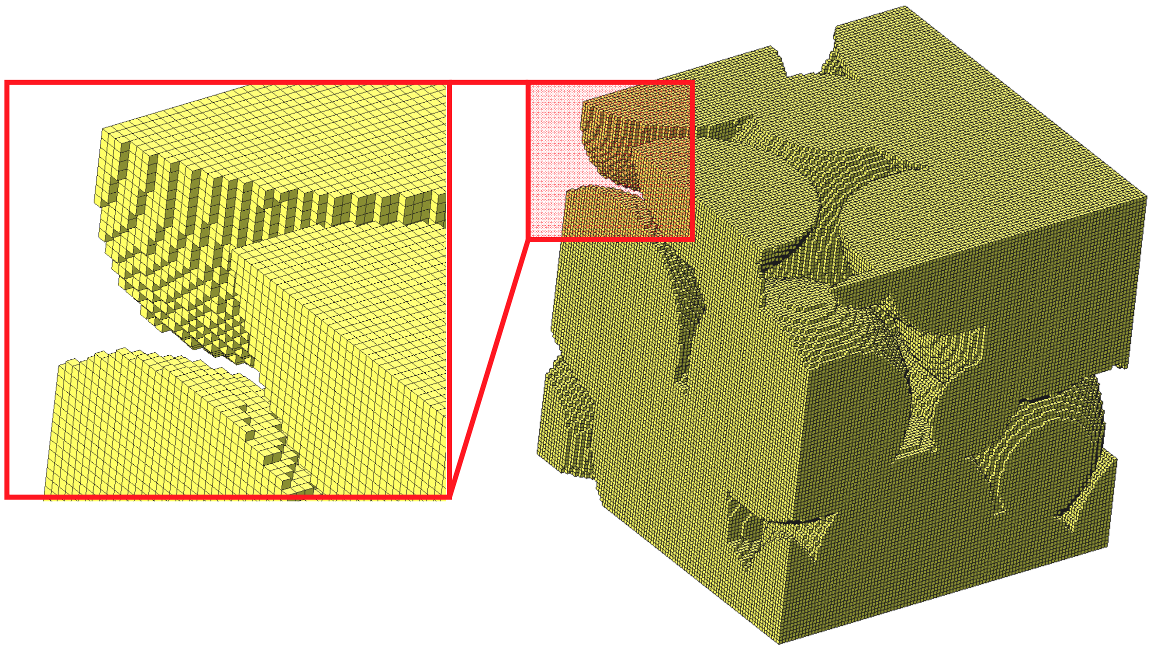
for the Computation of the Load Cases

FEM is the most popular numerical scheme for evaluating discrete microgeometries.

Discretization by standard finite elements

Voxel discretization (or also brick elements)





H.J. Böhm: "A Short Introduction to Continuum Micromechanics"(2004)

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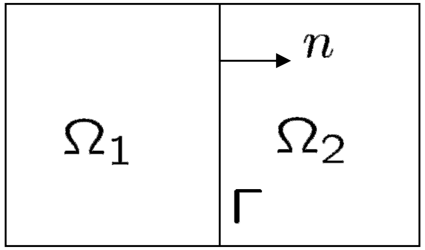
2. Effective Thermal Conductivity



Transmission problem with piecewise const. coefficients

$$
\begin{aligned}
-\nabla \cdot (\beta_i \nabla u_i) &= f && \text{in } \Omega_i \quad (i = 1, 2) \\
u_1 &= u_2 && \text{on } \Gamma \\
\beta_1 \frac{\partial u_1}{\partial n} &= \beta_2 \frac{\partial u_2}{\partial n} && \text{on } \Gamma
\end{aligned}
$$

and b.c.

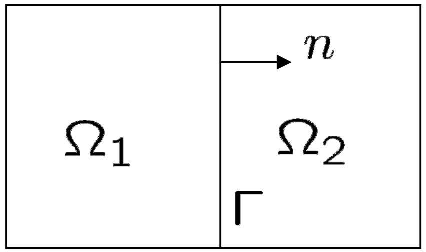
We introduce the jumps j as unknown variables:

$$j := \left[\frac{\partial u}{\partial n}\right] = \frac{\partial u_2}{\partial n} - \frac{\partial u_1}{\partial n}$$

$$
\begin{aligned}
-\nabla \cdot (\nabla u_i) &= \frac{f}{\beta_i} && \text{in } \Omega_i \quad (i = 1, 2) \\
u_1 &= u_2 && \text{on } \Gamma \\
j &= \left(\frac{\beta_1}{\beta_2} - 1\right) \frac{\partial u_1}{\partial n} && \text{on } \Gamma
\end{aligned}
$$

and b.c.

2. Effective Thermal Conductivity
Variational Formulation



Transmission problem with piecewise const. coefficients

Find $(u_1, u_2, j) \in \mathcal{U}_{ad}$ such that

$$\sum_{i=1}^{2} \int_{\Omega_i} \nabla u_i \cdot \nabla v_i dx + \int_\Gamma jw ds = \sum_{i=1}^{2} \int_{\Omega_i} \frac{f}{\beta_i} v_i dx + \int_{\Gamma_N} \frac{q}{\beta_i} v_i ds$$

$$\int_\Gamma (u_1 - u_2)\chi ds = 0$$

$$\int_\Gamma (S(u_2) - S(u_1) - j) w ds = 0$$

are satisfied for all test functions $(v_1, v_2, w, \chi) \in \mathcal{V}$.

