A Flexible Scheme for the Numerical Homogenisation in Linear Elasticity

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Background and motivation

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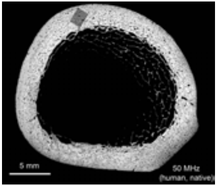
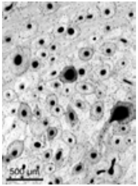
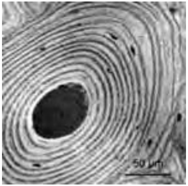
Bone-like materials

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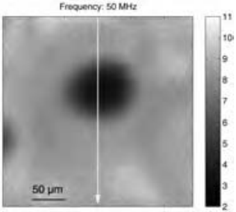
- Scanning Acoustic Microscopy (SAM)
  $\rightsquigarrow$ acoustic impedance map $Z(x)$ of bone cross section.
- Frequency of the acoustic beam determines scan resolution.
- $Z(x)$ strongly correlated with elastic stiffness coefficient in probing direction.

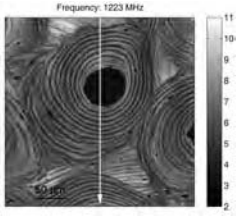
$\rightsquigarrow$ (with some additional assumptions): the elastic stiffness tensor $C(x)$.



$\Leftarrow$ coarse resolution

fine resolution $\Rightarrow$

$\Leftarrow$ experimental homogenisation $\Leftarrow$

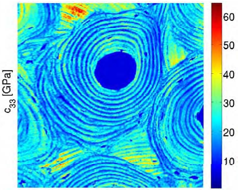


Details: [Raum, in: *Bone Quantitative Ultrasound*, Laugier & Haïat (Eds.), Springer, 2011]

Overview homogenisation

Numerical homogenization approach

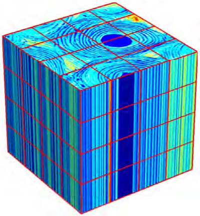
2D SAM data → $c_{33}(x)$



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

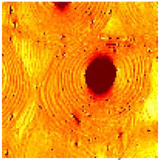
Translate to 3D RVE

Project on **regular** FE mesh



FE simulation of 6 independent loadings

σ_y @ 100 με



Reduction of complexity

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

$\int$ For each loading, average stress & strain over RVE

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

PDE problem: equations of linear elasticity

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Given:

- cuboid domain $\Omega \subset \mathbb{R}^3$, the representative volume element (RVE) and
- stiffness tensor $C(x)$ for $x \in \Omega$.

Determine displacement field $u = (u_1, u_2, u_3) : \Omega \to \mathbb{R}^3$ from

$$-\partial_j(\underbrace{C_{ijkl}(x)\epsilon_{kl}(x)}_{\text{stress } \sigma(x)}) = 0\,,\ x \in \Omega\,, \quad \text{where } \underbrace{\epsilon(x)}_{\text{strain}} := \frac{1}{2}\left(\nabla u(x) + (\nabla u(x))^{\mathsf{T}}\right) \qquad \text{(LE)}$$

subject to given boundary conditions (displacement, traction, periodic).

Comsol: Structural Mechanics Module, Solid stress-strain (static analysis).

Remark: for our application we only need zero volume forces in (LE).

Numerical homogenisation: RVE approach

[Zohdi & Wriggers, *An Introduction to Computational Micromechanics*, Springer, 2008]

1. Solve (LE) for six independent sets of boundary conditions (BCs)
   $\rightsquigarrow u^{(i)}(x), \epsilon^{(i)}(x), \sigma^{(i)}(x), i = 1, 2, \ldots, 6$.
2. The symmetric tensors $\epsilon^{(i)}(x)$ and $\sigma^{(i)}(x)$ are rearranged as vectors $\underline{\epsilon}^{(i)}(x), \underline{\sigma}^{(i)}(x) \in \mathbb{R}^6$.
3. Compute volume averages $\left\langle \underline{\epsilon}^{(i)} \right\rangle$ and $\left\langle \underline{\sigma}^{(i)} \right\rangle$ over Ω and arrange the vectors columnwise as matrices $\langle \underline{\epsilon} \rangle$ and $\langle \underline{\sigma} \rangle$.
4. The apparent stiffness tensor (in matrix form) is then defined by

$$\langle \underline{\sigma} \rangle = \underline{\underline{C}}^{\text{app}} \langle \underline{\epsilon} \rangle \ .$$

$\underline{\underline{C}}^{\text{app}} \approx \underline{\underline{C}}^{\text{eff}}$, the effective stiffness of the material at the scale of the RVE Ω.
$\rightsquigarrow \underline{\underline{C}}^{\text{app}}$ captures smaller-scale information.

Sets of boundary conditions (1)

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1. Pure linear displacements boundary conditions

$$u(x) = M^{(i)}x \quad \text{for all } x \in \partial\Omega\,.$$

2. Pure tractions boundary conditions ($n(x)$ = unit outer normal at $x \in \partial\Omega$)

$$\sigma(x)n(x) = M^{(i)}n(x) \quad \text{for all } x \in \partial\Omega\,.$$

Remark: requires additional constraint for a unique solution u.

