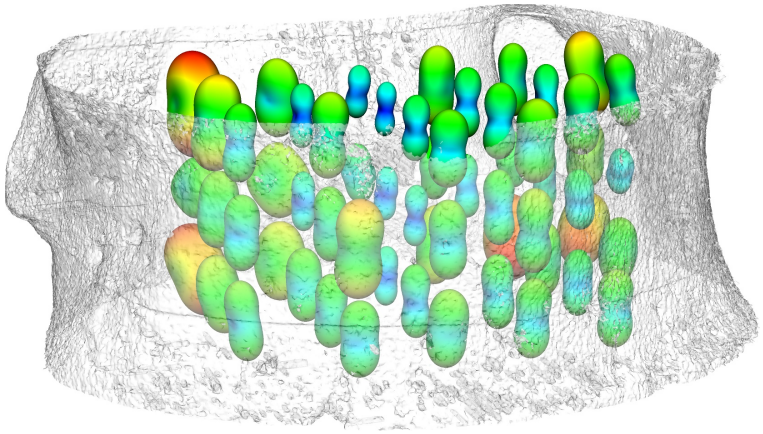
MULTISCALE ELASTICITY MODELING OF TRABECULAR BONE

Lecture Series on Reductionism in Physics and its Relation to Philosophy
Jacobs University, Spring 2014

Lars Ole Schwen
Fraunhofer MEVIS

2014-02-28



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1. Introduction

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1. Introduction

Overview

- example of multiscale modeling
- biomechanical problem
- mathematical simulation tools

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- biomechanical problem
- mathematical simulation tools

Cooperation Partners:

Martin Rumpf (INS, U Bonn)
Torben Pätz (Jacobs U and MEVIS)
Tobias Preusser (Jacobs U and MEVIS)
Stefan Sauter (U Zurich)
Hans-Joachim Wilke (UFB, U Ulm)
Uwe Wolfram (UFB, U Ulm and U Bern)

MULTISCALE ELASTICITY MODELING OF TRABECULAR BONE

2. Trabecular Bone

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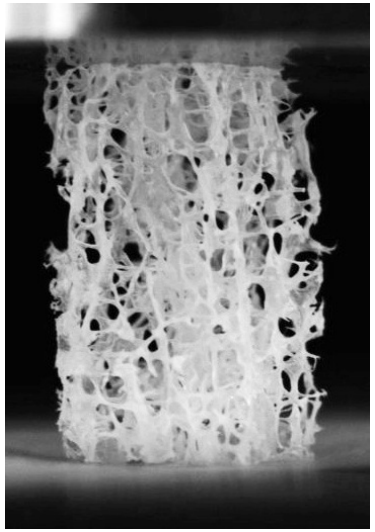
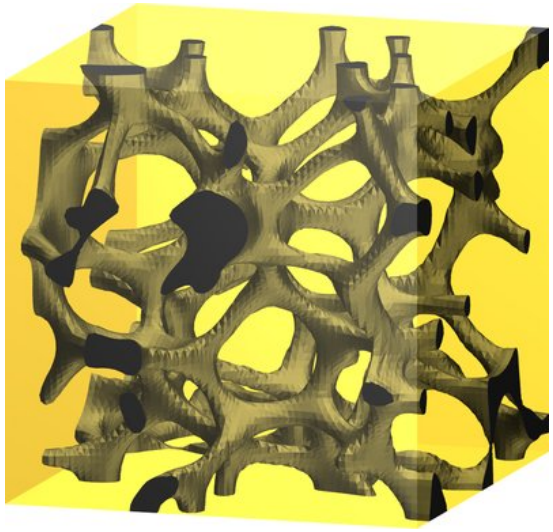
2. Trabecular Bone

Specimens

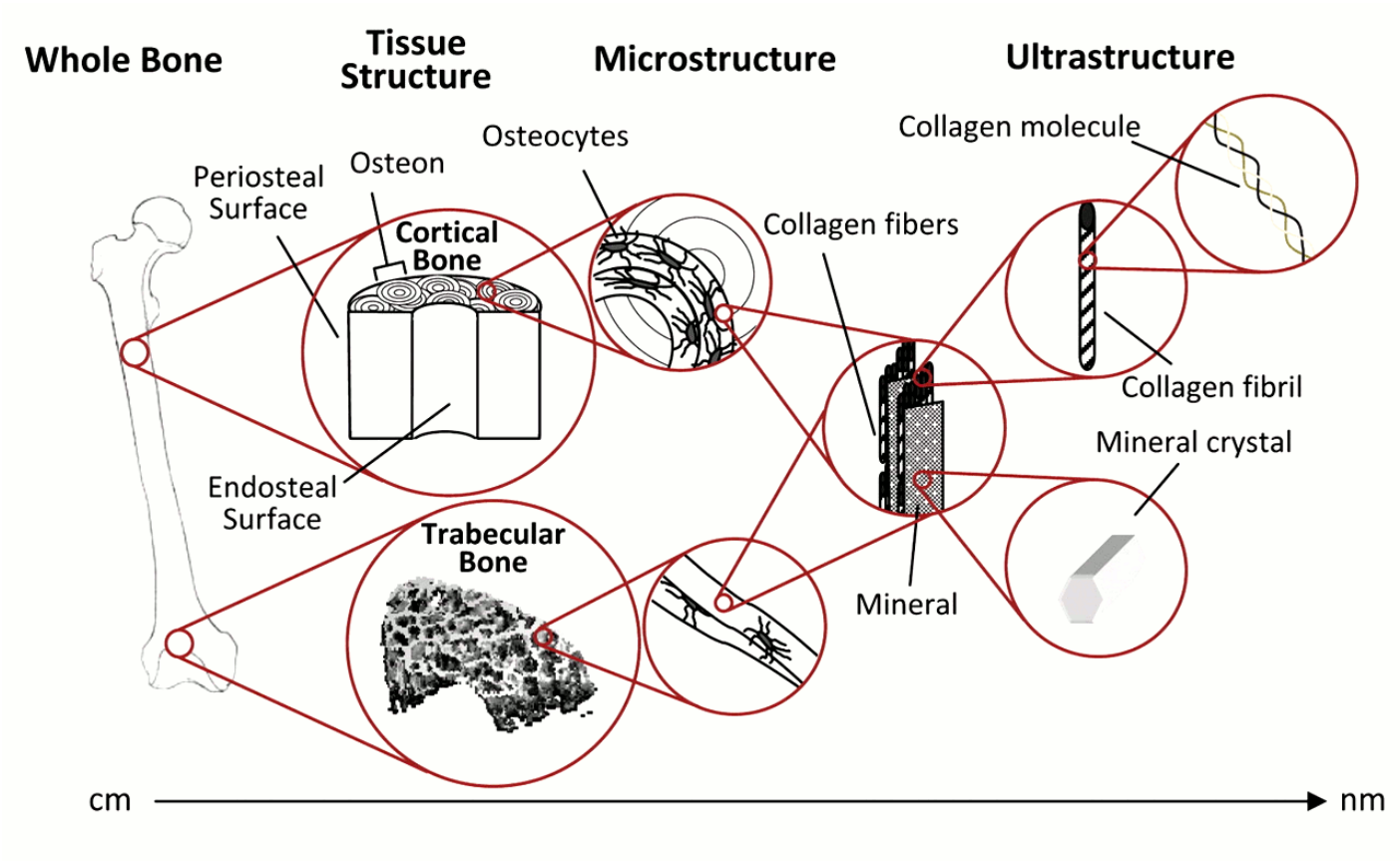




Specimens of trabecular bone obtained from vertebrae

2. Trabecular Bone

Scales



A. Boskey and R. Coleman, Journal of Dental Research 89 (2010), pp. 1333–1348
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3. Modeling Linearized Elasticity

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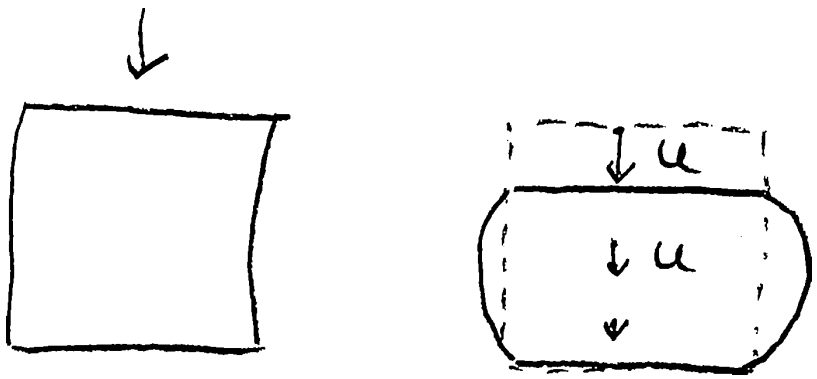
3. Modeling Linearized Elasticity

Basics of Linearized Elasticity



- **Displacement** deformation of elastic body described by displacement
  $u : \Omega \to \mathbb{R}^3$
  Where is a point shifted to?

3. Modeling Linearized Elasticity

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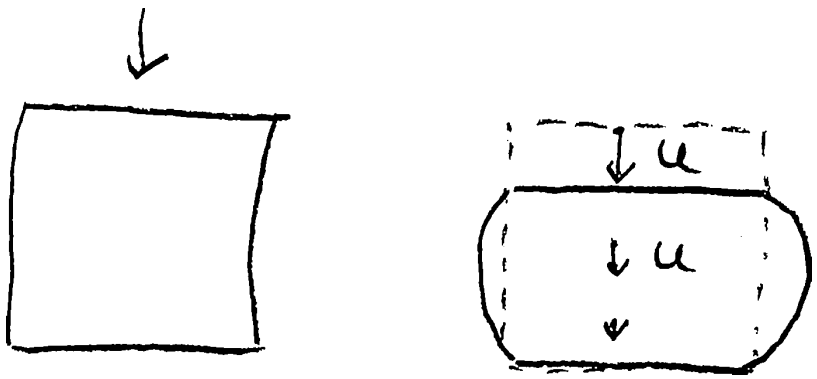

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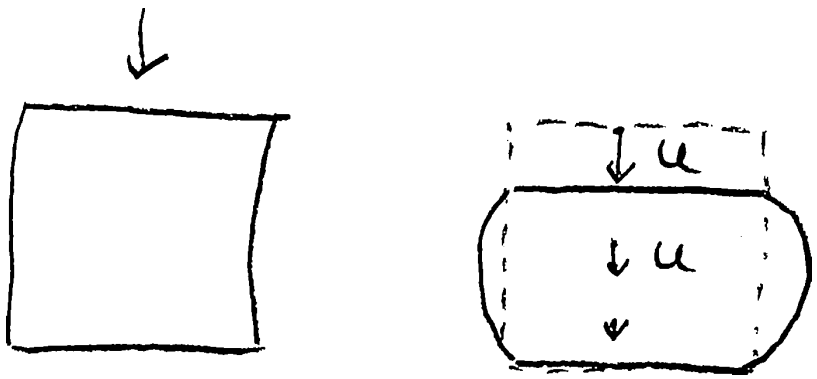

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  1D: How much is a spring compressed?

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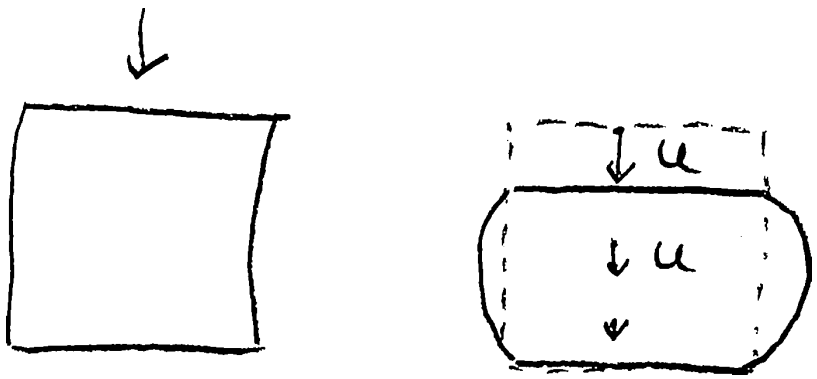

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  1D: How much is a spring compressed?
- **Stress** related to strain via elasticity tensor, $\sigma = C : \epsilon$, $C \in \mathbb{R}^{3\times 3\times 3\times 3}$
  1D: force needed for compressing spring

3. Modeling Linearized Elasticity

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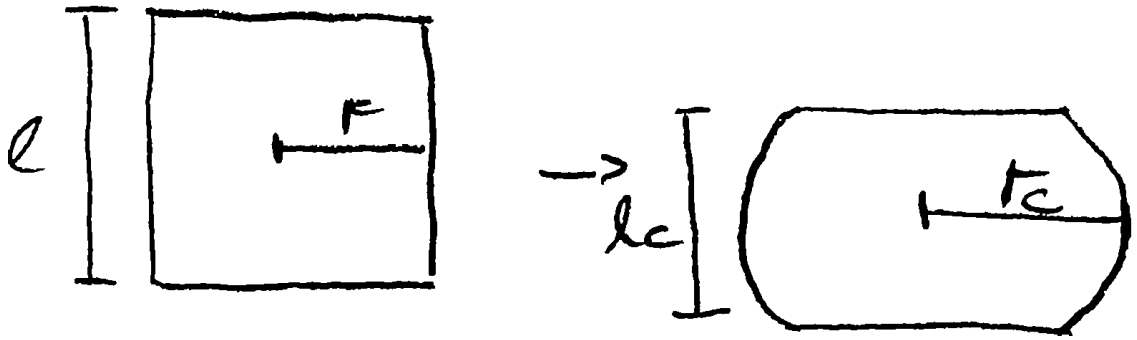

Simplest case of elasticity tensor C

- **Young's modulus** E describes stiffness
  How strong do I need to pull for a fixed elongation?
  How much does the object elongate for a given force?

