# Modeling and Simulation of Surfactant Effects on Finely Resolved Alveolar Structures

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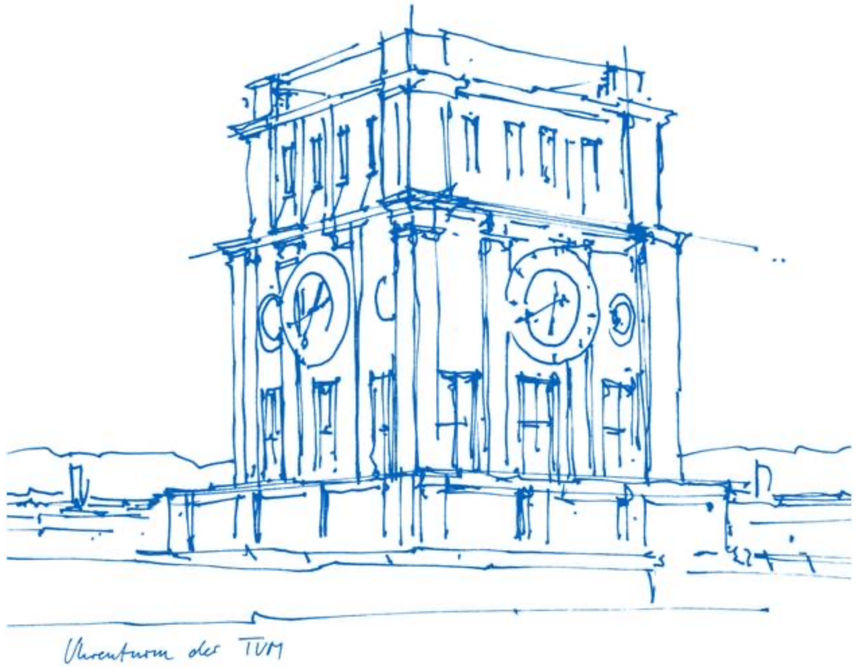
dealii-X Seminar Series: Lung Application

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## Motivation

- Respiratory diseases are common.
- Lung injuries can be deadly.
- Ventilation-induced lung injury (VILI) is a critical problem in patient care.
- Better understanding of respiratory mechanics is necessary.
- Personalized medicine is not the future, but the present.

# Approaches to Lung Modeling

Lung mechanics incorporates extreme scale differences, as well as many different quantities of interest and questions.

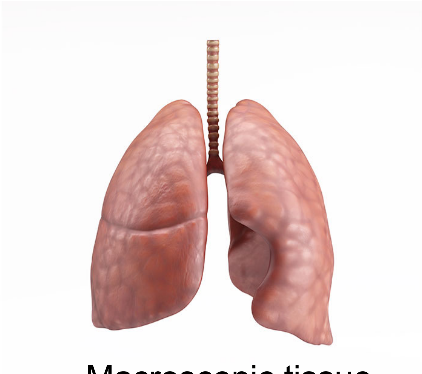
- Local strains
- Local oxygenation
- Drug distribution
- Diseases
- Collapse/Recruiting
- Perfusion

Macroscale

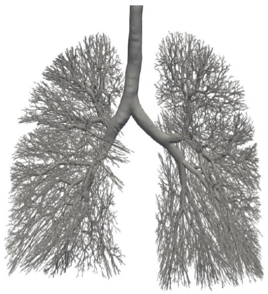
Microscale

- Reduced order models
- Elasticity problems
- Porous media – coupled problems
- Incompressible flow and transport