S : Steklov-Poincaré operator (D-N map)

FE or FD discretization leads to:

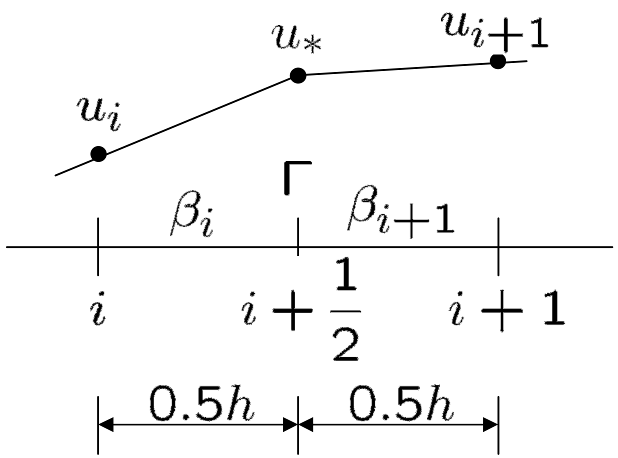
$$\begin{bmatrix} A & \Psi \\ D & H \end{bmatrix} \begin{bmatrix} U \\ J \end{bmatrix} = \begin{bmatrix} F_1 \\ F_2 \end{bmatrix}$$

$$\frac{\partial u_i}{\partial n} = S(u_i)$$

Hsiao, Schnack, Wendland and "Mixed Methods in Elasticity"

2. Effective Thermal Conductivity

- 1D case, first order FD approximation, equidistant mesh with parameter h



Discrete Steklov-Poincaré operator (D-N map) via extrapolation

$$J_i := [u_x]_{i+\frac{1}{2}} = \frac{u_{i+1} - u_*}{0.5h} - \frac{u_* - u_i}{0.5h}$$

$$\beta_i \frac{u_* - u_i}{0.5h} = \beta_{i+1} \frac{u_{i+1} - u_*}{0.5h}$$

(transmission condition)

$$\Rightarrow \quad J_i = 2 \frac{\beta_i - \beta_{i+1}}{\beta_i + \beta_{i+1}} \frac{u_{i+1} - u_i}{h}$$

$$-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \frac{J_i + J_{i-i}}{2h} = \frac{f_i}{\beta_i}$$

$$2\frac{\beta_{i+1} - \beta_i}{\beta_i + \beta_{i+1}} \frac{u_{i+1} - u_i}{h} + J_i = 0$$

$$\Longleftrightarrow \quad \begin{bmatrix} A & \Psi \\ D & I \end{bmatrix} \begin{pmatrix} U \\ J \end{pmatrix} = \begin{pmatrix} F_1 \\ 0 \end{pmatrix}.$$

β: piecewise constant

FD scheme is equivalent to standard FD scheme with harmonic averaging.

2. Effective Thermal Conductivity: EJIIM system for the computation of effective conductivity

Periodic boundary conditions lead to the system:

$$
\begin{aligned}
-\frac{u_{i+1} - 2u_i + u_{i-1}}{h^2} + \frac{J_i + J_{i-1}}{2h} &= \boxed{0} \\
2\frac{\beta_{i+1} - \beta_i}{\beta_{i+1} + \beta_i}\frac{u_{i+1} - u_i}{h} + J_i &= \boxed{-2\frac{\beta_{i+1} - \beta_i}{\beta_{i+1} + \beta_i}}
\end{aligned}
$$

This is an explicit jump (immersed interface method) system or EJIIM system in the case of periodic boundary conditions:

$$
\begin{bmatrix} A & \Psi \\ D & I \end{bmatrix} \begin{bmatrix} U \\ J \end{bmatrix} = \begin{bmatrix} 0 \\ F_2 \end{bmatrix}
$$

2. Effective Thermal Conductivity: Solution of EJIIM system, 3D Case, Voxel Mesh

$$\begin{bmatrix} A & \Psi \\ D & I \end{bmatrix} \begin{bmatrix} U \\ J \end{bmatrix} = \begin{bmatrix} 0 \\ F_2 \end{bmatrix}$$

A is the 7-point Laplacian with periodic boundary conditions, i.e. singular! The magic is:

$\sum DU = 0$ for all $U \in \mathbb{R}^n$, also $\sum F_2 = 0$. Thus $\sum J = 0 \Rightarrow \sum \Psi J = 0 \Rightarrow A^\dagger$, the FFT-based "inverse" on $\mathbb{R}^n \setminus \{\mathbf{x} \in \mathbb{R}^n : \sum \mathbf{x} = 0\}$ can be used.