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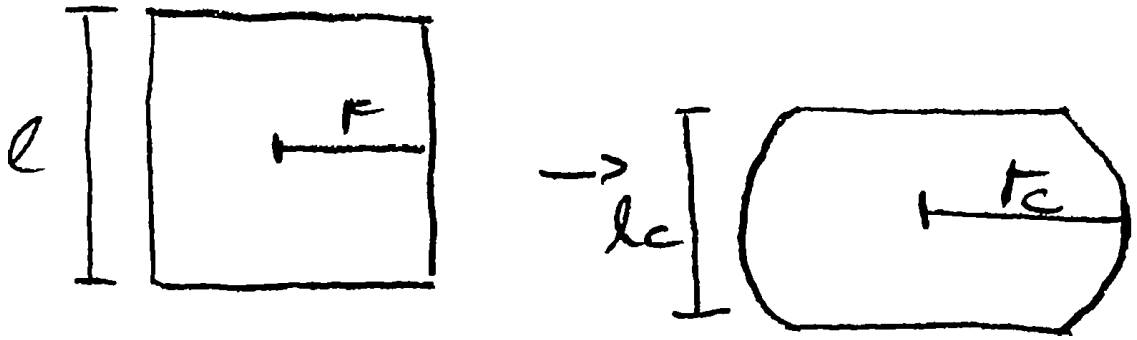

Simplest case of elasticity tensor C

- **Young's modulus** E describes stiffness
  How strong do I need to pull for a fixed elongation?
  How much does the object elongate for a given force?
- **Poisson's ratio** ν describes bulging, i.e. coupling between directions
  no 1D analogon

3. Modeling Linearized Elasticity

Voigt Notation

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} C_{00} & C_{01} & C_{02} & C_{03} & C_{04} & C_{05} \\ & C_{11} & C_{12} & C_{13} & C_{14} & C_{15} \\ & & C_{22} & C_{23} & C_{24} & C_{25} \\ & & & C_{33} & C_{34} & C_{35} \\ & \text{sym} & & & C_{44} & C_{45} \\ & & & & & C_{55} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix}$$

- can write C as symmetric 6×6 matrix with 21 constants

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- can write C as symmetric 6×6 matrix with 21 constants
- strain tensor ϵ is symmetric due to physical reasons, i.e. have 6 instead of 9 entries
- same for stress tensor σ

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Isotropy to Anisotropy

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- …
- **fully anisotropic** most general case
  21 constants

$$\begin{bmatrix} \sigma_{xx} \\ \sigma_{yy} \\ \sigma_{zz} \\ \sigma_{yz} \\ \sigma_{xz} \\ \sigma_{xy} \end{bmatrix} = \begin{bmatrix} C_{00} & C_{01} & C_{02} & C_{03} & C_{04} & C_{05} \\ & C_{11} & C_{12} & C_{13} & C_{14} & C_{15} \\ & & C_{22} & C_{23} & C_{24} & C_{25} \\ & & & C_{33} & C_{34} & C_{35} \\ & \text{sym} & & & C_{44} & C_{45} \\ & & & & & C_{55} \end{bmatrix} \begin{bmatrix} \epsilon_{xx} \\ \epsilon_{yy} \\ \epsilon_{zz} \\ 2\epsilon_{yz} \\ 2\epsilon_{xz} \\ 2\epsilon_{xy} \end{bmatrix}$$

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Visualization of Elasticity Tensors

6×6 matrix easier to understand than fourth order tensor $C \in \mathbb{R}^{3\times3\times3\times3}$, but still …

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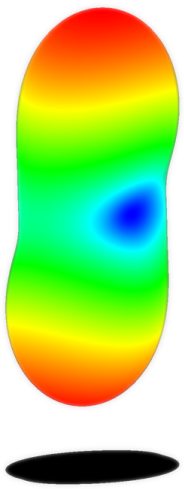
6×6 matrix easier to understand than fourth order tensor $C \in \mathbb{R}^{3\times3\times3\times3}$, but still …

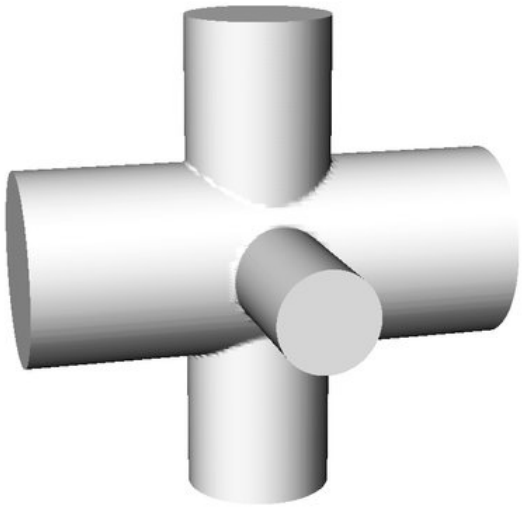
Tensors can be visualized as deformed (encoding uniaxial stiffness) and colored spheres (“colored peanuts”).

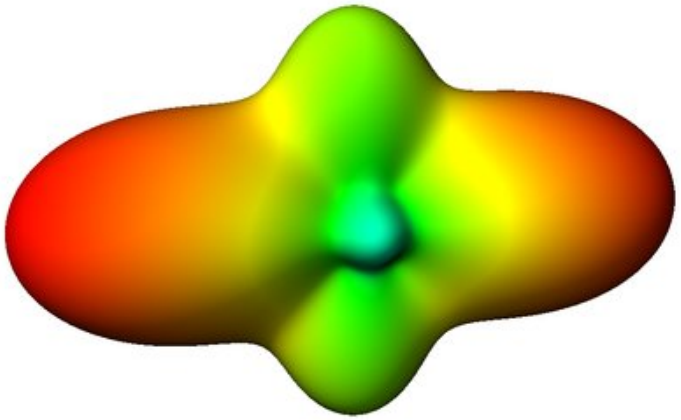


[He et al., Int J Solids and Structures 10(1995), Cazzani et al., Int J Solids and Structures 40(2003)]

3. Modeling Linearized Elasticity

Visualization of Elasticity Tensors, Example I

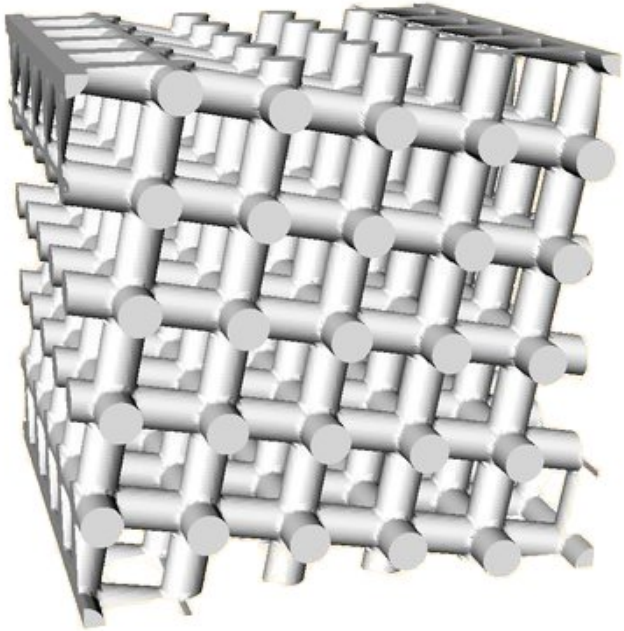


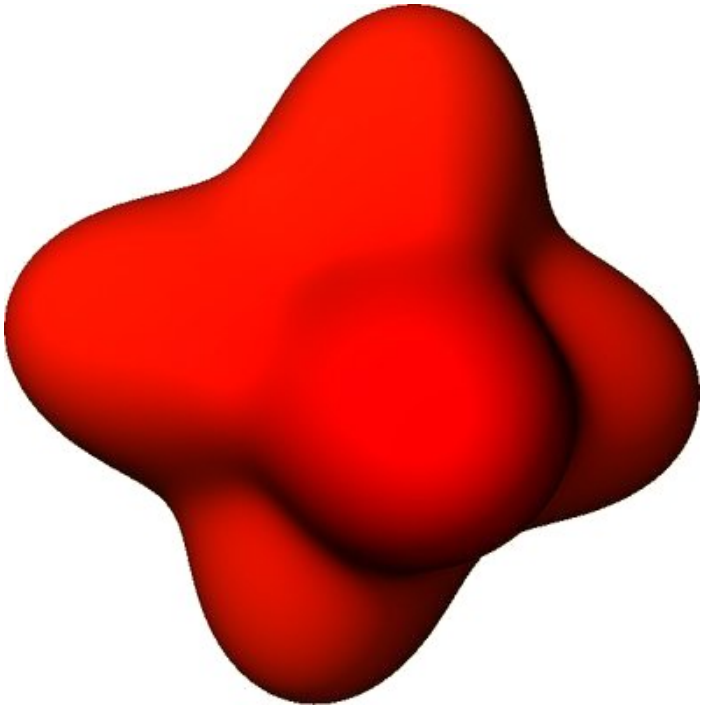


macroscopically orthotropic (⇐ geometry + microscopic isotropy)

3. Modeling Linearized Elasticity

Visualization of Elasticity Tensors, Example II

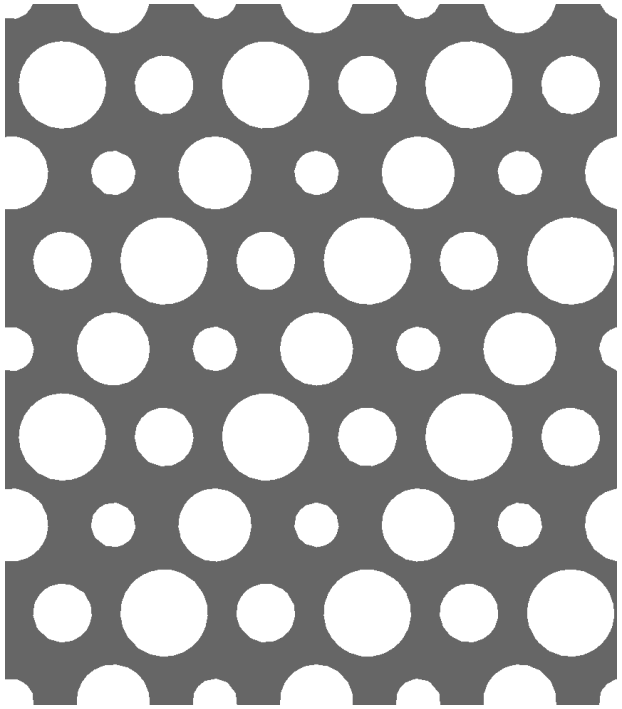


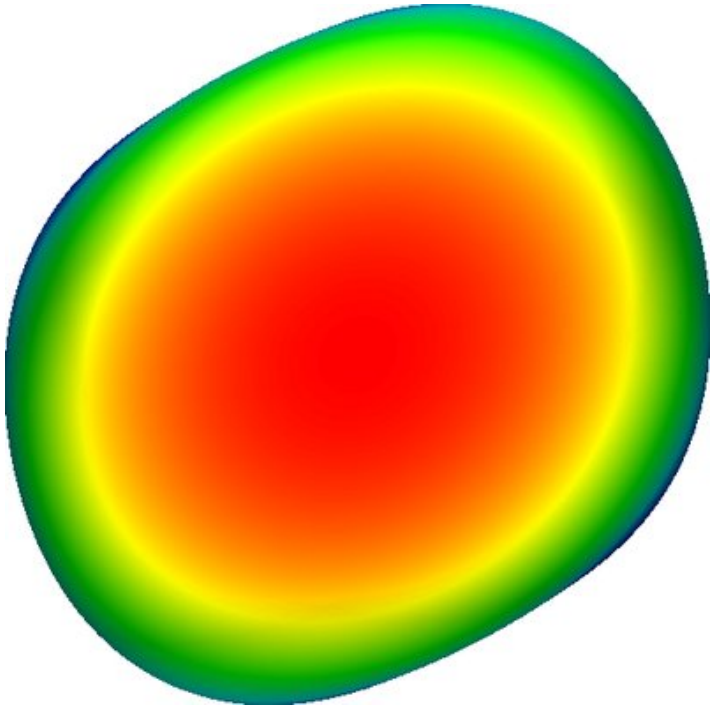


rotated – identify axes! Explained after examples …

3. Modeling Linearized Elasticity

Visualization of Elasticity Tensors, Example III

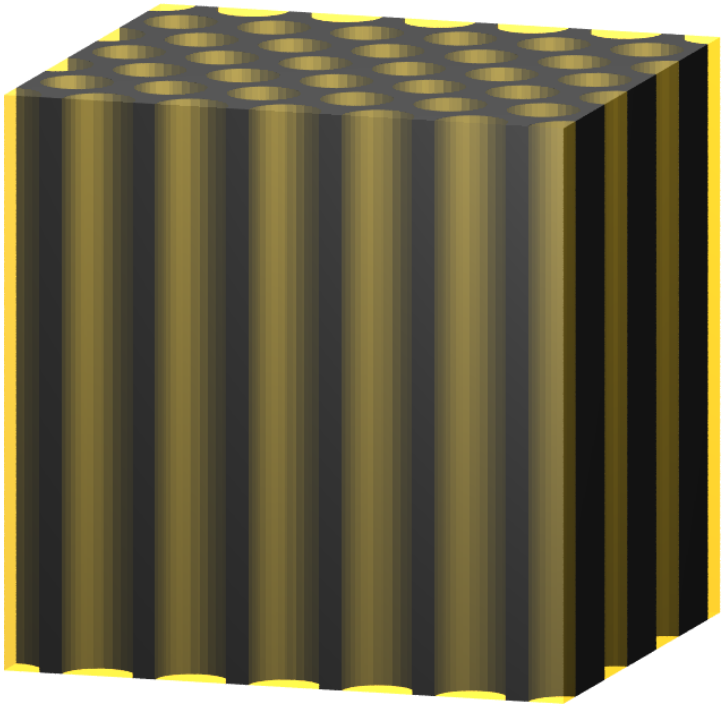


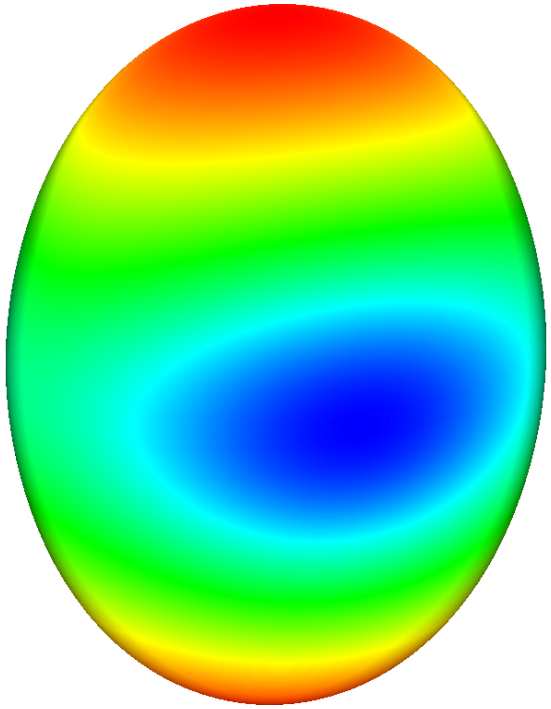


non-orthotropic (but I haven’t thought about how many constants are really necessary)

