Numerical homogenization in multi-scale models of musculoskeletal mineralized tissues

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This work was supported by the Deutsche Forschungsgemeinschaft within its priority program SPP1420 *Biomimetic Materials research: Functionality by Hierarchical Structuring of Materials* (grants GE1894/4 and Ra1380/7) and has been conducted within the framework of the European Associated Laboratory *Ultrasound Based Assessment of Bone* (ULAB).

Background and motivation

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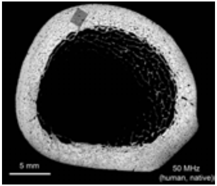
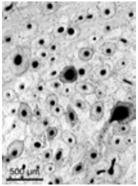
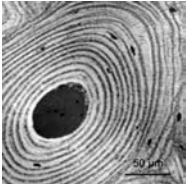
Bone-like materials

- are composed of simple constituents: collagen, mineral, water;
- are hierarchically structured across many length scales.

$\rightsquigarrow$ anisotropic materials displaying a great variety in mechanical function.







What is the importance of the hierarchical structure for mechanical function?

- Direct simulation across all length scales is not feasible.
- Homogenisation to “compress” information at fine scale.
- Use homogenised information at a coarser scale.

Experimental stiffness tensor

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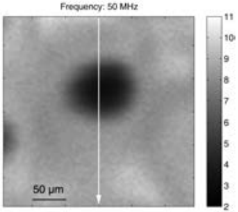
- Scanning Acoustic Microscopy (SAM)
  $\rightsquigarrow$ acoustic impedance map $Z(x)$ of bone cross section.
- Frequency of the acoustic beam determines scan resolution.
- $Z(x)$ strongly correlated with elastic stiffness coefficient in probing direction.

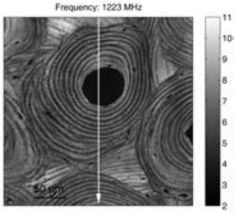
$\rightsquigarrow$ (with some additional assumptions): the elastic stiffness tensor $C(x)$.



$\Leftarrow$ coarse resolution

fine resolution $\Rightarrow$

$\Leftarrow$ experimental homogenisation $\Leftarrow$



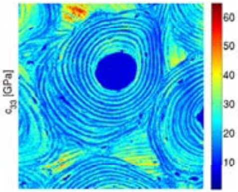
Details: [Raum, in: *Bone Quantitative Ultrasound*, Laugier & HaÃŕat (Eds.), Springer, 2011]

Numerische Mathematik

RVE-based homogenisation

Overview

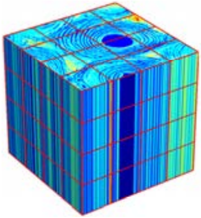
2D SAM data → $c_{33}(x)$



Extend $c_{33}(x)$ to $C(x)$

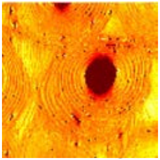
Translate to 3D RVE

Project on **regular** FE mesh



FE simulation of 6 independent loadings

σ_y @ 100 $\mu\varepsilon$



For each loading, average stress & strain over RVE

Computation of C^{eff} for equivalent homogeneous RVE from linear system

Reduction of complexity

$$\begin{pmatrix} C^{eff}_{11} & C^{eff}_{12} & \cdots & C^{eff}_{16} \\ C^{eff}_{21} & C^{eff}_{22} & \cdots & C^{eff}_{26} \\ \vdots & \vdots & & \vdots \\ C^{eff}_{61} & C^{eff}_{62} & \cdots & C^{eff}_{66} \end{pmatrix}$$

RVE-based homogenisation

Some Details

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- Solve equations of linear elasticity in cuboid domain for 6 independent loading cases, typically
  - linear displacement boundary conditions,
  - uniform traction boundary conditions, or
  - periodic boundary conditions

  to obtain apparent (=approximation of effective) material stiffness.