$$\Longrightarrow \left(I + DA^\dagger \Psi\right) J = F_2$$

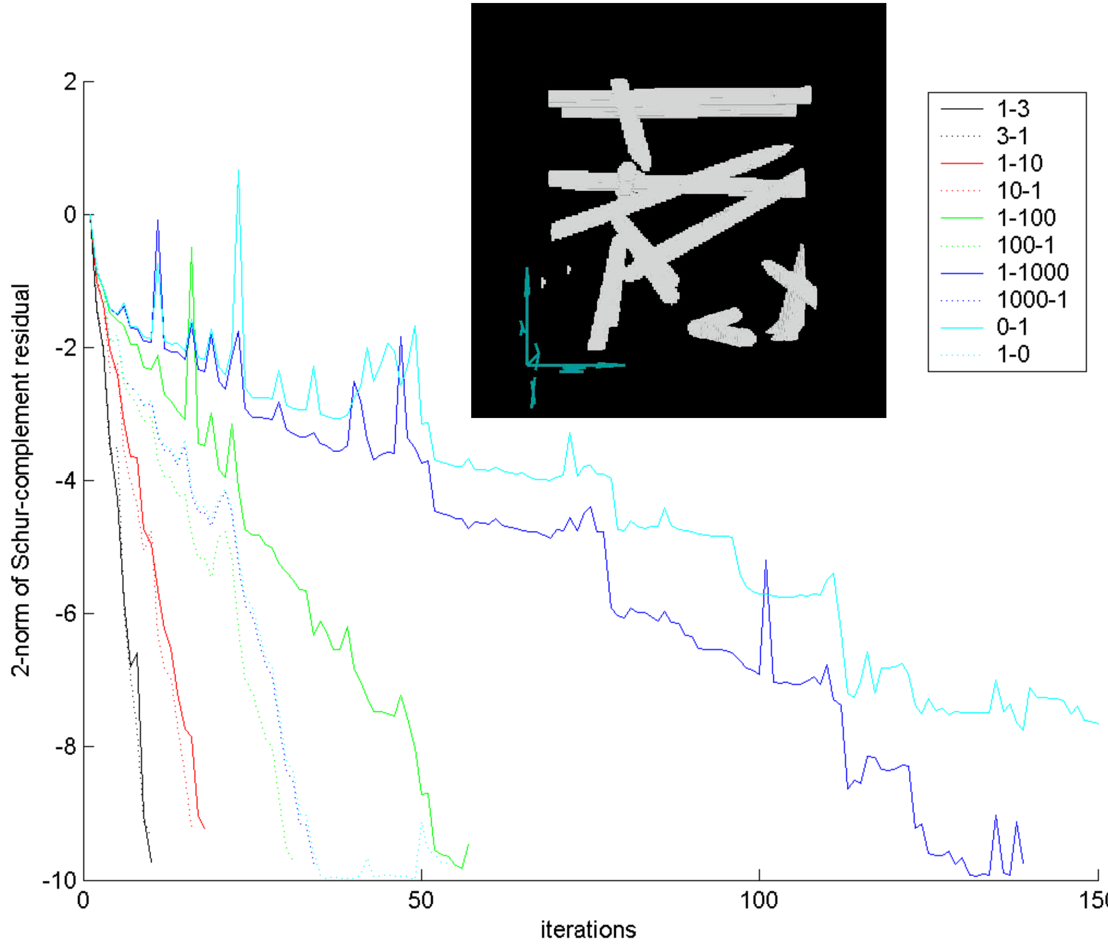
is a nonsymmetric regular linear system of equations on $\mathbb{R}^n \setminus \{\mathbf{x} \in \mathbb{R}^n : \sum \mathbf{x} = 0\}$.

Solve by BiCGStab. Matrix-vector multiplication is performed by applying operators, the "singular Schur-complement" is not formed.

2. Effective Thermal Conductivity:
Numerical Results: Composite Material with Long Fibers

128^3, 95% type 0, 5% type 1,
fibrous media,
required about 170MB RAM,
10 seconds / iteration

type	value	its
$0.\bar{3} : 1$	0.35	10
$0.1 : 1$	0.12	18
$0.01 : 1$	0.0185	57
$0.001 : 1$	0.0033	139
$0 : 1$	0.0	(*)150
$1 : 0.\bar{3}$	0.95	10
$1 : 0.1$	0.93	16
$1 : 0.01$	0.912	31
$1 : 0.001$	0.910	34
$1 : 0$	0.910	54



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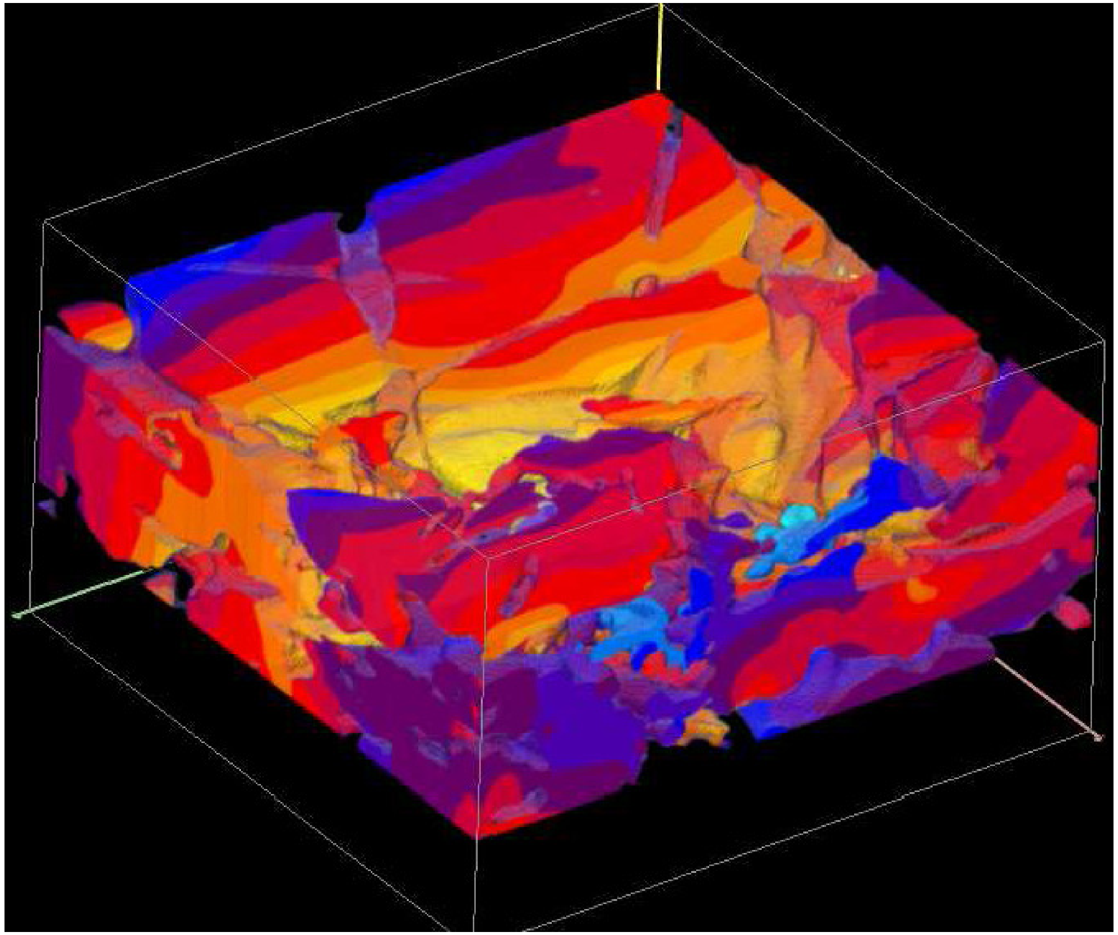
2. Effective Thermal Conductivity: Numerical Results for Real Life Problem