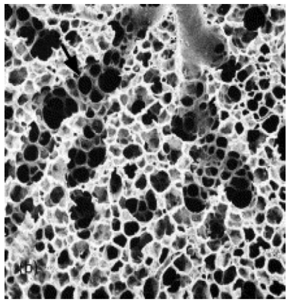
# Approaches to Lung Modeling



Macroscopic tissue



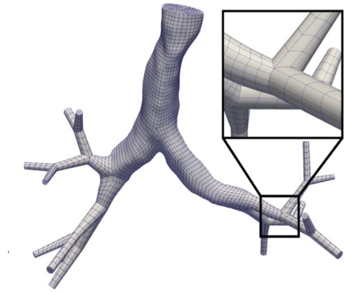
Airway tree



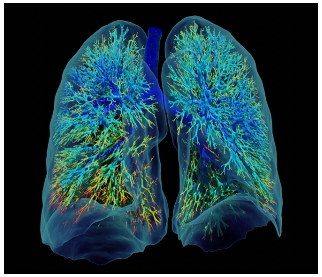
Lande et al., 2021

Microscopic tissue

Köglmeier et al., 2026



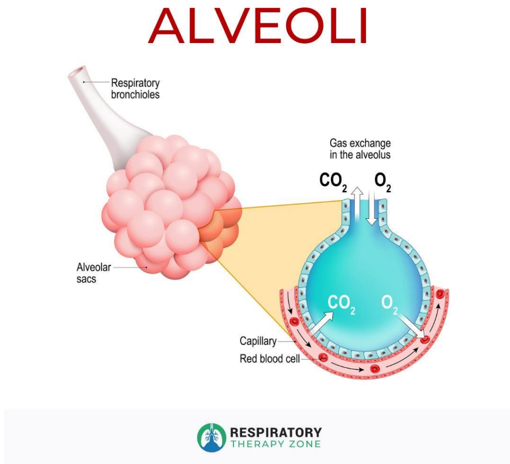
Kronbichler et al., 2021



Ebenbuild GmbH

# Surface Tension & Surfactant

- Lung models are very valuable and are currently being used to model many different effects.
- However, one vital effect is still missing: Surfactant
- Surfactant increases the compliance and keeps the lungs from collapsing.
- Its deficiency is fatal. External surfactant is classified as an essential medicine.
- Not clear, how to incorporate this into the very involved mathematics of homogenization for porous media models.



# Nonlinear Elastic Formulation

Balance equation and BCs:

$$\nabla_0 \cdot \boldsymbol{P} + \boldsymbol{b}_0 = \boldsymbol{0} \quad \text{in} \quad \Omega_0$$
$$\boldsymbol{d} = \hat{\boldsymbol{d}} \quad \text{on} \quad \Gamma_0^D$$
$$\boldsymbol{P} \cdot \boldsymbol{N} = \hat{\boldsymbol{t}} \quad \text{on} \quad \Gamma_0^N$$

Hyperelastic constitutive equation:

$$\boldsymbol{F}^{-1}\boldsymbol{P} = \boldsymbol{S} = 2\frac{\partial \Psi}{\partial \boldsymbol{C}}$$

Kinematic equation:

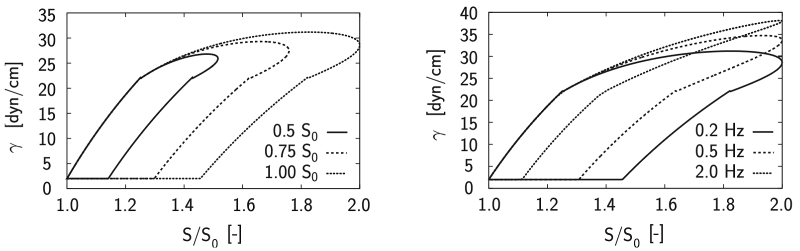
$$\boldsymbol{F} = \boldsymbol{I} + \frac{\partial \boldsymbol{d}}{\boldsymbol{X}}$$
$$\boldsymbol{C} = \boldsymbol{F}^T\boldsymbol{F}$$

Strain energy density function: [1]

$$\Psi = \frac{E(1-2\nu)}{4\nu + 4\nu^2}(I_3^{-\frac{\nu}{1-2\nu}} - 1) + \frac{E}{4-4\nu}(I_1 - 3)$$