3. Modeling Linearized Elasticity

Visualization of Elasticity Tensors, Example IV





non-orthotropic due to variable material properties

3. Modeling Linearized Elasticity

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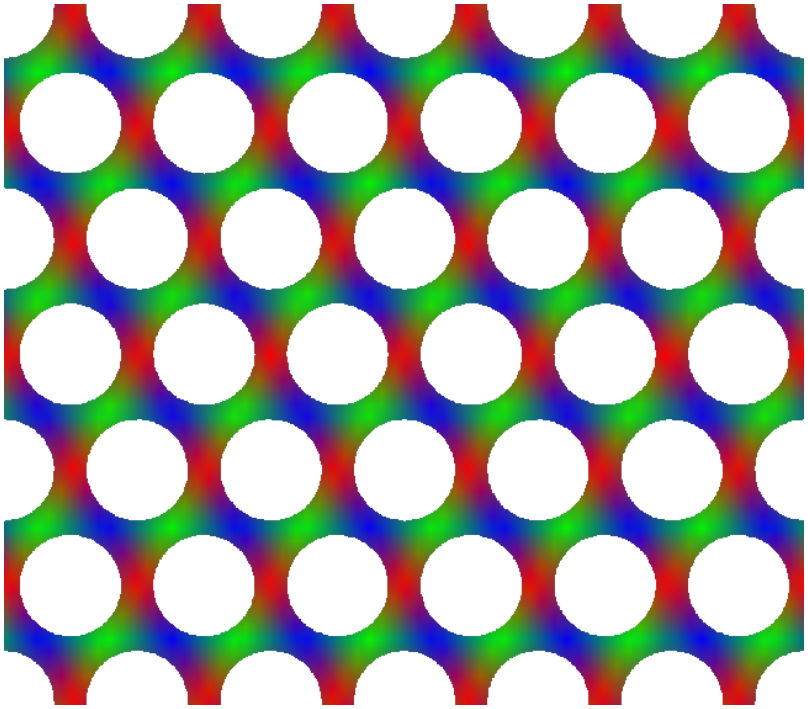

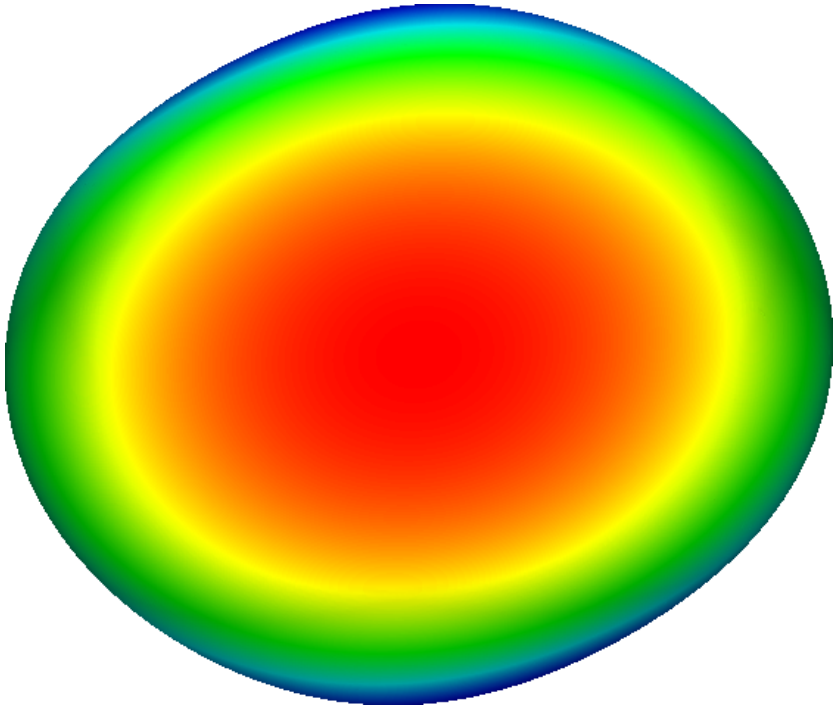

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Determining Axis Orientation I

Idea: view as an optimization problem.

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Here:

minimize $f(Q(C))$, the orthotropy violation (f) of rotated (Q) tensor C

where Q is a 3D rotation by $\pm 90°$ (to obtain uniqueness)

3. Modeling Linearized Elasticity

Determining Axis Orientation II

Aligned orthotropic Tensor

$$C = \begin{bmatrix} C_{00} & C_{01} & C_{02} & 0 & 0 & 0 \\ & C_{11} & C_{12} & 0 & 0 & 0 \\ & & C_{22} & 0 & 0 & 0 \\ & & & C_{33} & 0 & 0 \\ & \text{sym} & & & C_{44} & 0 \\ & & & & & C_{55} \end{bmatrix}$$

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Building blocks

- orthotropy violation

$$f(C) = \frac{\sum C_{ij}}{\sum C_{ij}} = \frac{\text{undesired entries}}{\text{desired entries}}$$

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Building blocks

- orthotropy violation

$$f(C) = \frac{\sum C_{ij}}{\sum C_{ij}} = \frac{\text{undesired entries}}{\text{desired entries}}$$

- rotation $Q(C)$
- minimization procedure for $f(Q(C))$

3. Modeling Linearized Elasticity

Determining Axis Orientation II

4. Numerical Homogenization for Multiscale Modeling

Contents

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Outline

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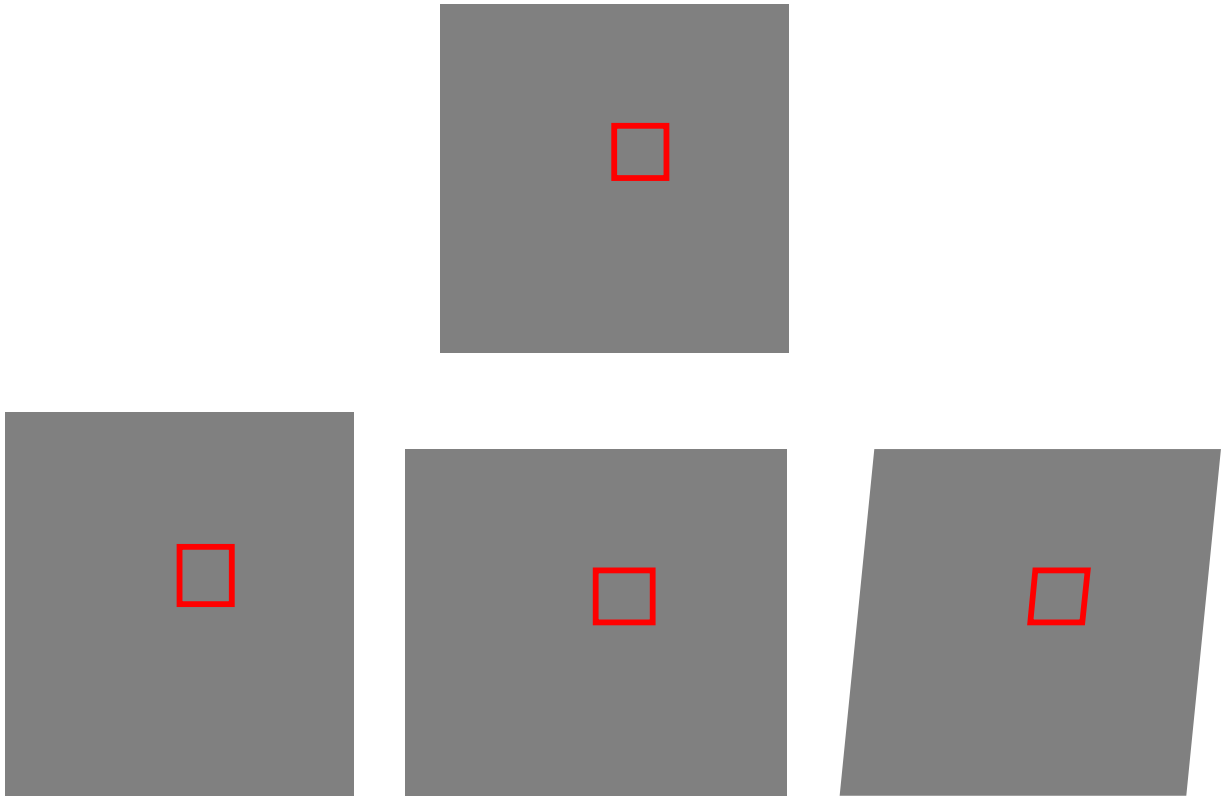
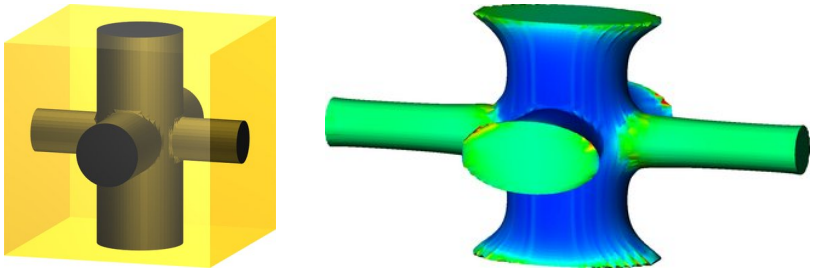


4. Numerical Homogenization for Multiscale Modeling

Statistically Periodic Objects

Problem

- artificial stiffening near the boundary by enforcing displacement boundary conditions (middle)



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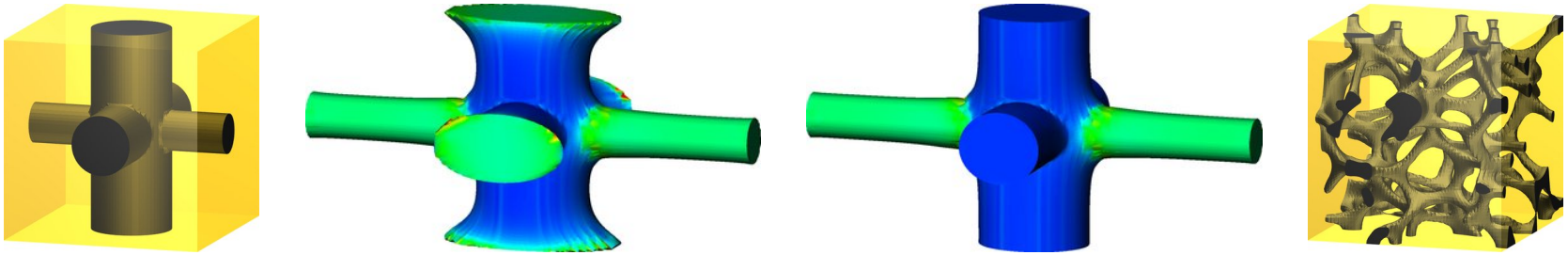
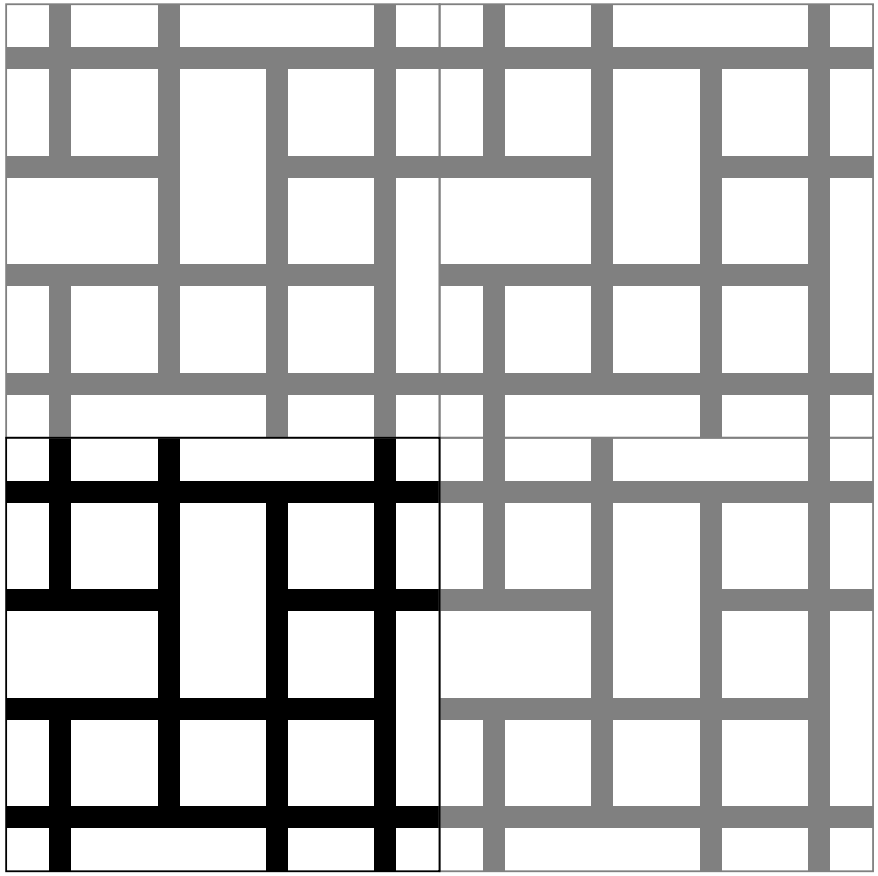


- cannot enforce periodic boundary conditions on non-periodic objects

4. Numerical Homogenization for Multiscale Modeling

Periodic Boundary Conditions?