Temperature field in an industrial medium



~ 34.000.000 grid points

~ 2.600.000 jumps

3.5 GB memory

80 min CPU time

70 BiCGStab iterations

$$\varepsilon = 1.0E-8$$

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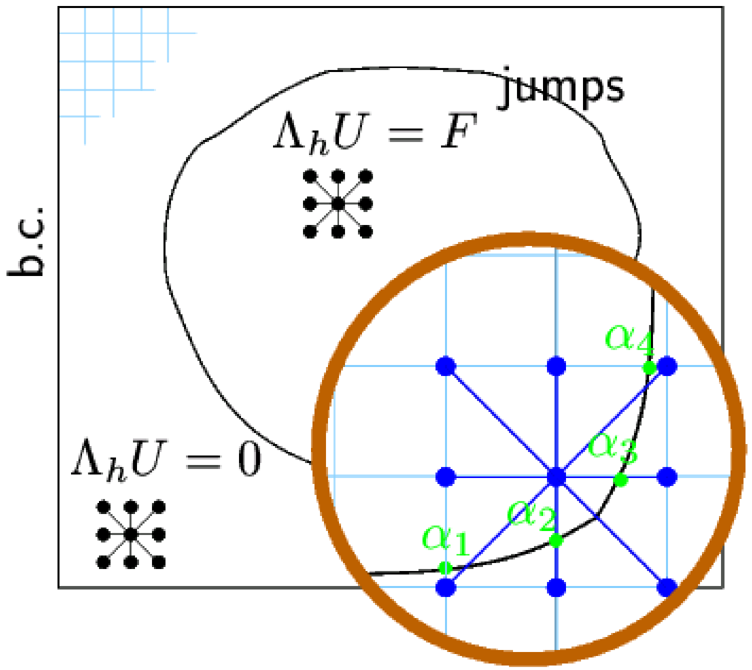
EJIIM Solver for Linear Elasticity (Second Order)



1. Embed the original domain in a "box". B.C.$\Rightarrow$ Jumps
2. Standard FD in the regular points

Irregular points:

$$\Lambda_h U + \text{correction} = F$$

$$\text{correction} = \sum_s \sum_{m=0}^{2} \psi_{m,s} [\partial^m u]_{\alpha_s}$$

Extrapolation + B.C. $\Rightarrow$

$$[\partial^m u]_{\alpha_s} = \tilde{F}_s - \sum_{i \in \text{grid}} d_{s,i} U_i$$

EJIIM system

$$\begin{pmatrix} \mathbf{A} & \mathbf{\Psi} \\ \mathbf{D} & \mathbf{I} \end{pmatrix} \begin{pmatrix} U \\ J \end{pmatrix} = \begin{pmatrix} F \\ \tilde{F} \end{pmatrix}$$

U	: grid function	J	: jumps
$\mathbf{A}$	: standard FD matrix	F	: extended rhs
$\mathbf{\Psi}$	: corrections	$\mathbf{I}$	: identity
$\mathbf{D}$, $\tilde{F}$	: extrapolation		