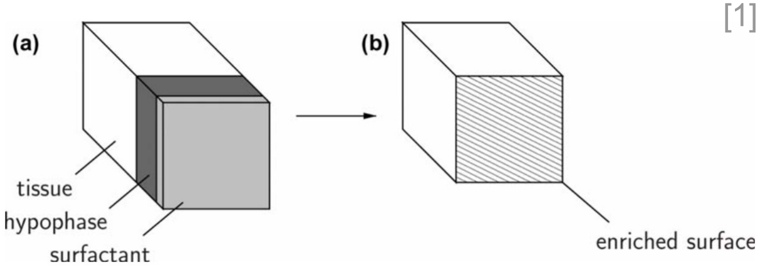
[1] Rausch et al. “Material model of lung parenchyma based on living precision-cut lung slice testing”. Journal of the Mechanical Behavior of Biomedical Materials (2011)

# Modeling the Surfactant Behavior




[1]

Surfactant effects are highly nonlinear.




[1]

- We couple structural and interfacial mechanics in terms of an enriched surface on structural elements.[2]

$$W_{\text{surf}} = \int_{S_0}^{S} \gamma(S^*)\mathrm{d}S^*$$

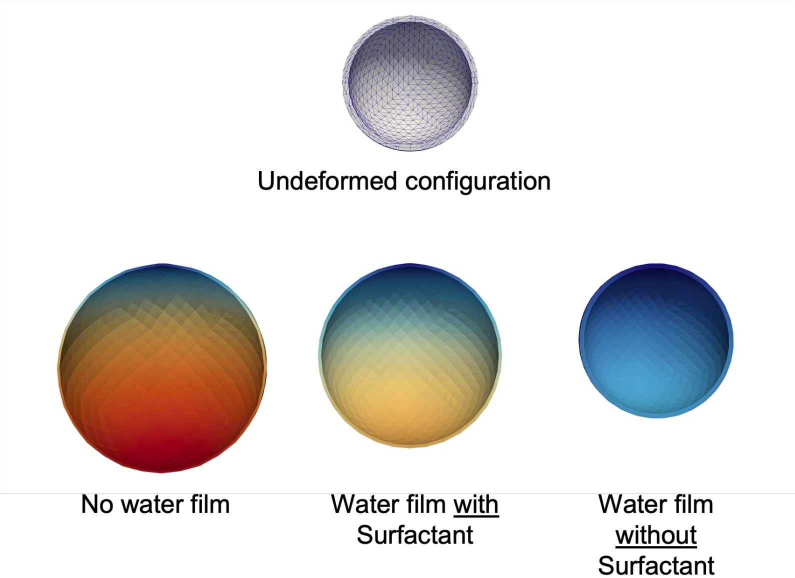
- Stress-term on the boundary

$$\boldsymbol{P}_\gamma := \gamma(S)||\boldsymbol{n}^*||(\boldsymbol{I} - \boldsymbol{n} \otimes \boldsymbol{n}) \cdot \boldsymbol{F}^{-T}$$

- Evolutionary model for the surface tension $\gamma$ and surfactant concentration.

[2] Wiechert et al. “Modeling the Mechanical Behavior of Lung Tissue at the Microlevel”. Journal of Engineering Mechanics (2009)

# Surfactant Model




- The surfactant model contains many parameters:

$$\gamma = \gamma\left(\gamma_0, \gamma_{\mathrm{eq}}, \gamma_{\mathrm{min}}, \Gamma_{\mathrm{max}}, k_1, k_2, C\right)$$ [3]

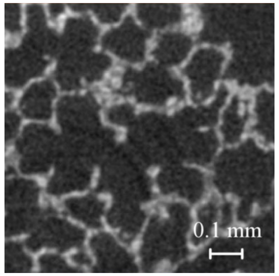
- These parameters are uncertain, for example:

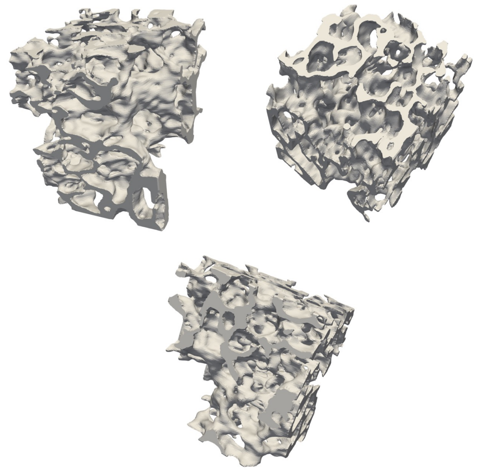
$$\gamma_{\mathrm{min}} = 10\ \mathrm{dyn/cm} \quad \mathrm{OR} \quad \gamma_{\mathrm{min}} = 2\ \mathrm{dyn/cm}$$

[3] Denny & Schroter "Viscoelastic Behavior of a Lung Alveolar Duct Model". Journal of Biomechanical Engineer (2000)

# Surfactant Effects on the Alveolar Structures

- Dynamic surface tension renders the structural problem very non-linear and time-dependent.
- Very large number of simulations on a huge domain is necessary to extract enough relevant information for homogenization.



[4]

Computational mesh of the alveolar structures

Is enabled by current developments in HPC.

[4] Rausch et al. “Local Strain Distribution in Real Three-Dimensional Alveolar Geometries”. Annals of Biomedical Engineering (2011)

# Development: ExaDG & deal.II

- We use ExaDG for our application. Why?
  - Nicely abstracted use of the matrix-free infrastructure in deal.II,
  - Tried and tested in large-scale computations,
  - Extensible software,
  - Affinity to biomechanics applications,
  - Developments on hyperelasticity are very promising for our use case. [5]

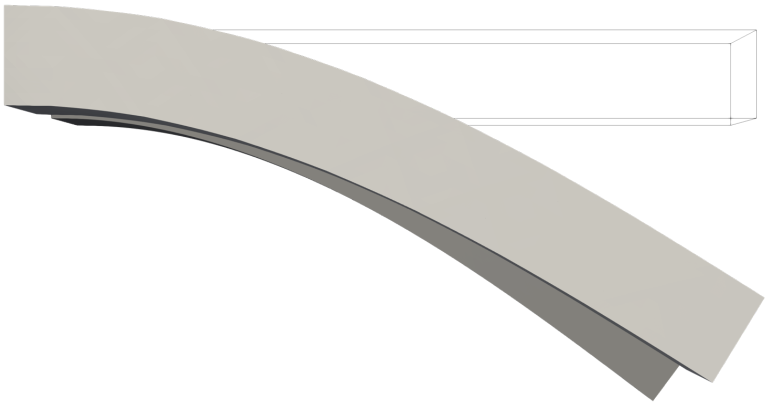
**dealii-X/exadg**

[5] Schussnig et al. “Matrix-Free Higher-Order Finite Element Methods for Hyperelasticity”, Computer Methods in Applied Mechanics and Engineering (2025)

# Locking

The alveolar simulations are prone to both:

- Shear locking due to the thin alveolar walls, and
- Volumetric locking due to the nearly incompressible biological tissue.

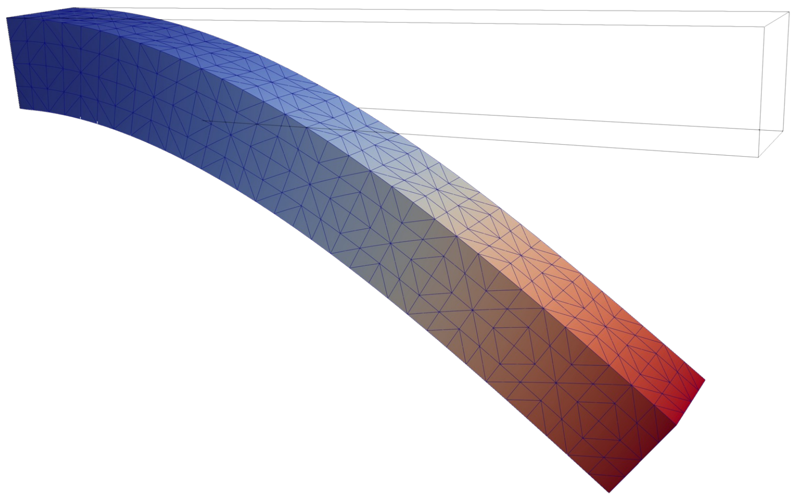


TET4 (light) vs. TET10 (dark)

➡ Using higher-order elements, e.g., TET10 or TET20, can remedy locking for nearly incompressible materials.