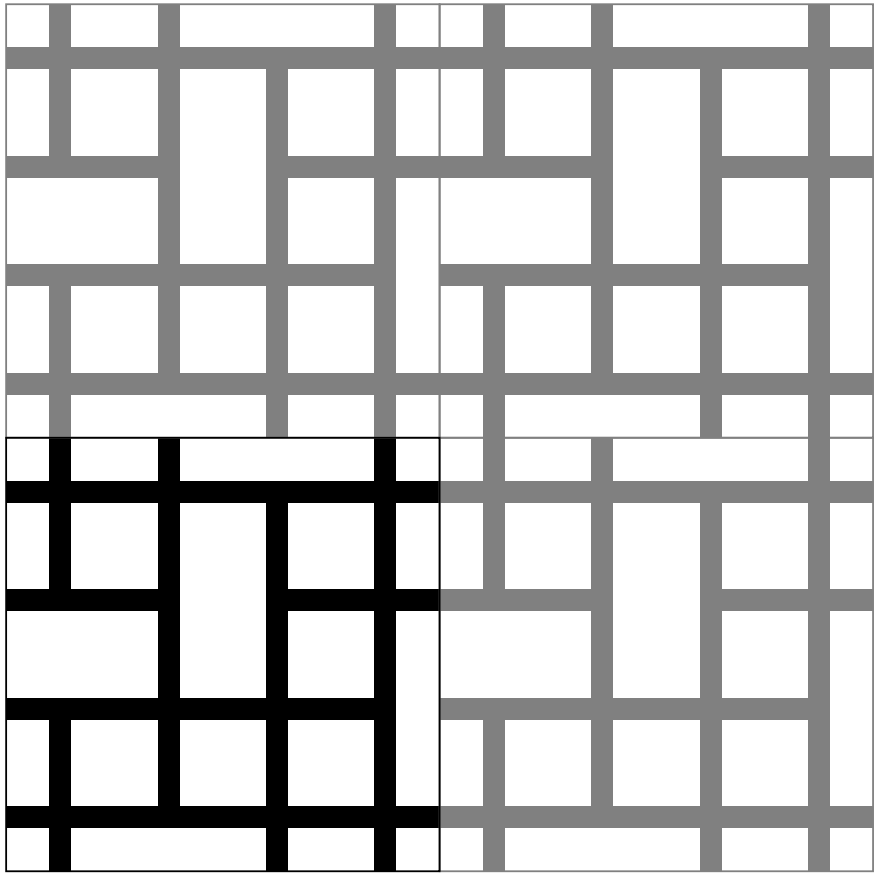
Problem: cannot enforce periodic boundary conditions.



4. Numerical Homogenization for Multiscale Modeling

Periodic Boundary Conditions?

Could make structure periodic by mirroring



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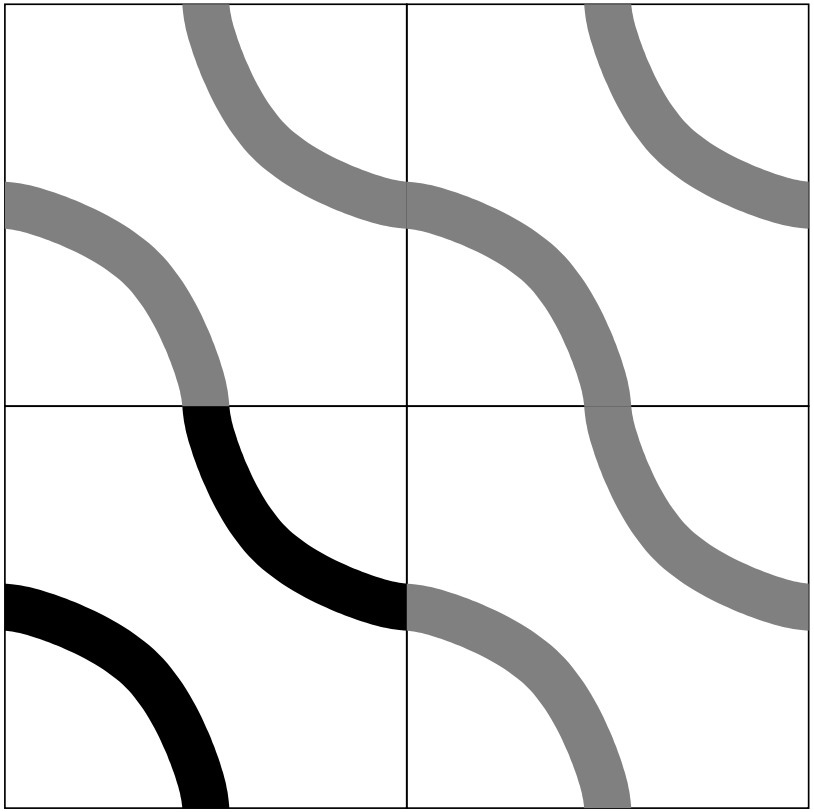
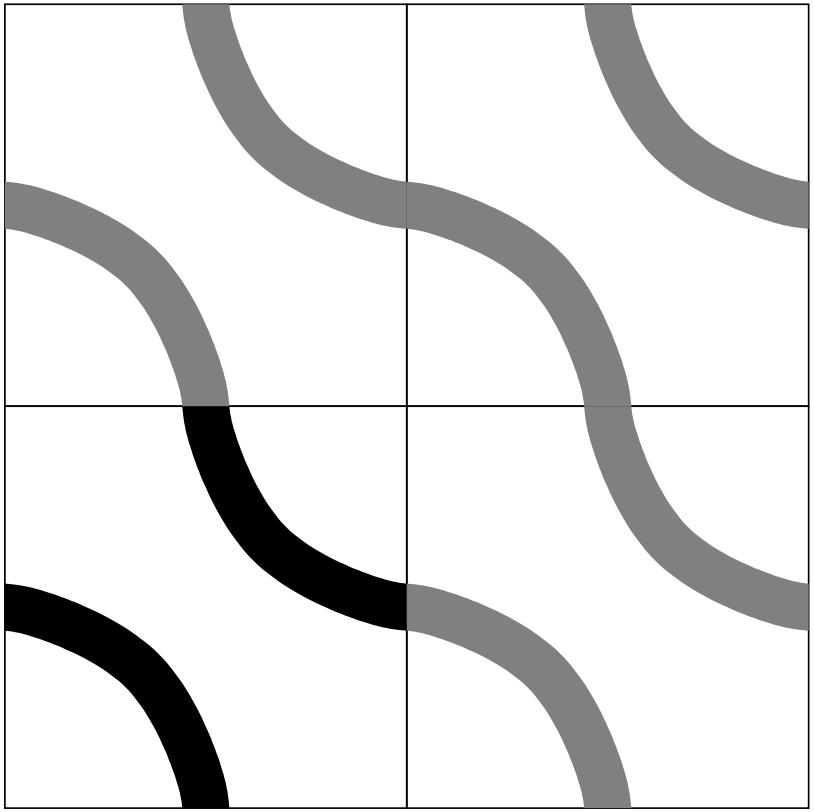
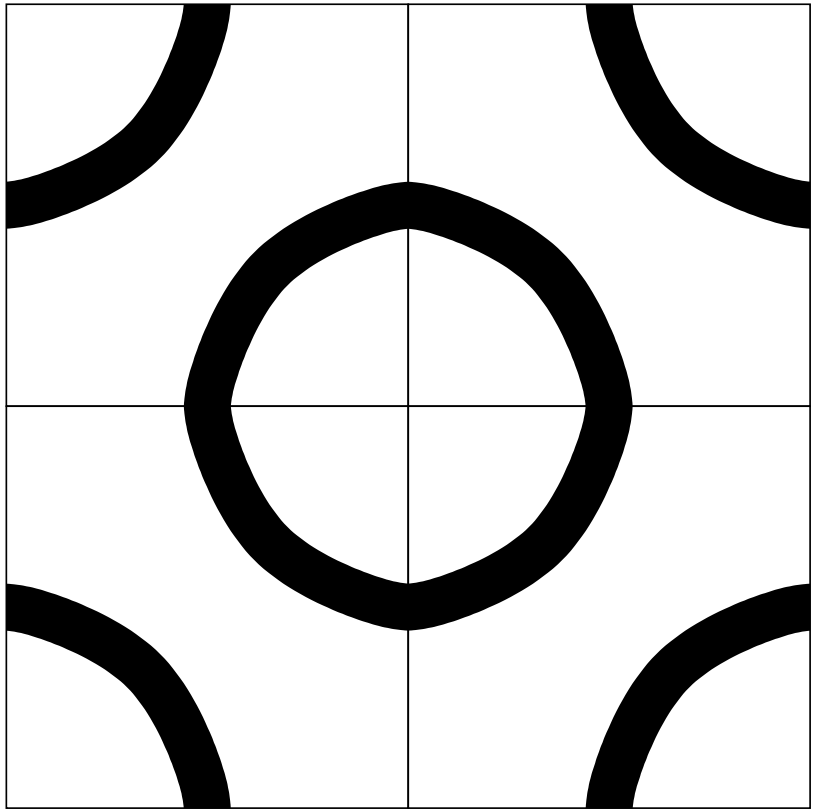


4. Numerical Homogenization for Multiscale Modeling

Periodic Boundary Conditions?

Could make structure periodic by mirroring, but that is a bad idea!



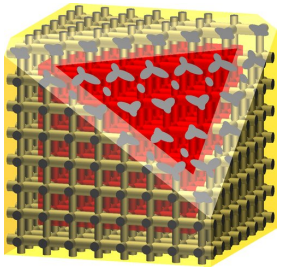


4. Numerical Homogenization for Multiscale Modeling

Statistically Periodic Objects

Solution

- ignore boundary layer β for stress evaluation
- evaluate stress only in interior



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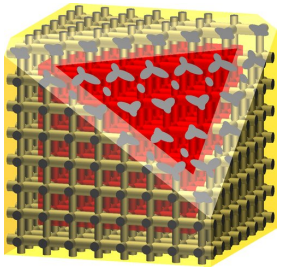

- typically $\beta = 1/8$ cf. [Ün, Bevill, Keaveny J Biomech 39:1955]
- interior still needs to be representative
- trade-off between accuracy and workload

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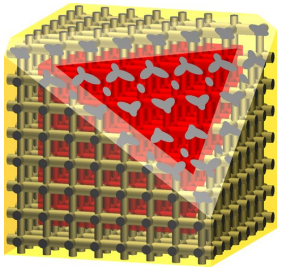


- typically $\beta = 1/8$ cf. [Ün, Bevill, Keaveny J Biomech 39:1955]
- interior still needs to be representative
- trade-off between accuracy and workload

In case of non-periodic microstructures, need statistically representative fundamental cell of at least 5 inter-trabecular distances.