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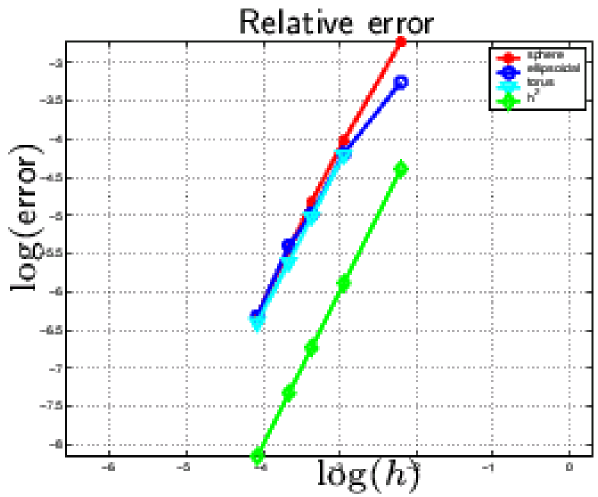
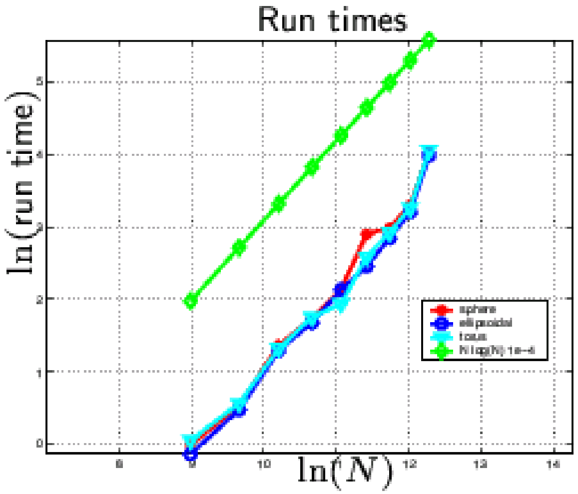
EJIIM Solver for Linear Elasticity (Second Order)

- is second order convergent w.r.t. the grid refinement in maximum norm





- takes $N \log N$ time

The concrete test problem:

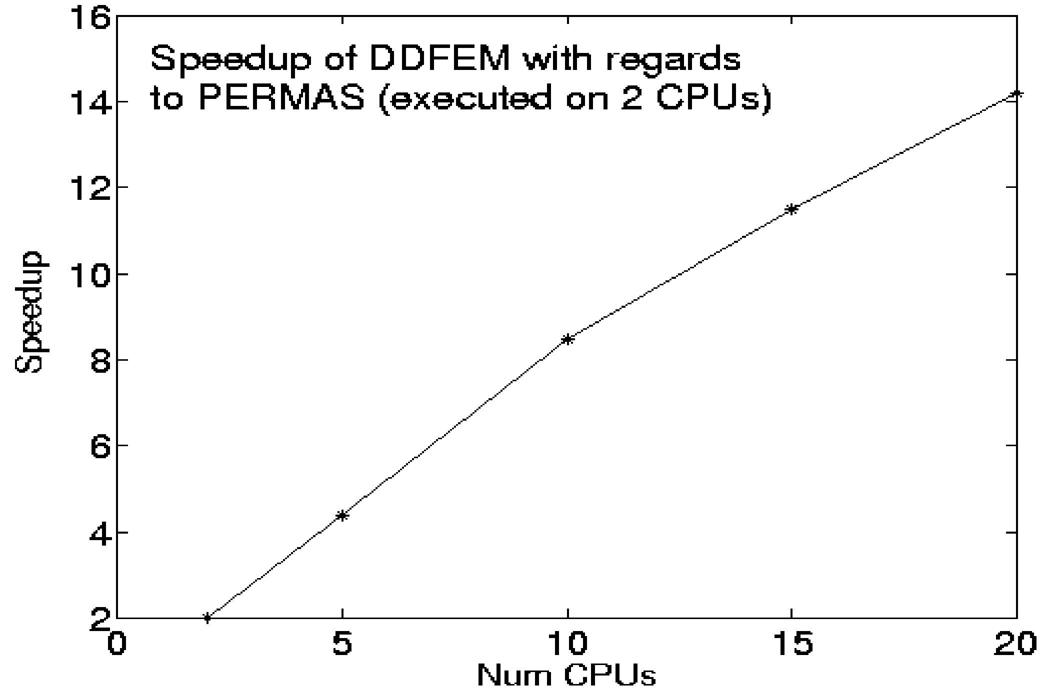
– three different geometries: sphere, ellipsoidal and torus

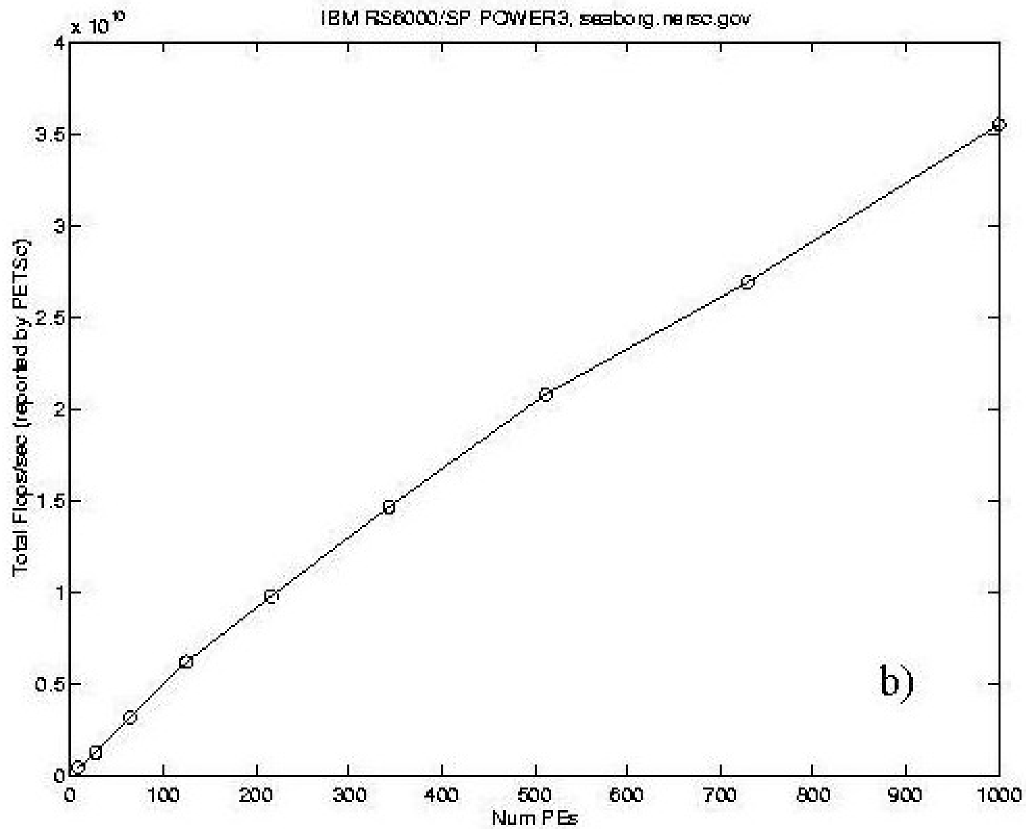
– Dirichlet boundary conditions, isotropic material

