Lehrstuhl für Numerische Mechanik

SuperMUC-NG – Next-Gen Science Symposium

November 22nd, 2018 – Garching, Germany

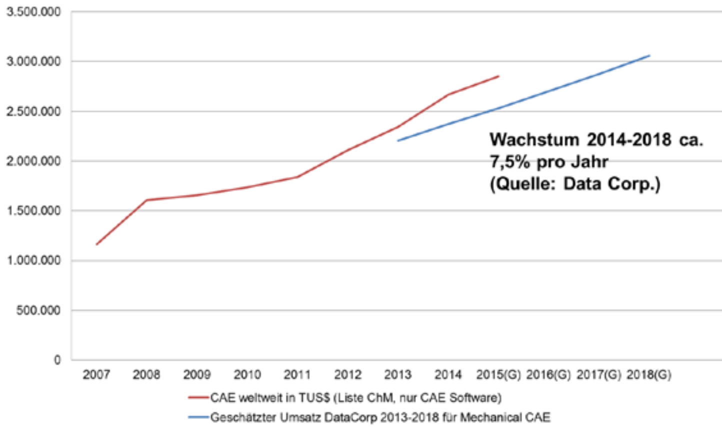
Predictive HPC Engineering – Towards a paradigm shift in healthcare

Wolfgang A. Wall & Martin Kronbichler
& many more members of the LNM team

B. Svetnik (2006)

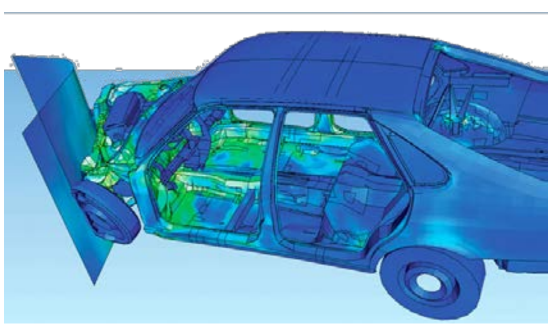
Institute for Computational Mechanics @ Technical University of Munich

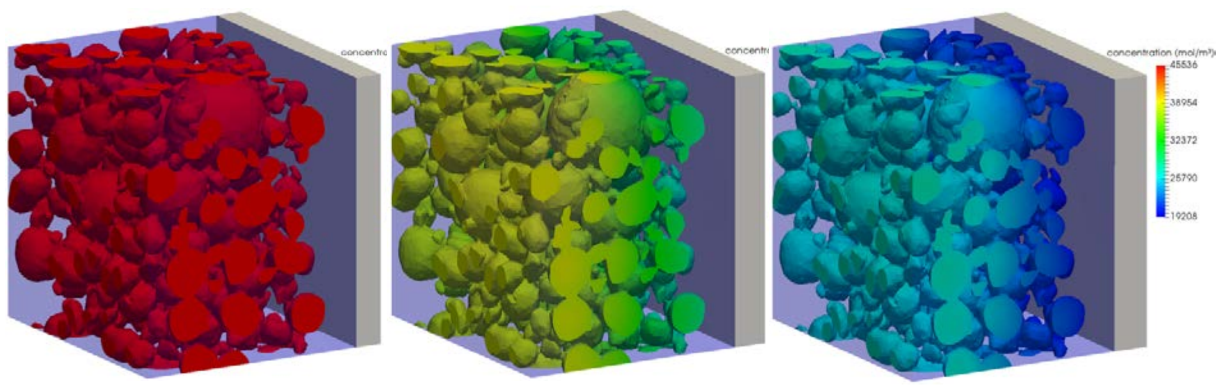
Importance of CAE



„The Global CAE market is mainly driven by discrete manufacturing industries worldwide. In terms of geography, the majority of the growth comes from the Americas, which is followed by the EMEA and the APAC regions. The overall market is expected to grow at a CAGR of ***11.34 percent from 2014-2019***."