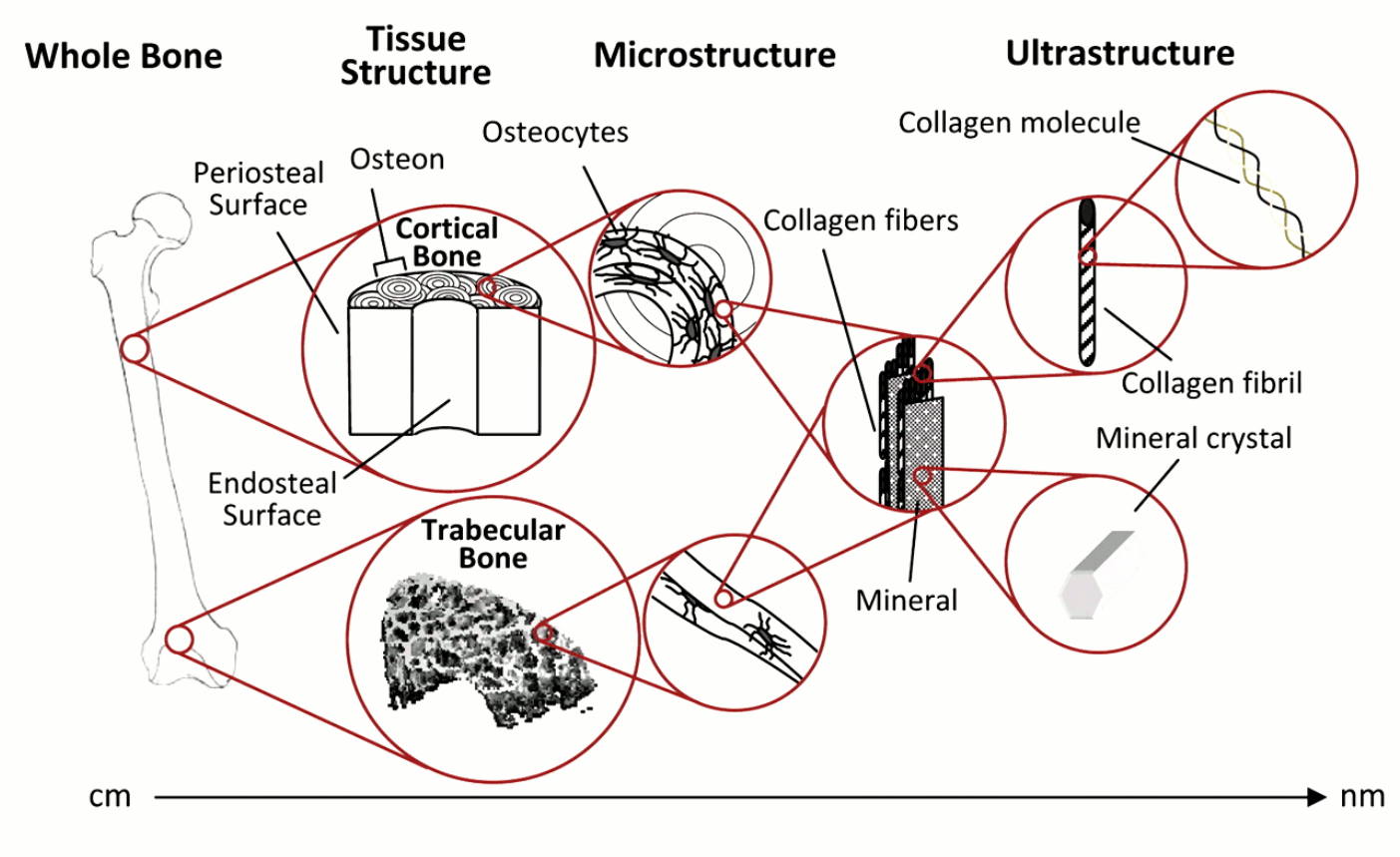
[Harrigan et al, JBiomech 21:269]

5. From Experiment To Model

Contents

5. From Experiment To Model

Trabecular Scale



A. Boskey and R. Coleman, Journal of Dental Research 89 (2010), pp. 1333–1348
Copyright © by International & American Associations for Dental Research

5. From Experiment To Model

Measuring Elasticity Properties

Elasticity Tensor on the trabecular scale measured using **nanoindentation**

- small pyramid-shaped object pressed into trabecula
- allows calculating elasticity properties of trabeculae

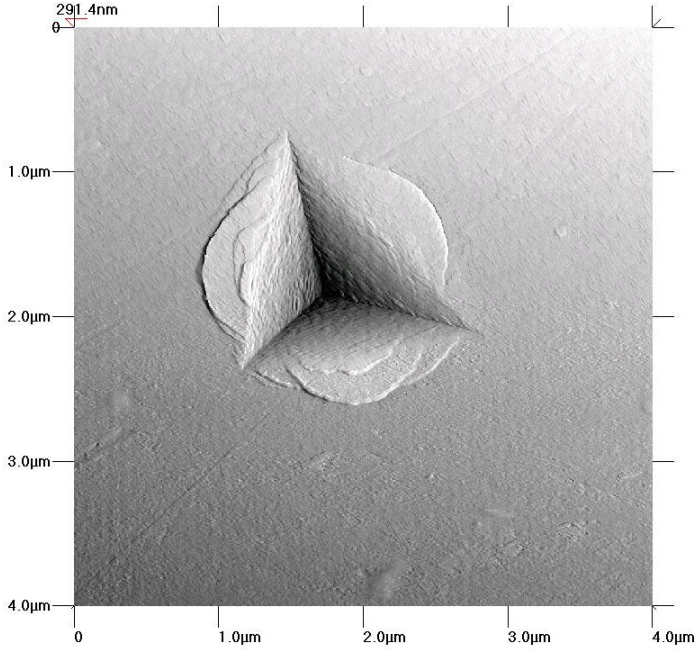


image by Jonathan Puthoff from http://en.wikipedia.org/wiki/File:Nanoindent.JPG

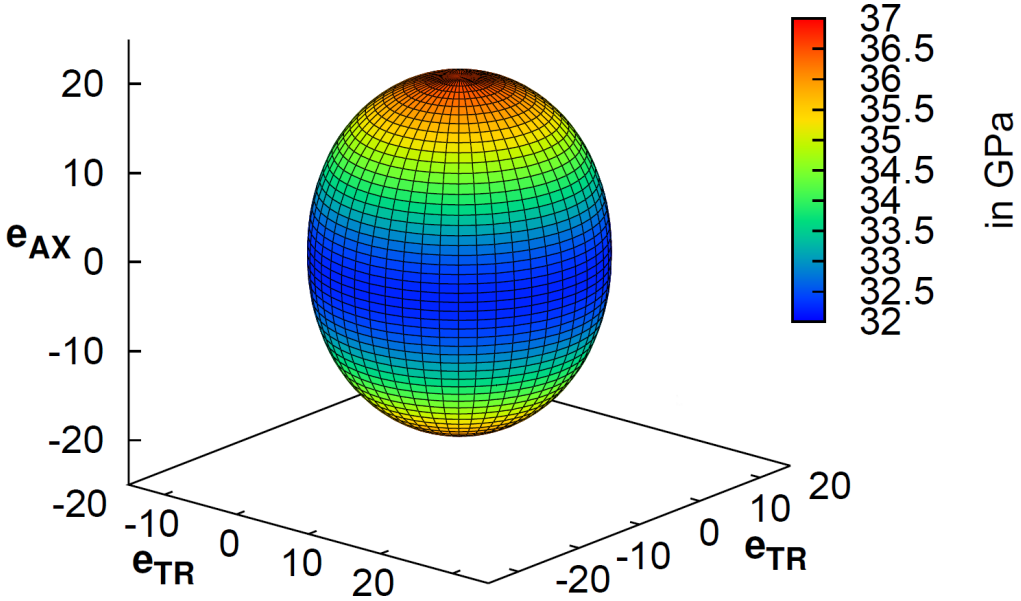
5. From Experiment To Model

Measuring Elasticity Properties

Result

[U. Wolfram et al, J. Biomech. 43 (2010), 1731–37]

- obtain transversely isotropic tensor



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Measuring Elasticity Properties

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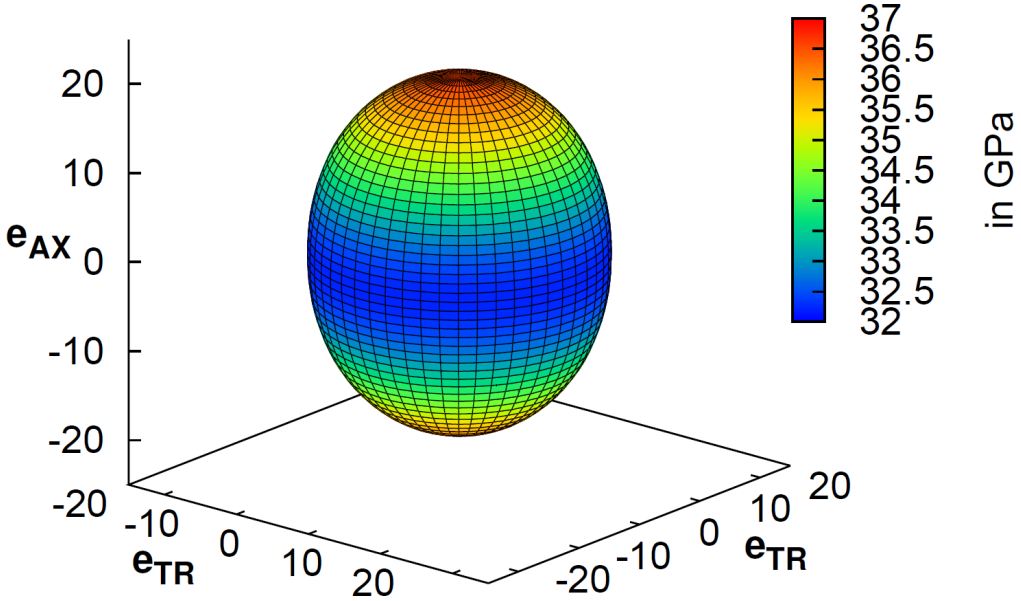


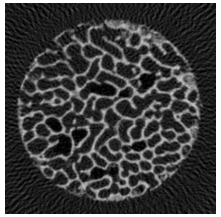
- we did not yet determine trabecular orientation but only used isotropic tensor

5. From Experiment To Model

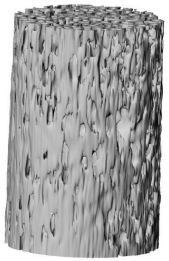
3D Imaging

↓ extract

↓ µCT scan



↓ segment



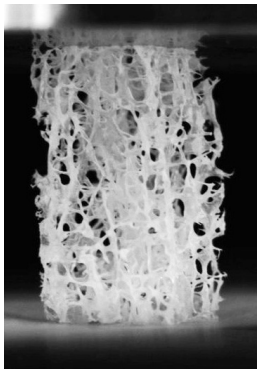
- extract trabecular from spine
- drill cylindrical specimen
- scan in µCT
- image processing (segmentation) to obtain geometry information

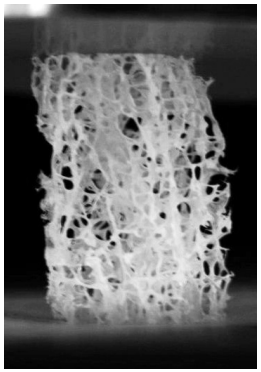
5. From Experiment To Model

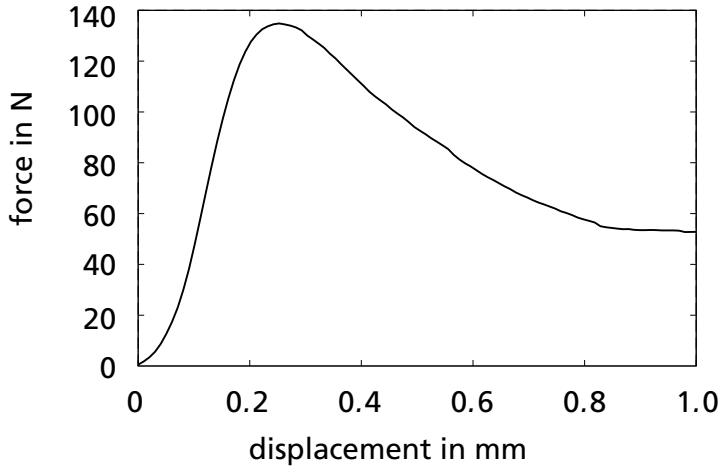
Elasticity Simulation and Validation

- simulation using Composite Finite Elements
- validated experimentally

⇓







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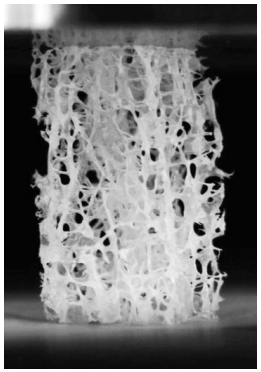

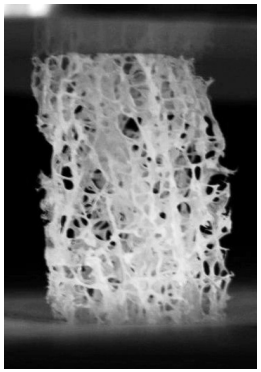

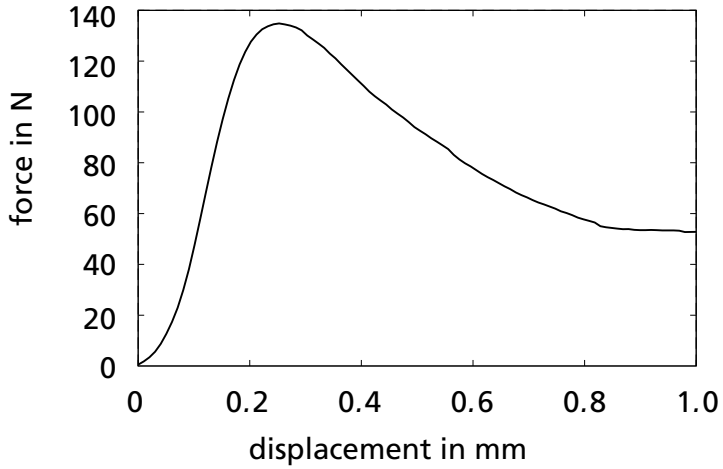

compare simulated uniaxial stiffness to experimentally measured stiffness in linear range

[L. O. Schwen, U. Wolfram, Comp. Meth. Biomech. Biomed. Eng]