– exact solution: $u = e^x \sin(y) z^4$, $v = \frac{y^5 \cos(z)}{x+1}$, $w = \frac{\sqrt{x+1} e^z}{y^2+1}$

3. Effective Elastic Coefficients: FEM solver DDFEM

- Specialized parallel FEM code
- Hierarchical shape functions on tetrahedrons (for a-posteriori error estimation)
- Linear algebra routines from PETSc
- A-priori geometrical DD or use of METIS for a-posteriori geometrical decomposition
- Variant of all-floating FETI algorithm
- Developed for benchmarking parallel computers (*IPACS*)





DDFEM = Domain Decomposition Finite Element Method

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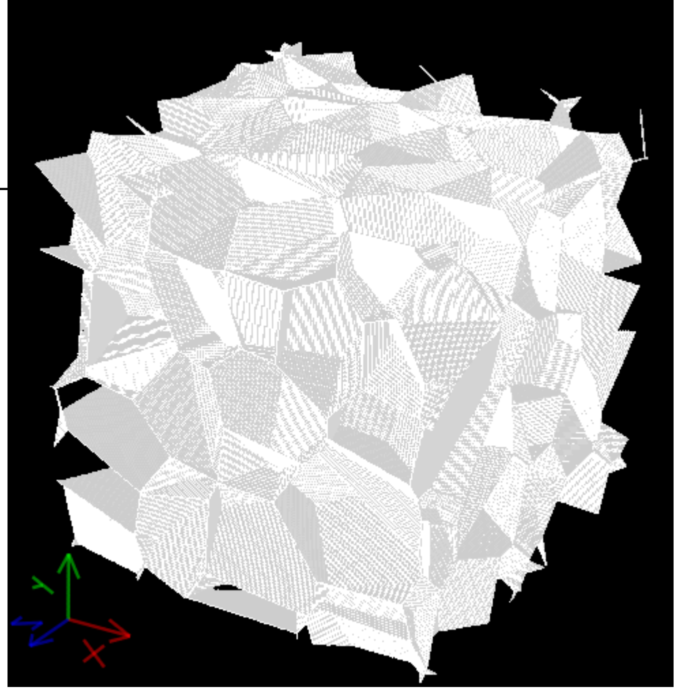
3. Effective Elastic Coefficients: Numerical results and Computational Effort

Name	Resolution	Porosity	SVF	Elements	CPU	Time
Foam_400	400X400X400	96,45%	3,55%	11.375.590	32	1:46
Foam_500	500X500X500	96,45%	3,55%	22.199.675	50	2:56
Foam_600	600X600X600	96,46%	3,54%	38.269.680	75	5:06

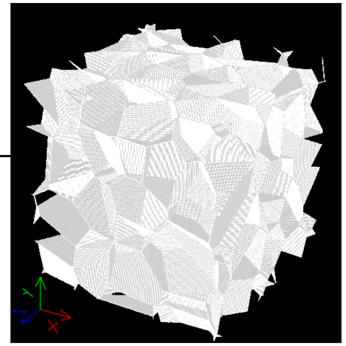


Statistically reconstructed closed-cell foam

6 load cases

DDFEM = Domain Decomposition Finite Element Method

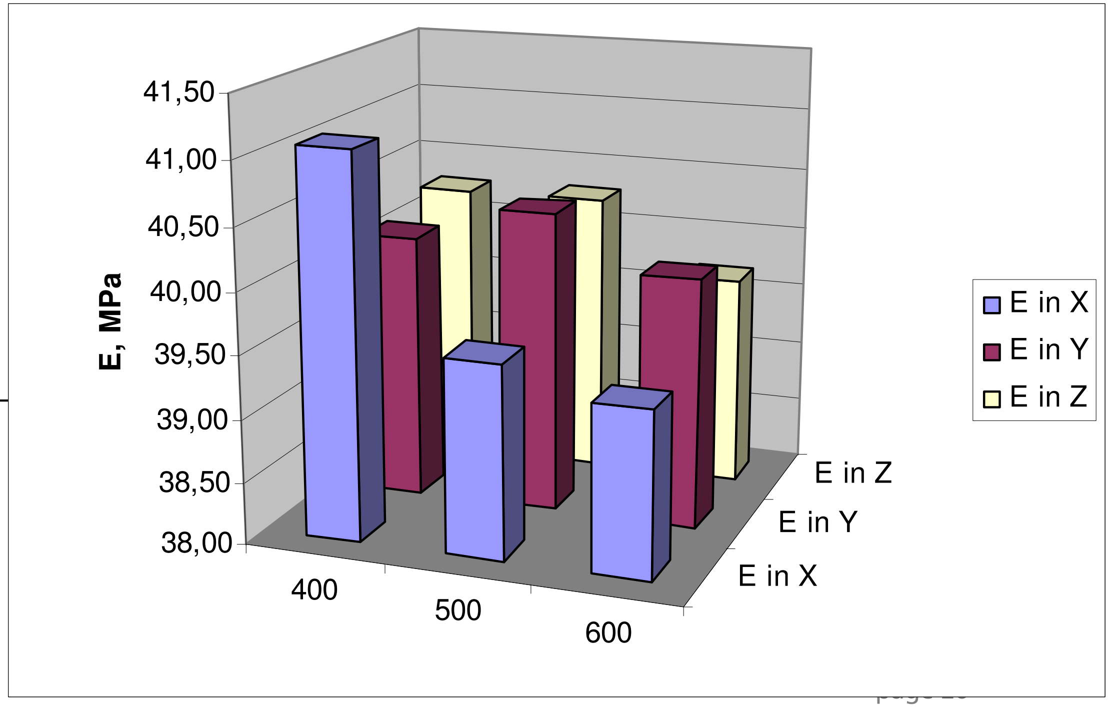
3. Effective Elastic Coefficients: Size of RVE