Choice of matrices $M^{(i)}$:

$$\begin{pmatrix}\beta & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & 0\end{pmatrix},\begin{pmatrix}0 & 0 & 0\\ 0 & \beta & 0\\ 0 & 0 & 0\end{pmatrix},\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & 0\\ 0 & 0 & \beta\end{pmatrix},\begin{pmatrix}0 & \beta & 0\\ \beta & 0 & 0\\ 0 & 0 & 0\end{pmatrix},\begin{pmatrix}0 & 0 & 0\\ 0 & 0 & \beta\\ 0 & \beta & 0\end{pmatrix},\begin{pmatrix}0 & 0 & \beta\\ 0 & 0 & 0\\ \beta & 0 & 0\end{pmatrix}$$

Sets of boundary conditions (2)

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3. Periodic boundary conditions

$$u(x) - P^{(i)}(x) \quad \text{is periodic for } x \in \partial\Omega \quad \text{and } \left\langle u - P^{(i)} \right\rangle = 0\,.$$

Here:

$$P^{(i)}(x) = \begin{pmatrix} x \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ y \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ z \end{pmatrix}, \begin{pmatrix} y \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ z \\ 0 \end{pmatrix}, \begin{pmatrix} z \\ 0 \\ 0 \end{pmatrix}.$$

Details: [Cioranescu & Donato, *An Introduction to Homogenization*, OUP, 1999]

Implementation issues

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Comsol, using its Matlab programming interface, provides the tools required to implement the computation of the apparent stiffness tensor $\underline{\underline{C}}^{\text{app}}$.

- displacement and traction BCs: implemented in “solid” application mode;
- periodicity constraints: implemented using extrusion coupling variables and boundary constraints;
- volume average constraints: implemented using integration coupling variables and point constraints;
- stress/strain averages: implemented using integration coupling variables.

Remarks:

- Higher accuracy for periodic BCs on periodic (unstructured) boundary mesh.

Numerical results: the lamellar unit (1)

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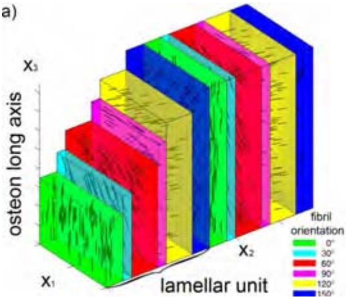
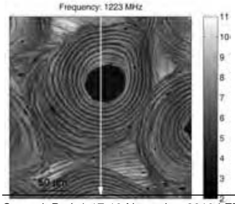
The lamellar unit

- is the structural building block of an osteon;
- is a layered structure with fixed orientation θ_i of mineralised collagen fibrils in each layer i;
- the orientation changes from layer to layer.





Model input data:

- SAM at 1.2 GHz is used to derive a transverse isotropic stiffness tensor $C(\theta)$ for $\theta = 0$;
- b the stiffness tensor $C(\theta_i)$ in layer i is obtained by rotating $C(0)$.

Numerical results: the lamellar unit (2)

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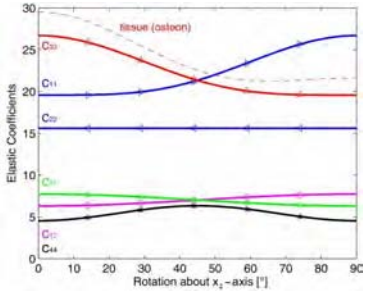
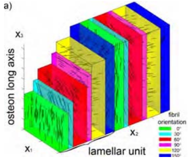
- The LU model: *asymmetric plywood*, twist angle 30°. Homogenisation recovers (experimental) anisotropy at osteon scale.
- Other LU models: symmetric or orthogonal plywood ⇝ do not result in this characteristic anisotropic feature.

⇝ *asymmetric plywood*: strong candidate for real structure at the LU-level of organisation.





Self-consistent RVE scheme

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The effective stiffness of an RVE is independent of applied BCs.

Goal: Reduce influence of applied BCs in computation of apparent stiffness $\underline{\underline{C}}^{\text{app}}$.

Method: embed RVE Ω in domain $\tilde{\Omega}$ and use material with the (yet unknown) effective/apparent stiffness in $\tilde{\Omega} \setminus \Omega$.

$\rightsquigarrow$ iterative scheme computing $\underline{\underline{C}}^{\text{app},0}, \underline{\underline{C}}^{\text{app},1}, \ldots$

1. Set $i = 0$ and initial guess for apparent stiffness $\underline{\underline{C}}^{\text{app},0}$.
2. Solve (LE) in $\tilde{\Omega}$ with $\underline{\underline{C}}^{\text{app,i}}$ for given BCs.
3. Compute stress/strain averages in embedded RVE Ω and determine $\underline{\underline{C}}^{\text{app,i+1}}$.
4. IF distance($\underline{\underline{C}}^{\text{app,i}}, \underline{\underline{C}}^{\text{app,i+1}}$) $\leq$ tolerance (convergence test)
   THEN
   $\underline{\underline{C}}^{\text{app}} := \underline{\underline{C}}^{\text{app,i+1}}$, RETURN.
   ELSE
   $i := i + 1$ and GOTO step 2.

Implementation issues

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- The standard RVE approach can be fully utilised with minor changes.
- Reuse solution u of ith iteration as initial solution guess in iteration $i + 1$.
- In our application, a few (4–6) iterations are usually sufficient for convergence.
- If the RVE has void pores then the embedding of the RVE makes the computations more robust.

Conclusions

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- Developed a numerical homogenisation scheme within Comsol Multiphysics.
- In principle, any material or structure can be inside the RVE.
- Periodic grids improve accuracy with periodic BCs.

Open problems and outlook

- Periodic BCs:
  - the linear iterative solver has convergence problems;
  - occasionally, the grid does not turn out to be periodic.
- Further improvements in required CPU time by spatial adaptivity.
- But: Periodic grids prevent (simple) use of spatial adaptivity.
- Tests with other homogenisation problems (also non-bone).