"Interpolation / extrapolation" vs. *Predictive* (first principle based)

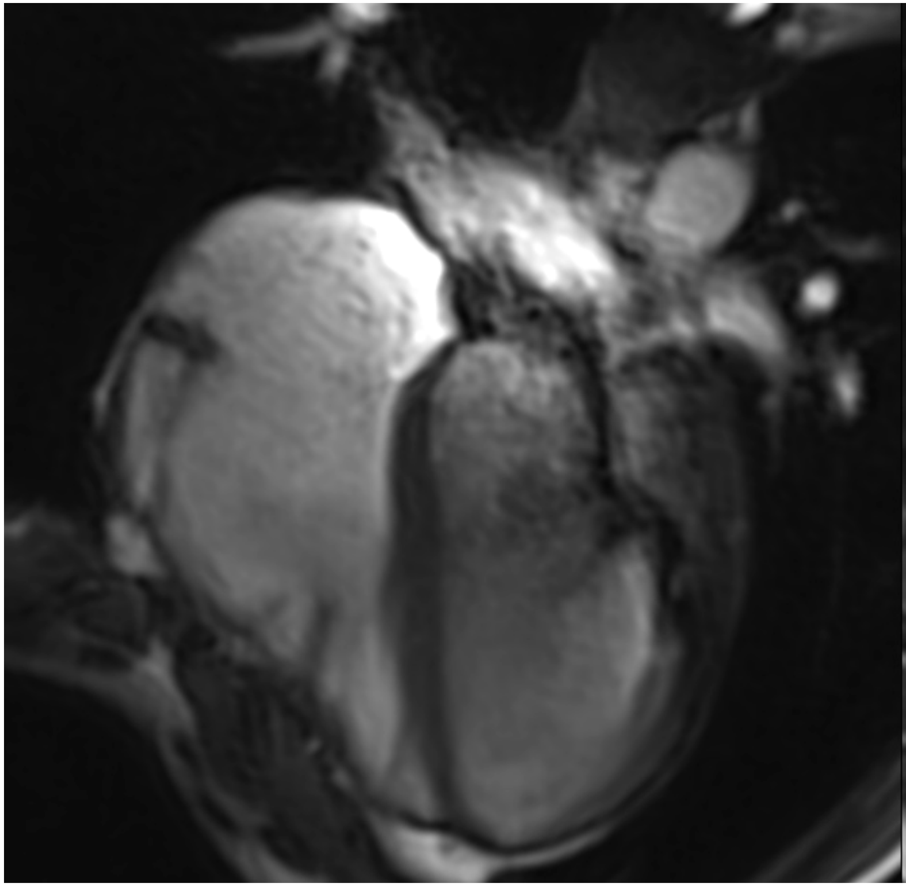




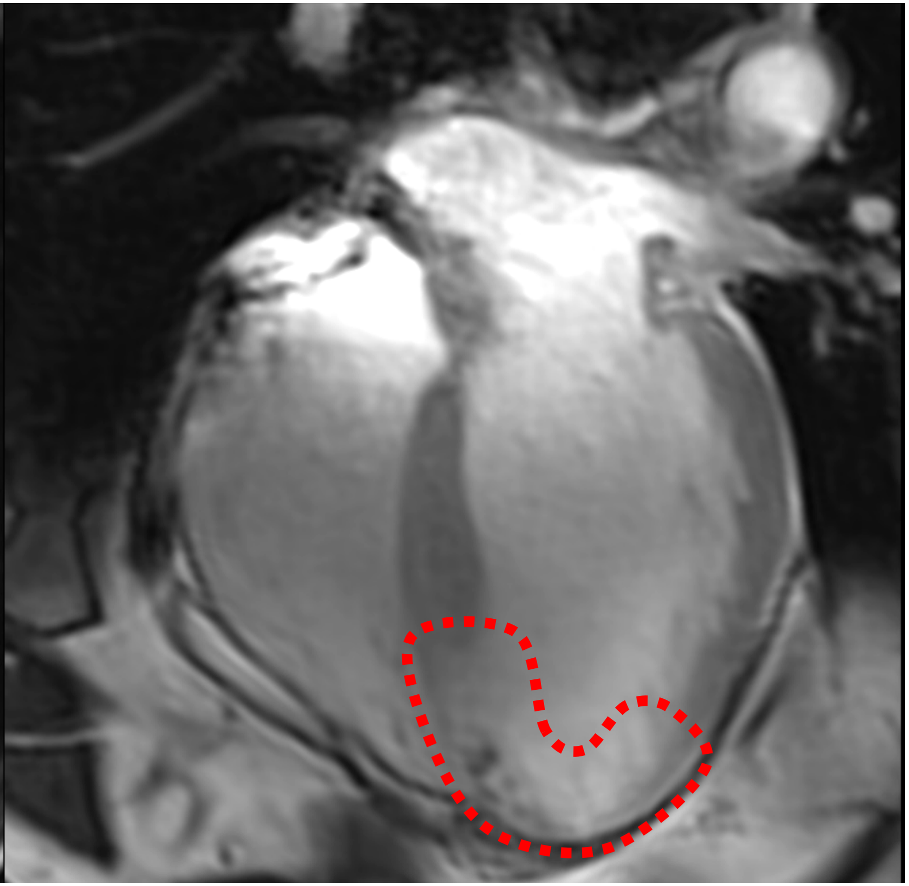
… not only individual, patient-specific, but