Name	Resolution	Porosity	SVF	e_x Strain in x	e_y Strain in y	e_z Strain in z	E [MPa] in x	E [MPa] in y	E [MPa] in z
Foam_400	400X400X400	96,45%	3,55%	-2,43%	-2,49%	-2,48%	41,07	40,13	40,27
Foam_500	500X500X500	96,45%	3,55%	-2,53%	-2,47%	-2,48%	39,55	40,42	40,28
Foam_600	600X600X600	96,45%	3,55%	-2,54%	-2,50%	-2,52%	39,33	40,00	39,70

RVEs with different size are considered:

If the differences between the results are relatively small then the size is large enough.



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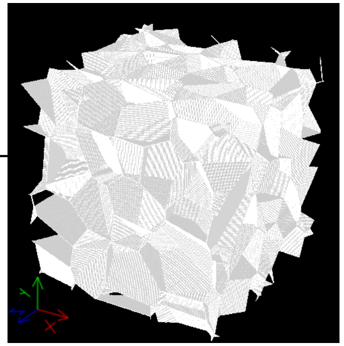
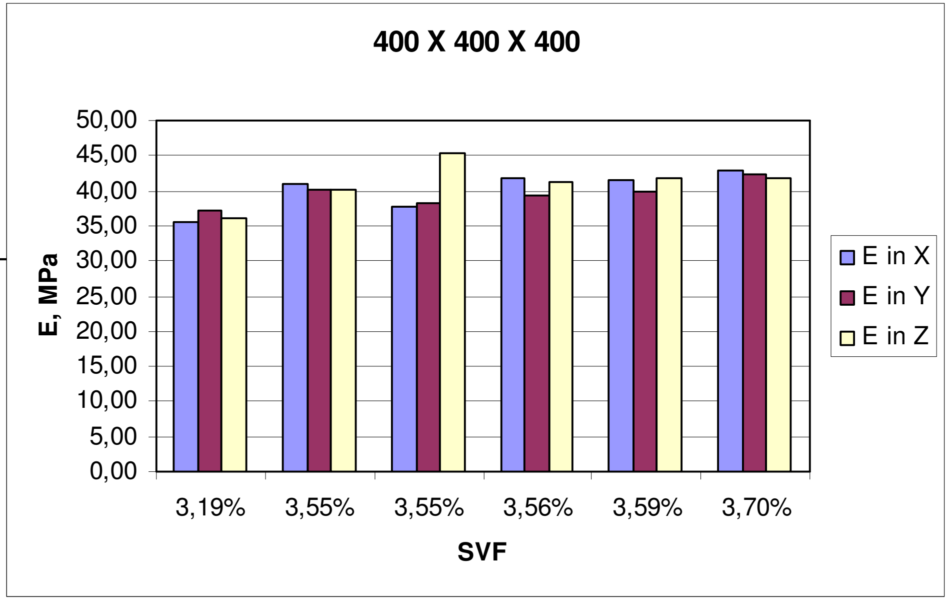
3. Effective Elastic Coefficients: Numerical Results for 6 Realizations of the Stochastic Microstructure

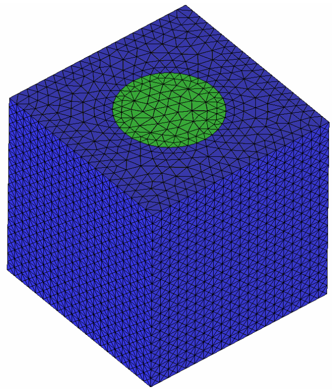


Resolution	Porosity	SVF	e_x Strain in x	e_y Strain in y	e_z Strain in z	E [MPa] in x	E [MPa] in y	E [MPa] in z
400X400X400	96,81%	3,19%	-2,81%	-2,70%	-2,77%	35,62	37,10	36,11
400X400X400	96,45%	3,55%	-2,43%	-2,49%	-2,48%	41,07	40,13	40,27
400X400X400	96,45%	3,55%	-2,66%	-2,61%	-2,20%	37,63	38,30	45,43
400X400X400	96,44%	3,56%	-2,39%	-2,55%	-2,42%	41,78	39,27	41,23
400X400X400	96,41%	3,59%	-2,41%	-2,50%	-2,40%	41,53	39,96	41,75
400X400X400	96,30%	3,70%	-2,34%	-2,36%	-2,40%	42,77	42,34	41,75

- The foam is almost isotropic.
- The stiffness strongly depends on the porosity.