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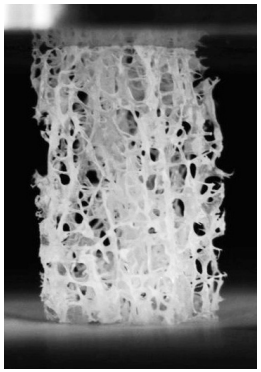
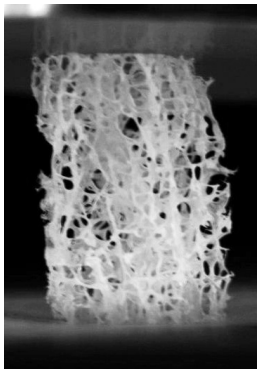
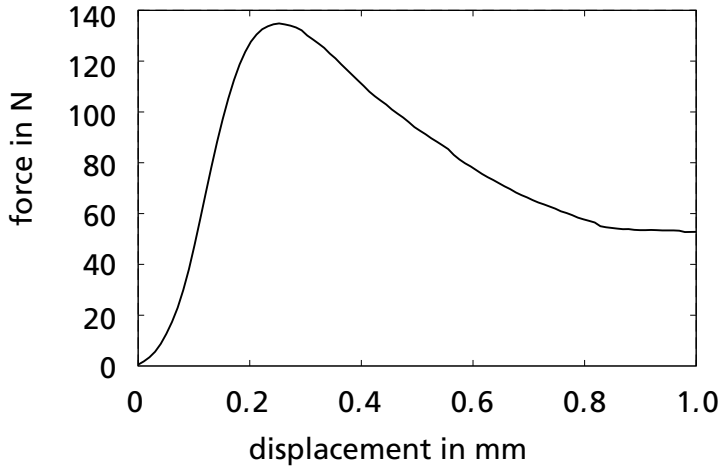






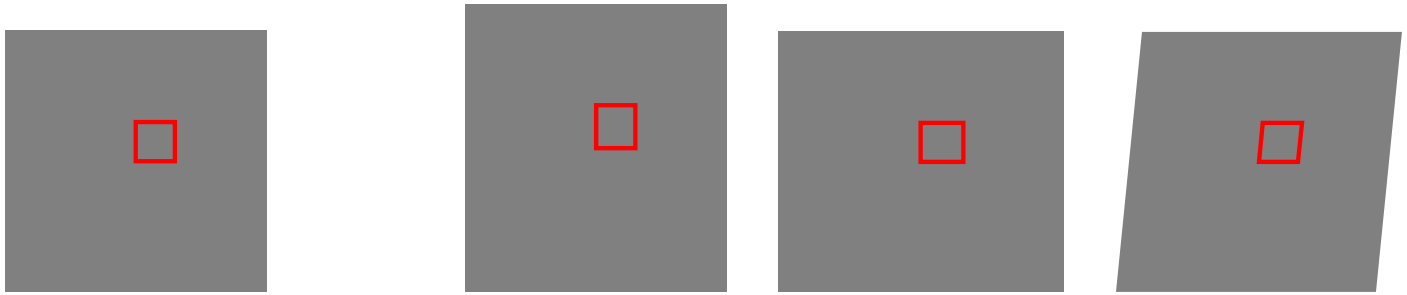
compare simulated uniaxial stiffness to experimentally measured stiffness in linear range

[L. O. Schwen, U. Wolfram, Comp. Meth. Biomech. Biomed. Eng]

So let's apply it for obtaining effective elasticity tensors …

5. From Experiment To Model

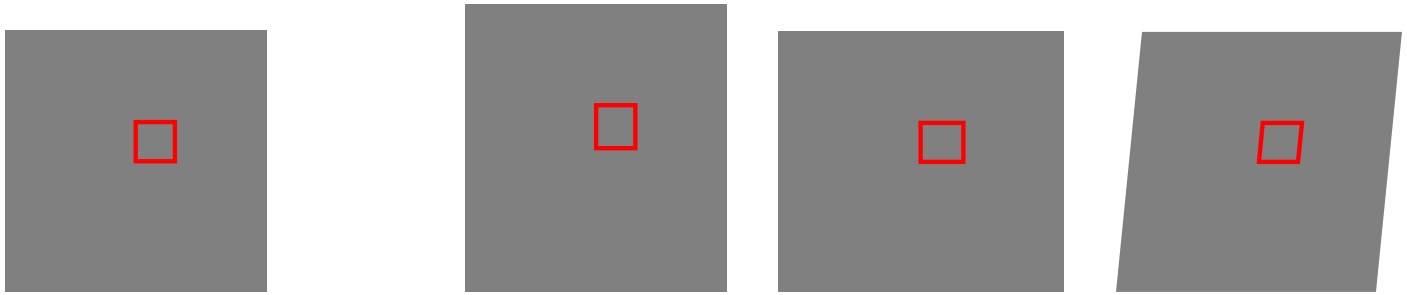
Numerical Homogenization Summarized



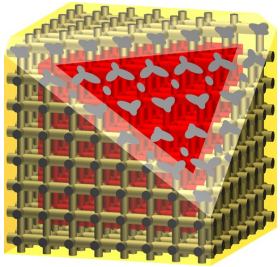
- run elasticity simulation for different unit strains

5. From Experiment To Model

Numerical Homogenization Summarized



- run elasticity simulation for different unit strains
- compute stress response on subdomain



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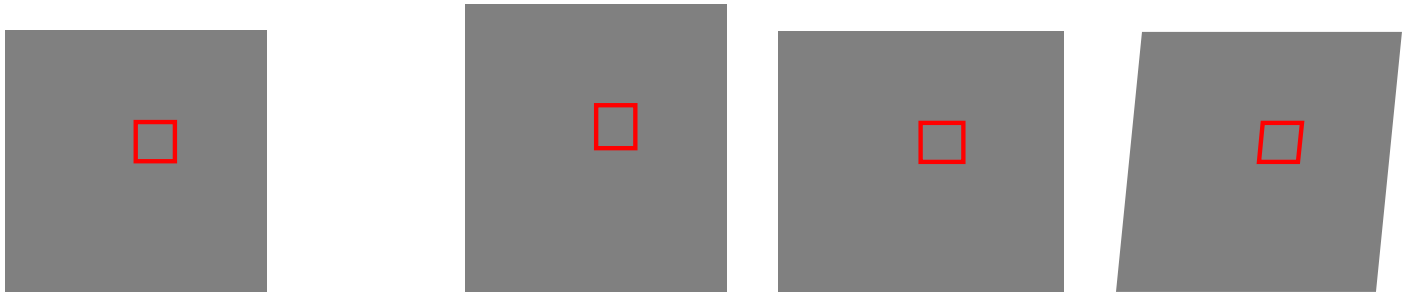
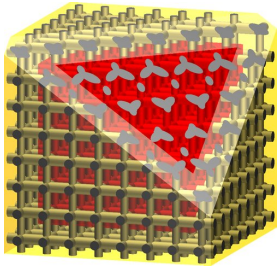
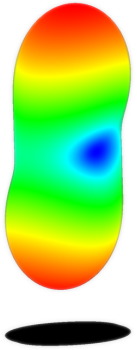


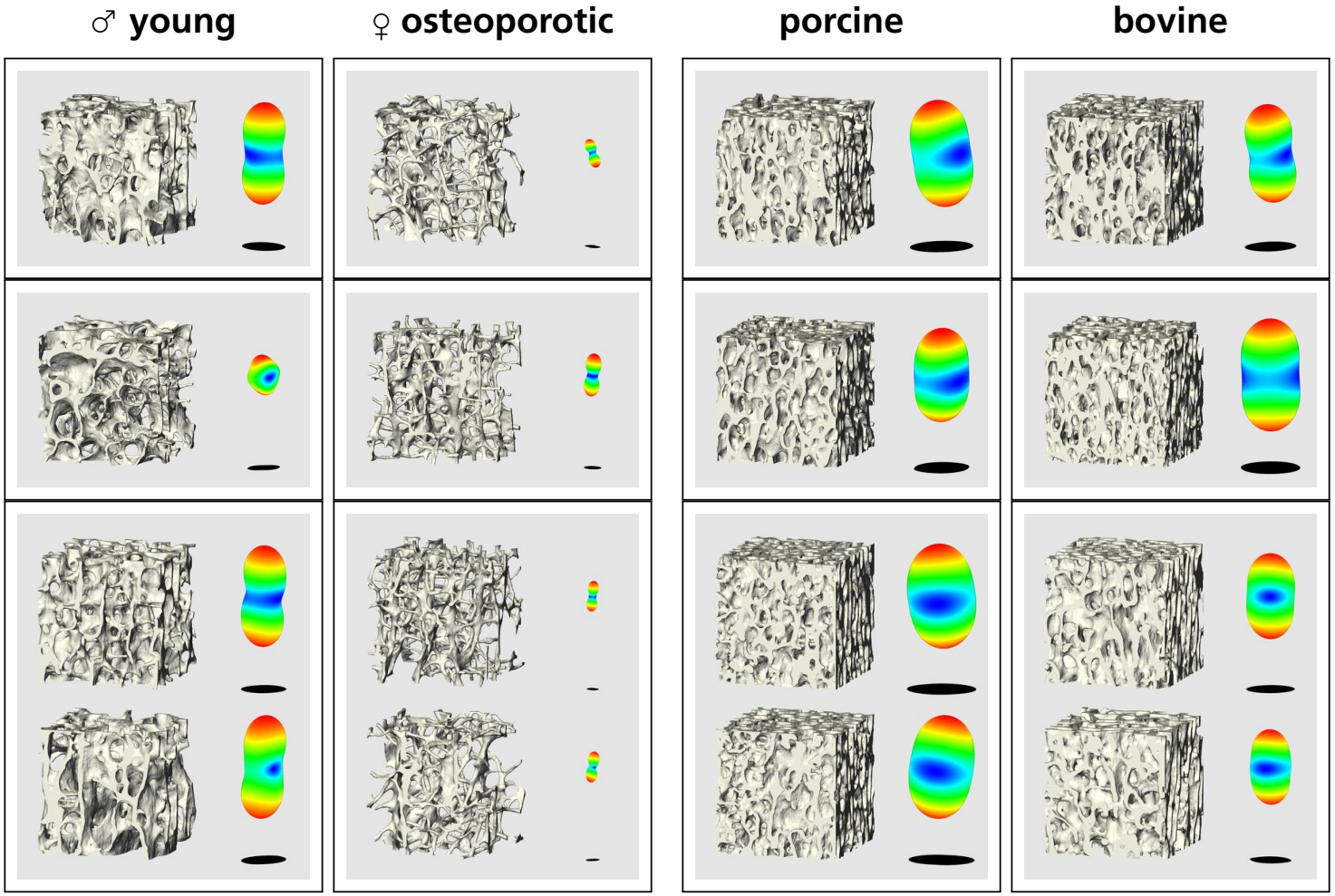
- run elasticity simulation for different unit strains
- compute stress response on subdomain
- obtain macroscopic elasticity tensor





5. From Experiment To Model

Results I: Differences between Species

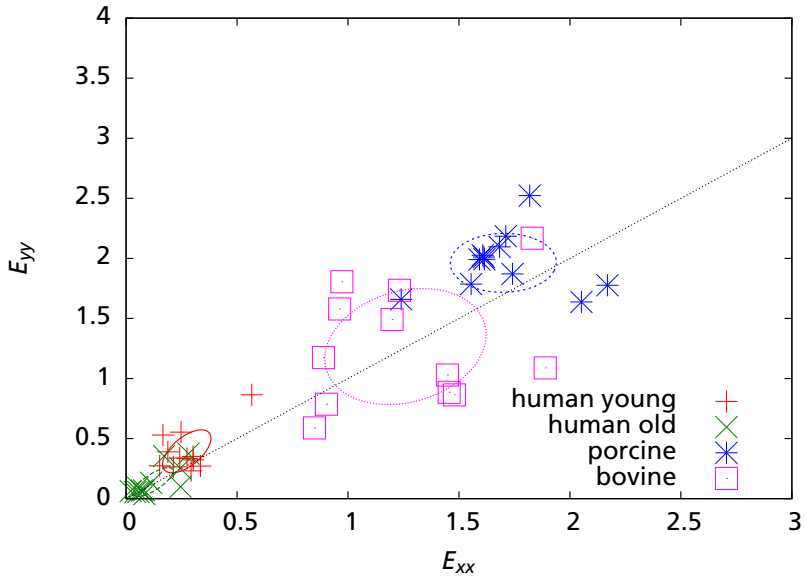


human tensors scaled by 4

[M. Rumpf et al., Int. J. Multiphys. 2010]

5. From Experiment To Model

Results I: Differences between Species



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(ellipses: 1 standard deviation obtained by PCA)

Interpretation:

- transverse isotropy?