Predictive Medicine

The human heart



Healthy (24y)



Myocardial Infarction (60y)

Images: Cristoph Rischpler, Department of Nuclear Medicine, TUM

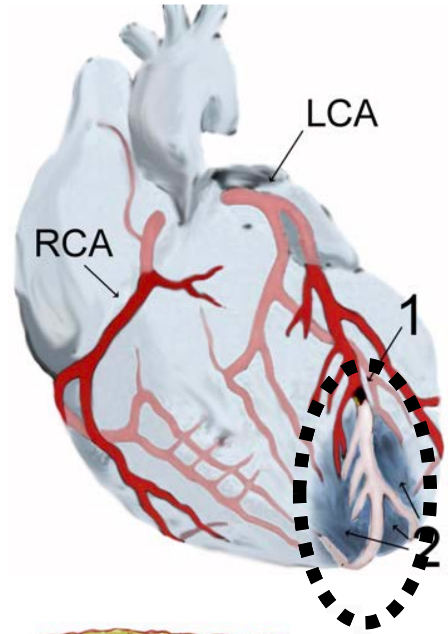
Cardiac modeling

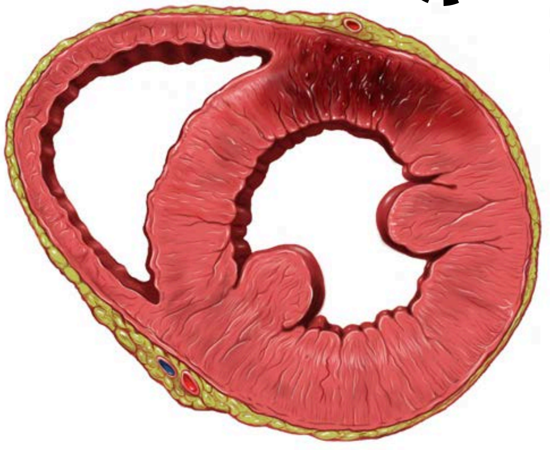
M. Pfaller, J. Hörmann, A. Nagler, C. Bertoglio

Governing physics
- Electrophysiology
- Active mechanics
- Fluid (reduced)

Modeling of post-infarction healing
- adaption to mechanical environment
- growth and remodeling

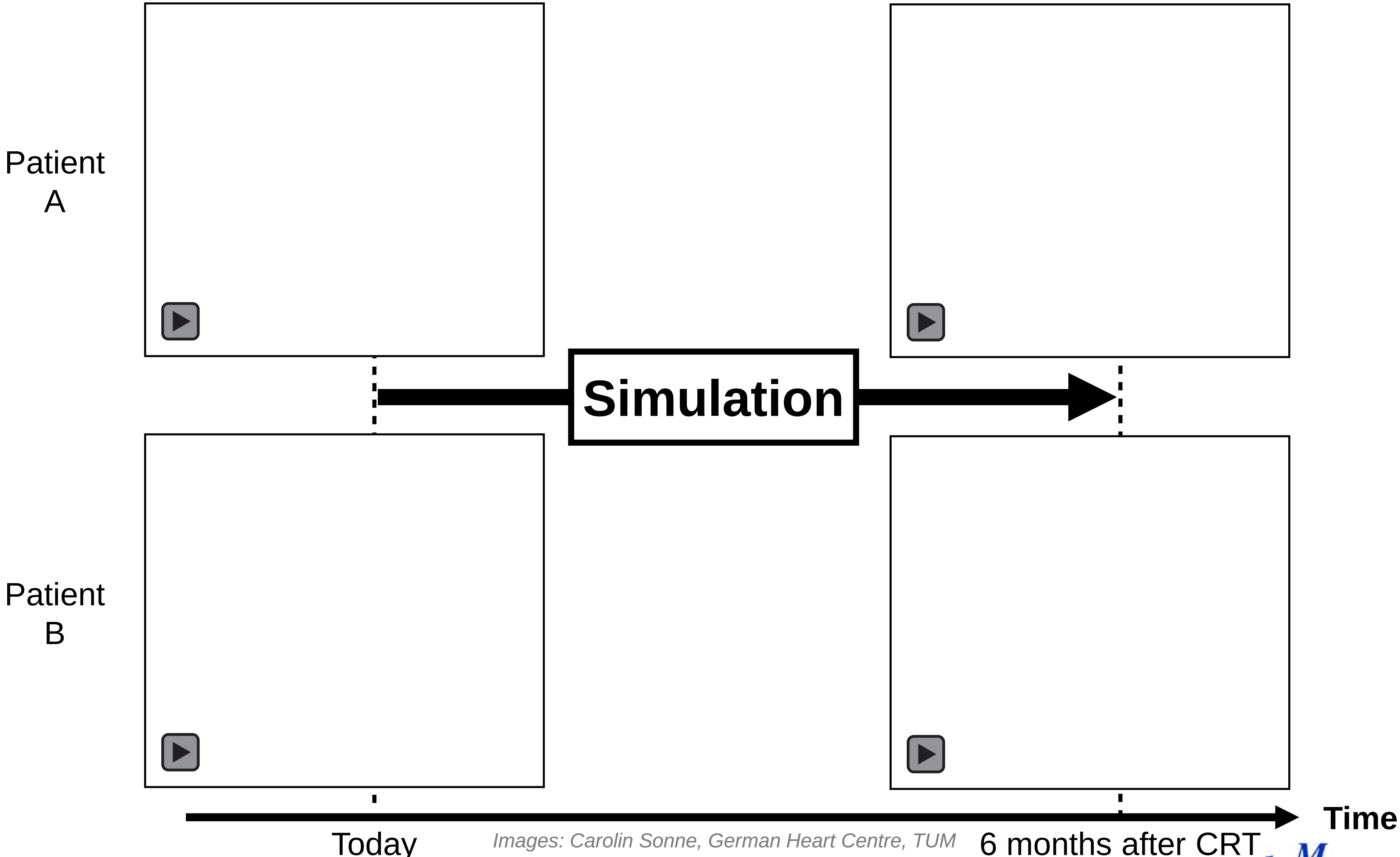
Some clinical applications
- predict long term patient response
- patient-specific therapy optimization
- select eligible patients
- …