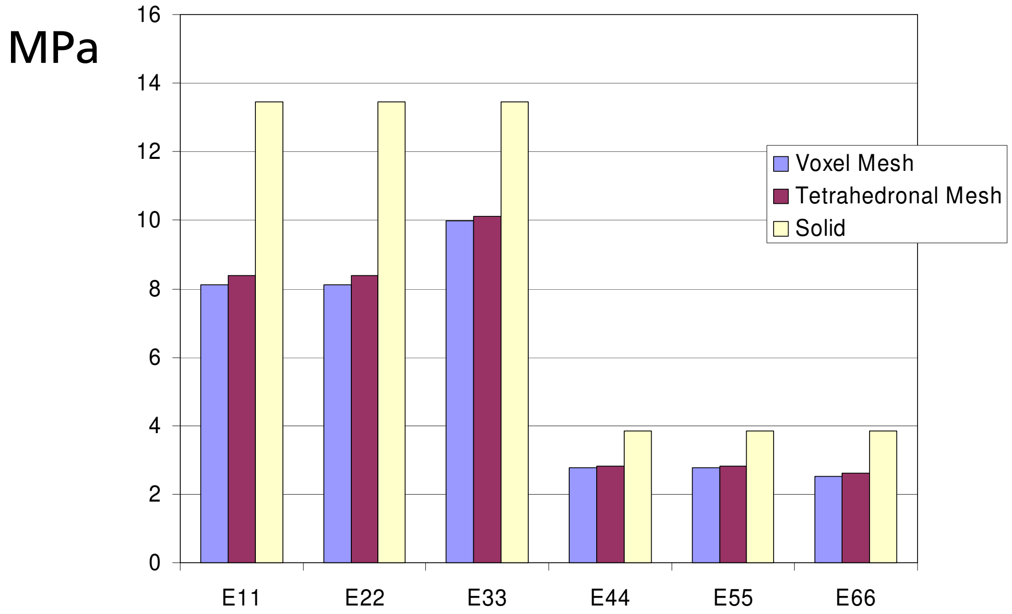


Comparison of Standard FEM and Voxel Discretization
Numerical Convergence of Effective Stiffness Tensor E*



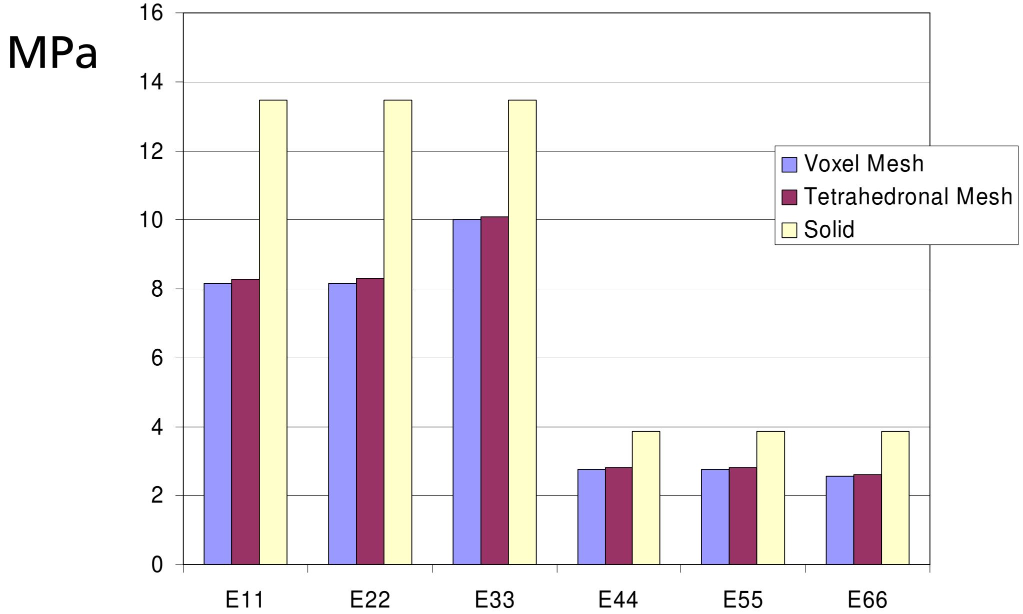
Mesh 1

20 x 20 x 20



Mesh 3

80 x 80 x 80



The effective stiffness tensor E* is almost transversely isotropic.

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$$E^* = \begin{pmatrix} E_{11} & E_{12} & E_{13} & E_{14} & E_{15} & E_{16} \\ & E_{22} & E_{23} & E_{24} & E_{25} & E_{26} \\ & & E_{33} & E_{34} & E_{35} & E_{36} \\ & & & E_{44} & E_{45} & E_{46} \\ & \text{symm} & & & E_{55} & E_{56} \\ & & & & & E_{66} \end{pmatrix}$$

Summary

- Effective tensors are defined in micromechanics to describe the macroscopic behavior of inhomogeneous materials.
- We study discrete microstructures to determine the effective material behavior.
- The effective tensor E* belongs in general to the triclinic symmetry class, but can be decomposed into a sum of orthogonal tensors belonging to different symmetry classes.
- One can compute E* and its decomposition together with the symmetry Cartesian coordinate system (SCCS) by voxel discretization (e.g. using GeoDict).