  Details: e.g. [Zohdi & Wriggers, *An Introduction to Computational Micromechanics*, Springer, 2008]
- Apparent stiffness tensor depends on choice of boundary conditions. The effective stiffness is, by definition, independent of it.
  - What is a suitable RVE size for the material at hand?

    See [Grimal et al., *A determination of the minimum sizes of representative volume elements for the prediction of cortical bone elastic properties*, Biomech Model Mechanobiol, 2011]
  - Self-consistent approach: embedding of RVE in homogenized material.

    $\rightsquigarrow$ leads to iterative procedure.

RVE-based homogenisation

Comsol implementation

Comsol Multiphysics with the Structural Mechanics Module and the Matlab LiveLink are the tools to implement the computation of the apparent stiffness tensor.

- Solid stress-strain physics mode (static analysis);
- Extrusion coupling variables and boundary constraints;
- Integration coupling variables and point constraints;

A first observation

The self-consistent approach requires only a few (4–6) iterations.
It is much more robust than the basic approach for materials with void pores.

Starting values for the linear/nonlinear solver

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For a homogeneous stiffness tensor, the exact solution of the PDE problem for all loading scenarios can be computed easily and used as starting value.

Which homogeneous stiffness tensor to use?

- Basic approach: estimate from heterogeneous stiffness data;
- Self-consistent approach: apparent stiffness estimate from previous iteration.

  This typically saves some iterations of the solver compared to starting with a zero solution but depends strongly on the microstructure!

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Larger efficiency gains:

Basic approach on increasingly finer grids:
transfer solution from coarser to starting values on finer grids.

Self-consistent approach:
use idea within each outer iteration but intricate interplay between outer iteration and grid refinement for efficient computation.

Choice of FE mesh

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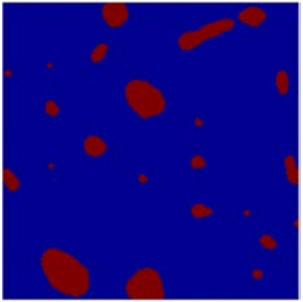
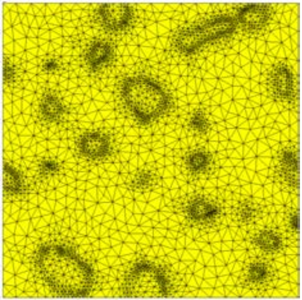
- Stiffness tensor at microscale often heterogeneous and a segmentation into fixed material classes (subdomains) not feasible.
- However, larger scale geometric features, like Haversian canals, should be resolved accurately by the mesh (this is where the action takes place!).





$\rightsquigarrow$ same accuracy at greatly reduced number of mesh elements compared to uniform mesh

- reduced CPU time
- reduced memory requirements

Comsol Version 3.5 vs. 4.x

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- Software implemented for both versions, but runs much faster in v3.5.
- Only difference: experimental data to compute stiffness tensor uses global Matlab variables set up before the Comsol run and used by model Matlab functions (v3.5) vs. the use of Comsol interpolation functions for the same purpose (v4.x).
- Problem: How to setup and use global variables in the Comsol Server Matlab in v4.x?
- Our (very recent) solution/workaround: Use a dummy Comsol model to set up and manage global variables for other models in the Comsol Server Matlab. (No timings yet.)

Does anybody have a nicer solution at hand?

Conclusions and future work

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- Developed a numerical homogenization scheme within Comsol Multiphysics with Matlab LiveLink.
- In principle, any structure or material can be inside the RVE, but
  - suitability and limitations have to be assessed for each application and
  - small and simple changes can improve the performance and reliability.

Future work:

Large RVE homogenization:

- large means too large to be solved as single instance on your computer;
- derive stiffness bounds from apparent stiffness of sub-RVEs;
- close bounds imply a good approximation of the effective stiffness of the large RVE.

Goal: establish technique and apply to human cortical bone to assess influence of pore network at mesoscale.