Images:
J. Heuser, commons.wikimedia.org/wiki/File:AMI_scheme.png
Patrick J. Lynch, commons.wikimedia.org/wiki/File:Heart_ant_wall_infarction.jpg

Myocardial infarction



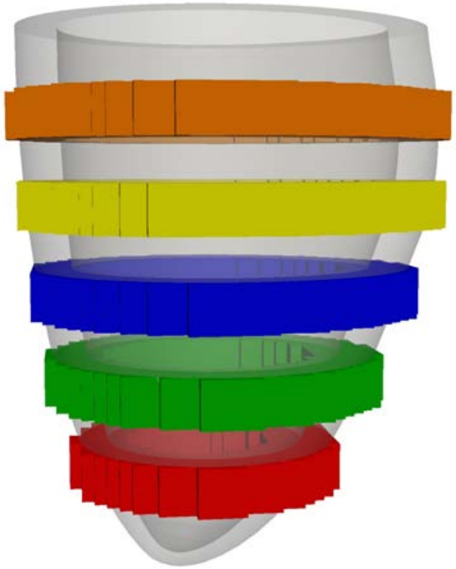
Images: Carolin Sonne, German Heart Centre, TUM

Fiber architecture

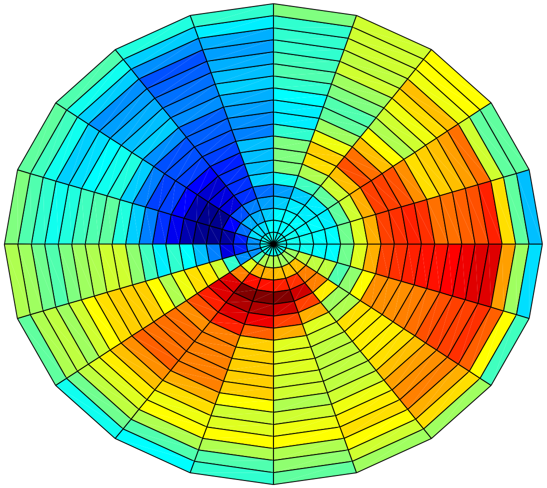
Maximum likelihood estimator

$$\widehat{\boldsymbol{\alpha}}_{k_h,k_t} = \underset{\boldsymbol{\alpha}}{\operatorname{argmin}} \left(\frac{N}{2} \log 2\pi\sigma^2 + \frac{1}{2\sigma^2} \sum_{i=1}^{N_{\mathrm{grad}}} \sum_{j=1}^{N^{(i)}} \left[\gamma_{i,j} - \mu_{i,j}(\boldsymbol{\Theta}, \boldsymbol{\Phi}, \beta, \boldsymbol{\lambda})\right]^2 \cdot \chi_{i,j} \right)$$