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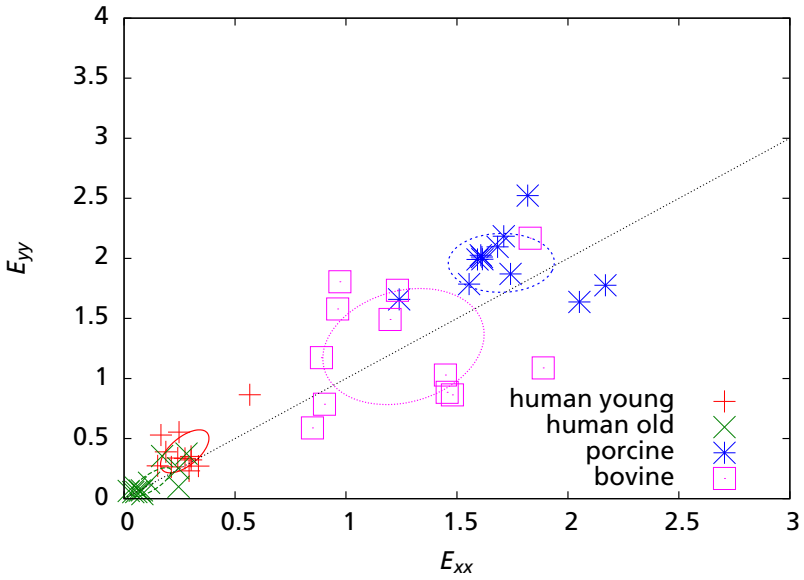

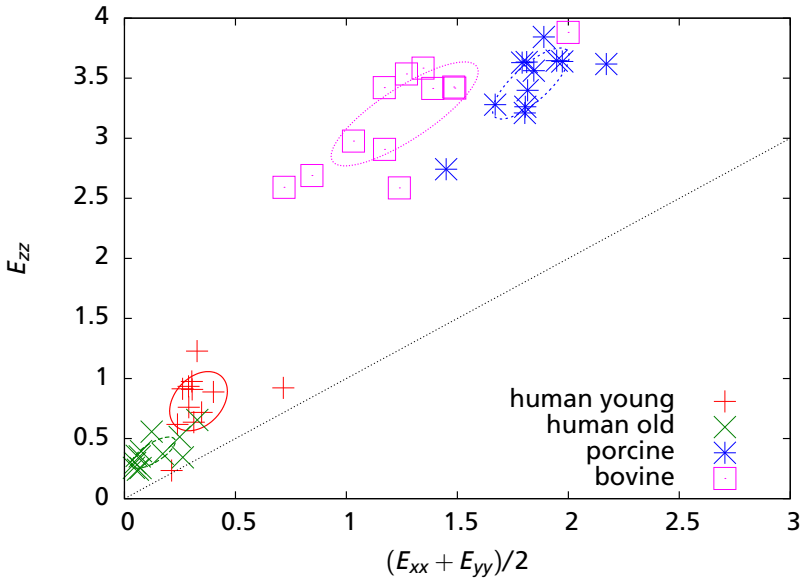

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(ellipses: 1 standard deviation obtained by PCA)

Interpretation:

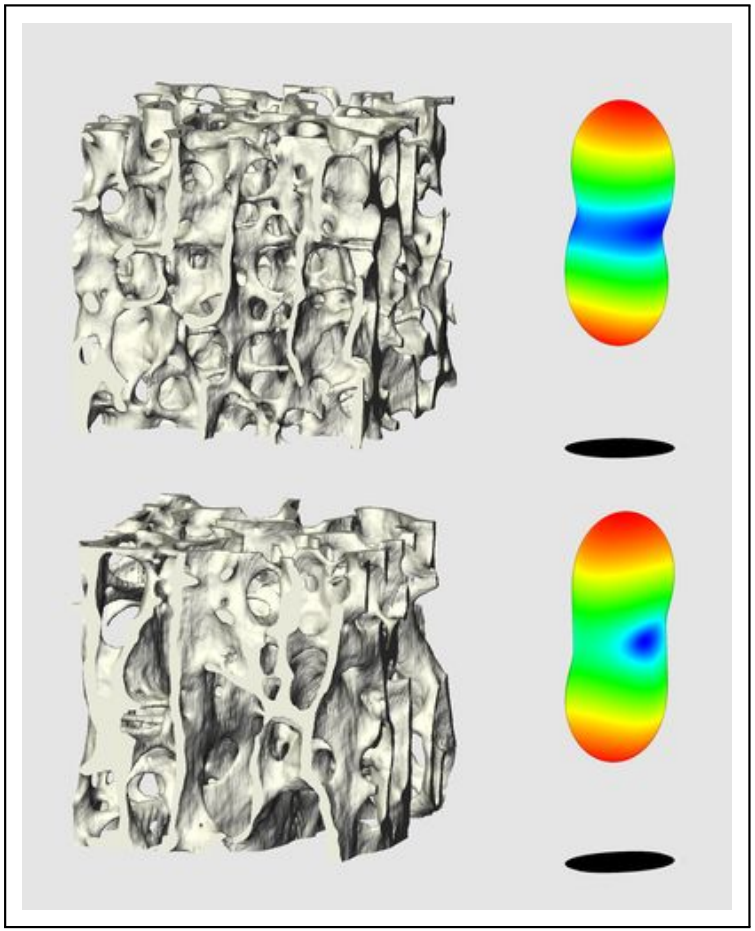
- transverse isotropy?
- anisotropy: craniocaudal/average transverse
- distinct clusters

5. From Experiment To Model

Results II: Intra-Specimen Variations

♂ young example from above

- effective elasticity tensor varies in space



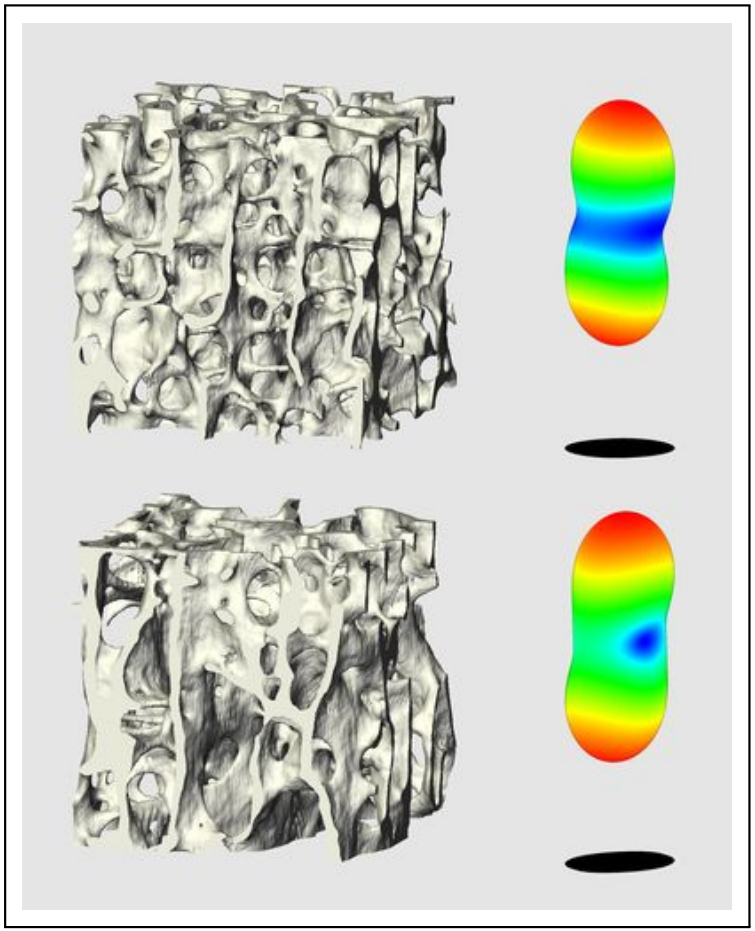
[M. Rumpf et al., Int. J. Multiphys.]

5. From Experiment To Model

Results II: Intra-Specimen Variations

♂ young example from above

- effective elasticity tensor varies in space
- can also consider a whole vertebra



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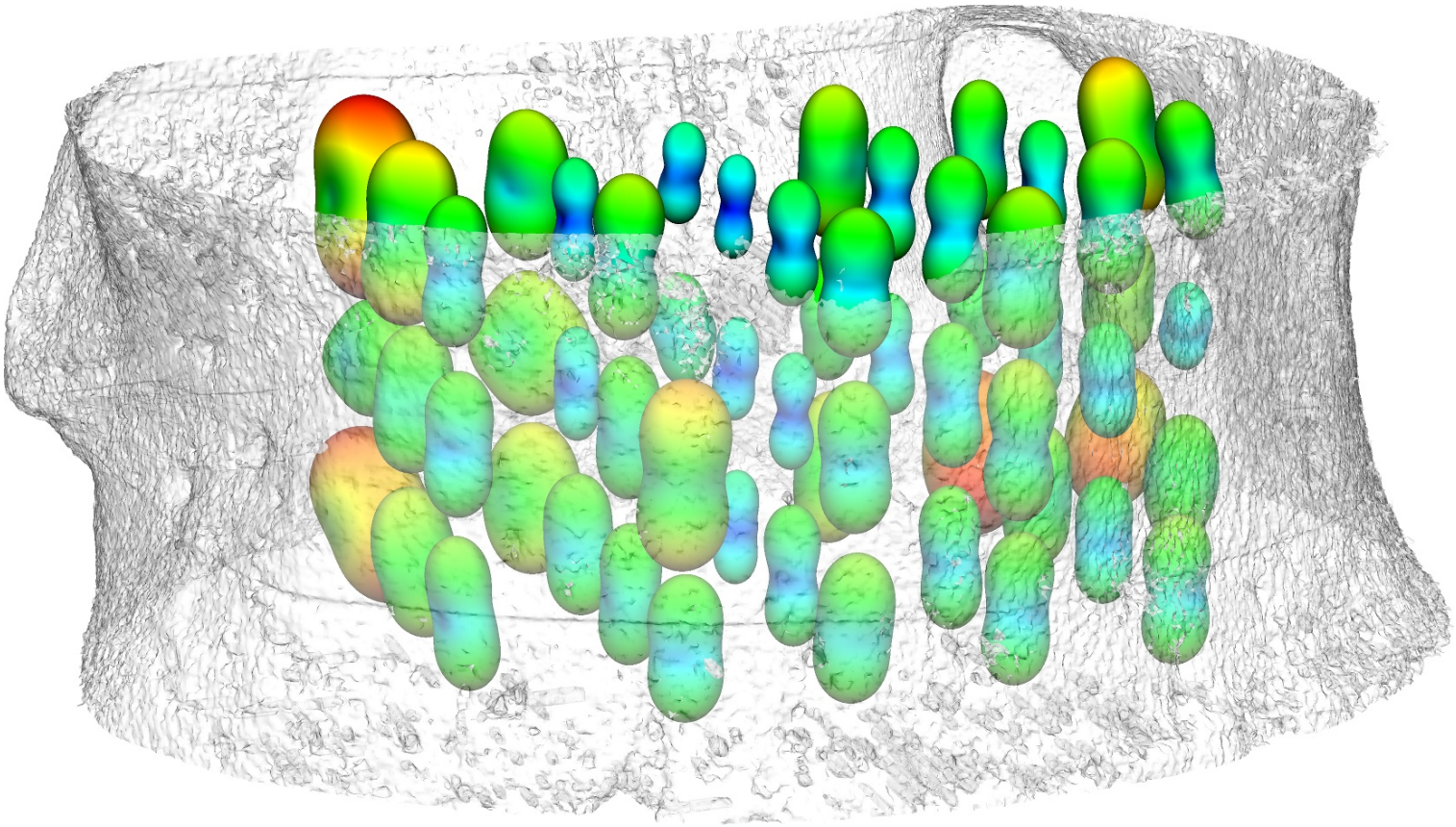
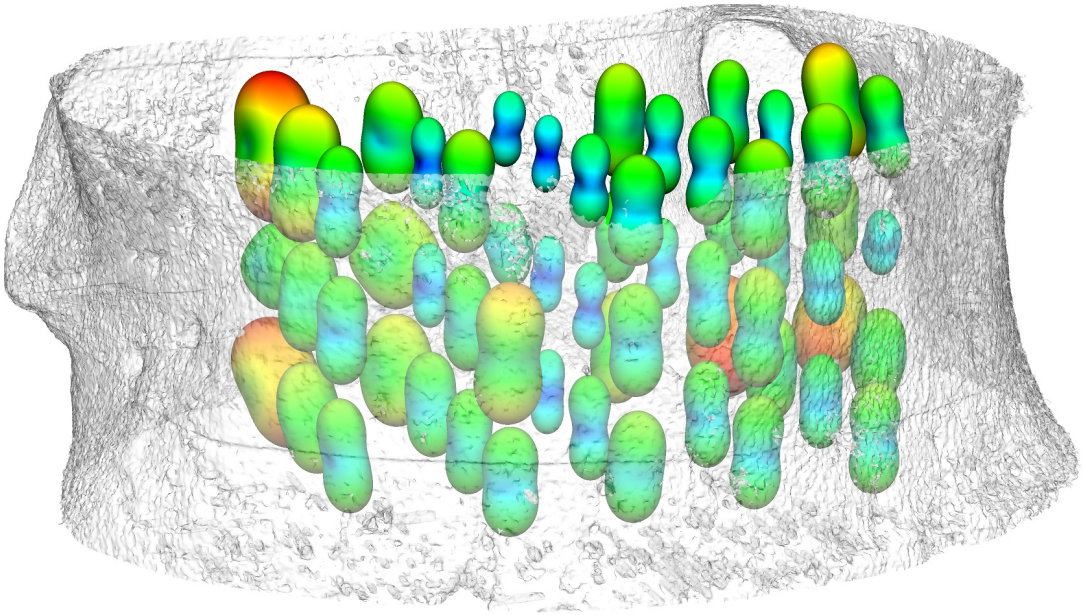


[L. O. Schwen et al, Proc. ECCOMAS 2012]

human ♀ L4 vertebra

5. From Experiment To Model

Two-Scale Simulation



[L. O. Schwen et al, Proc. ECCOMAS 2012]

- continuously varying elasticity tensor in trabecular interior (spongiosa)