# Bending Beam

Under the clear presence of locking with linear TETs, is the solver affected?



Preconditioner 1:
Algebraic Multigrid with a Chebyshev smoother and a direct solution of the coarse problem.

Preconditioner 2:
Polynomial Multigrid with a Chebyshev smoother and an application of Preconditioner 1 on the coarse problem (linear polynomials).

# Bending Beam

Solver statistics for a quasi-static bending beam problem.
100 load increments, ~14k DoFs, run serially on Intel Core i9-9900

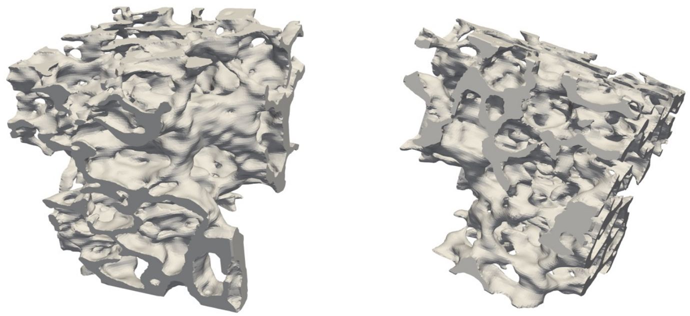
| | Compressible & AMG | Compressible & pMG | Incompressible & AMG | Incompressible & pMG |
|---|---|---|---|---|
| Avg. # of Newton iter. per load step | 2.00 | | 2.71 | |
| Avg. # of lin. iter. per Newton iter. | 22.2 | 10.2 | 67.8 | 28.9 |
| Wall time | 72.8 s | 39.8 s | 224 s | 135 s |

## Computational Mesh

Synchrotron-based X-ray tomographic microscopy.

- High-resolution 3D images of an approx. 300 $\mu$m x 300 $\mu$m cubic domain.

- ~3 million cells
- ~2 million DoFs for linear tetrahedra
- ~12.5 million DoFs for quadratic tetrahedra

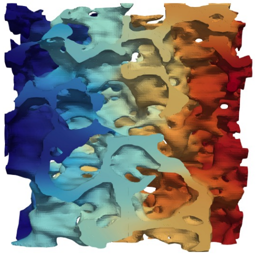


[4]

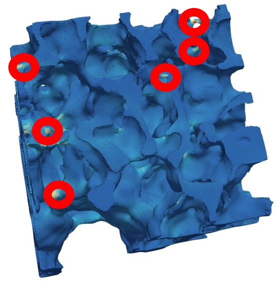
Cell refinement as well as higher order polynomials are required for sufficient resolution of thin walls and representation of smooth surfaces.

[4] Rausch et al. “Local Strain Distribution in Real Three-Dimensional Alveolar Geometries”. In: Annals of Biomedical Engineering 39.11 (2011)

## Initial Simulation Results



Unixial tension on the alveolar structure



Strain hotspots on thin walls

On an AMD EPYC 9354 with the quadratic TET mesh:

- pMG: 0.5 seconds per iteration with ~20 iterations per Newton step,
- AMG: 0.9 seconds per iteration with ~37 iterations per Newton step.

**Q:** How does the water film (+ surfactant) affect the results?

# Outlook

- Extensive numerical experiments with dynamic surfactant effects.
- Domain growth techniques.
- Performance optimization and GPU porting.
- Sensitivity analysis & homogenization study, possible use of learning approaches for material modelling.

**Thank you for your attention!**