5. From Experiment To Model

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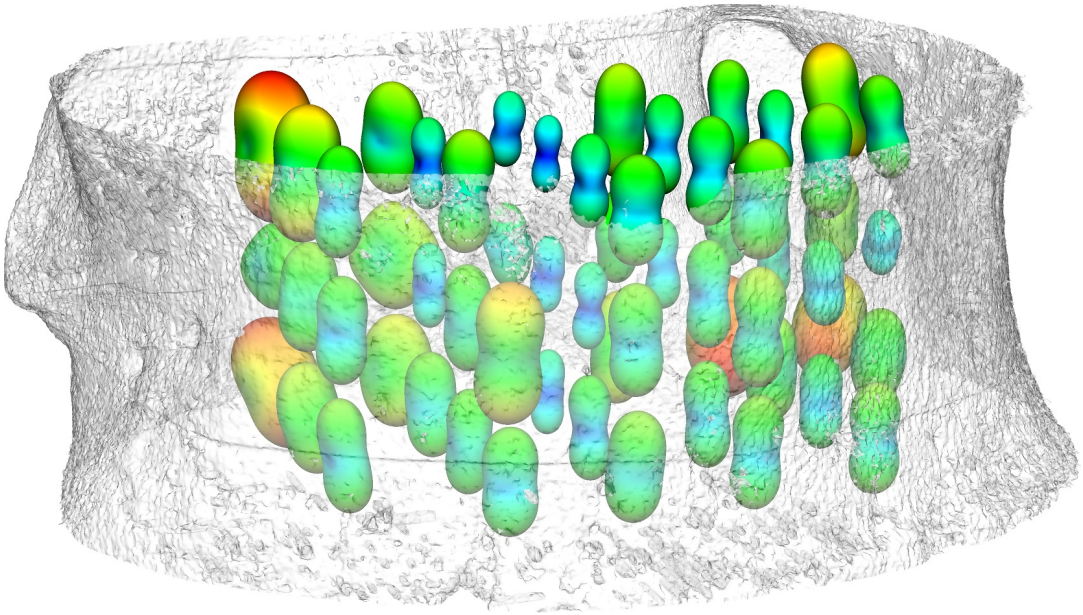

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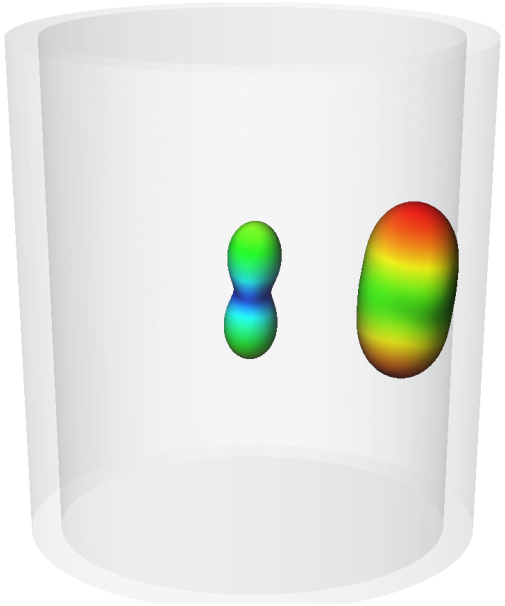
- higher stiffness in exterior wall (compacta)

5. From Experiment To Model

Two-Scale Simulation: Model Geometry



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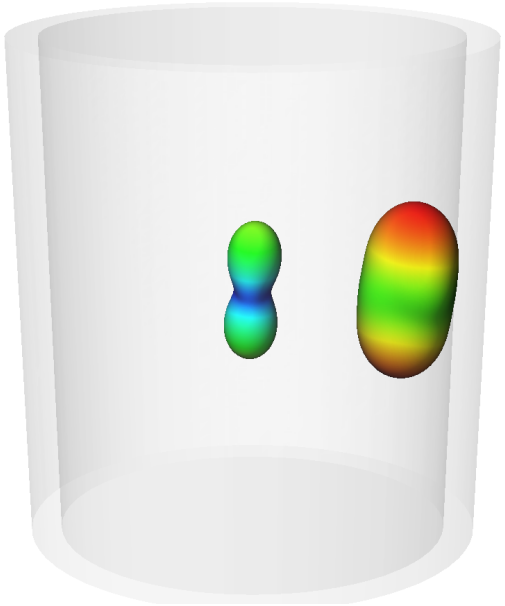

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- CFE elasticity simulation

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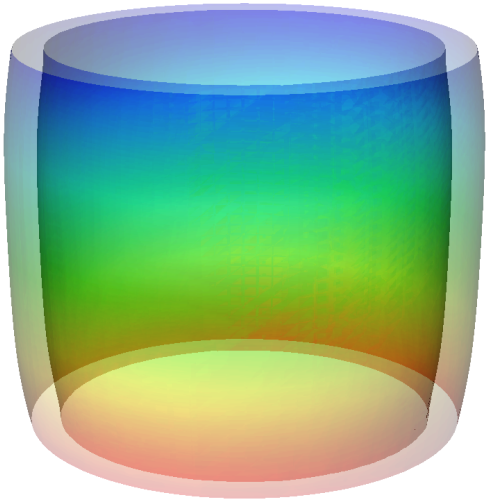

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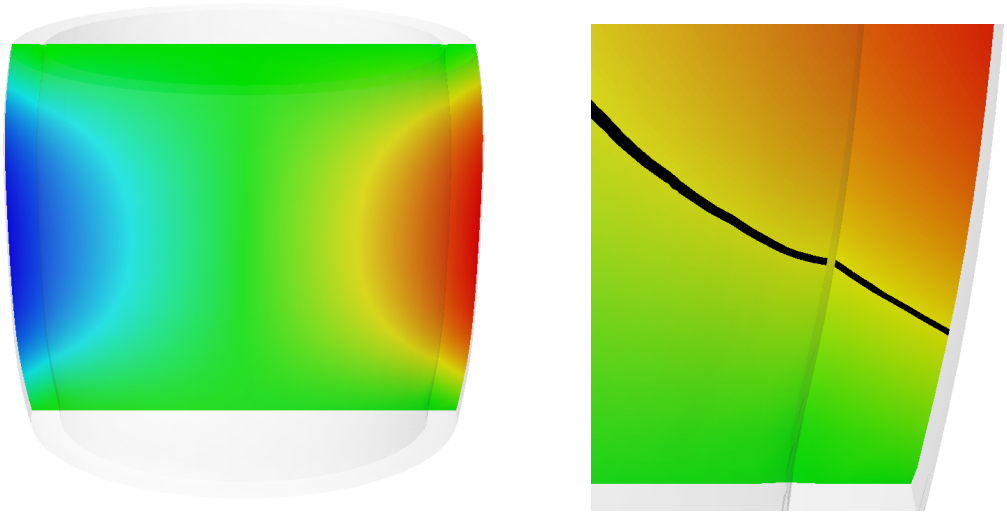

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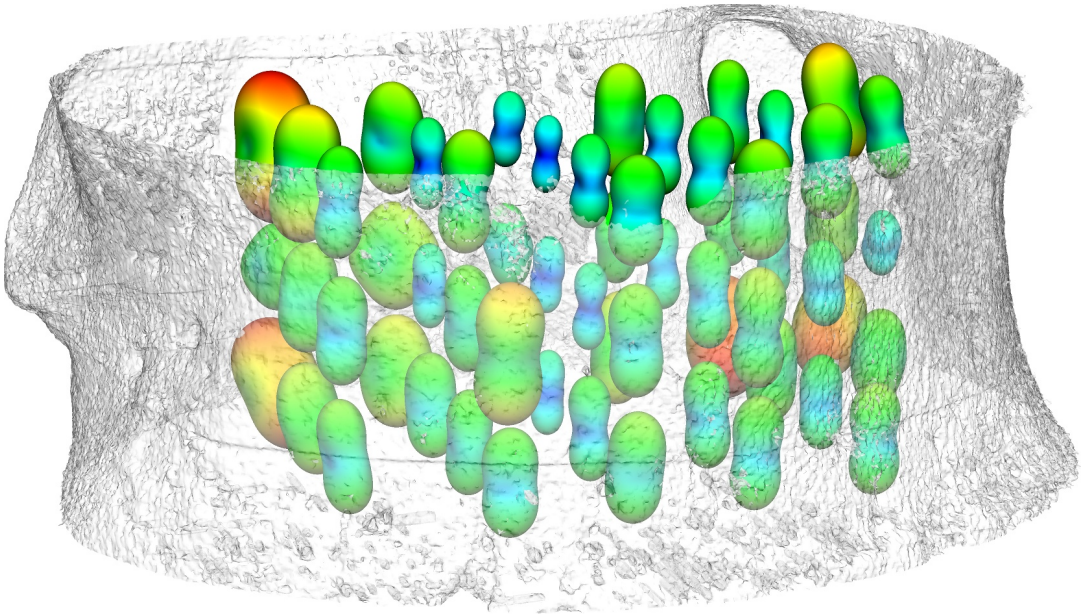
5. From Experiment To Model

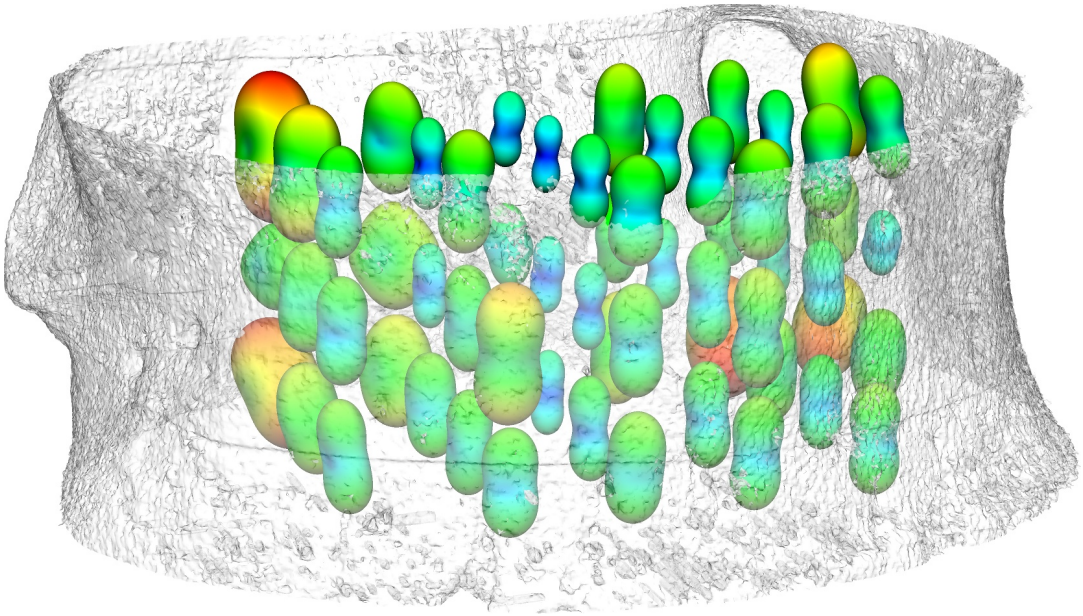
Outlook



- proper two-scale model

5. From Experiment To Model

Outlook



- proper two-scale model
- taking into account trabecular orientation
  (more realistic properties on the fine scale)

6. Summary

Contents

6. Summary

Elasticity Modeling of Trabecular Bone

- modeling and simulations require

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- trabecular bone has multiple scales
- homogenization yields effective material properties for coarser scales

6. Summary

Buzzword Check

6. Summary

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✔ **interdisciplinary** biomechanical experiments & mathematical simulation tools

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- ✔ **interdisciplinary** biomechanical experiments & mathematical simulation tools
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6. Summary

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- ✔ **interdisciplinary** biomechanical experiments & mathematical simulation tools
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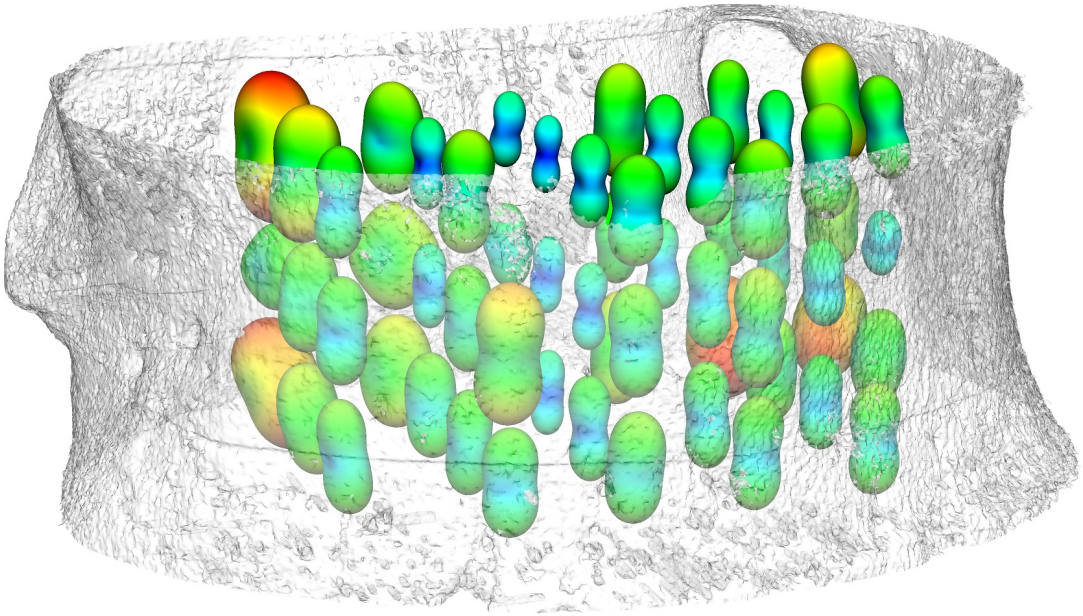
- ✘ **sustainable**

6. Summary

Buzzword Check

- ✔ **interdisciplinary** biomechanical experiments & mathematical simulation tools
- ✔ **nano** we did nanoindentation
- ✘ **real-time** unfortunately, we're far from that in terms of computational efficiency
- ✘ **sustainable**
- ■ **web 2.0** open source, but not more

6. Summary



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