Complex fiber anatomy



Diffusion tensor MRI



Estimated fiber angle

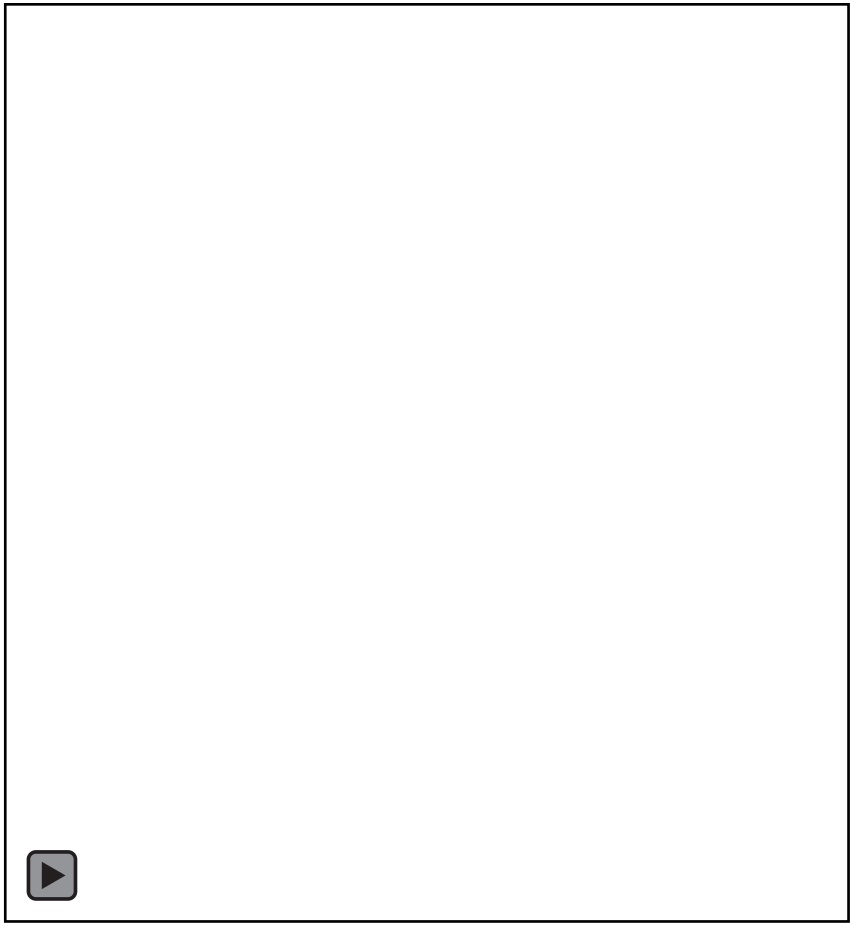
Electrophysiology

Monodomain model: Find transmembrane potential *u*

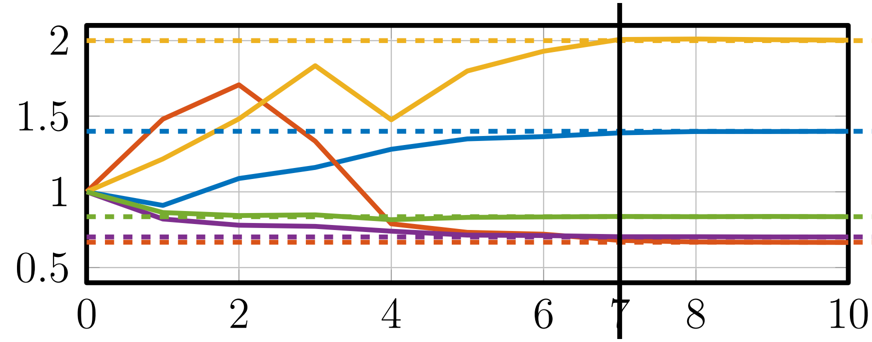
$$\begin{aligned}\chi(C_m \partial_t u - I_{ion}(u, \mathbf{w})) &= \nabla \cdot (\mathbf{D} \nabla u) && \text{in } \Omega \times (0, T], \\ \partial_t \mathbf{w} - \mathbf{g}(u, \mathbf{w}) &= 0 && \text{in } \Omega \times (0, T]\end{aligned}$$

Element degree | Electrical activation | Displacement

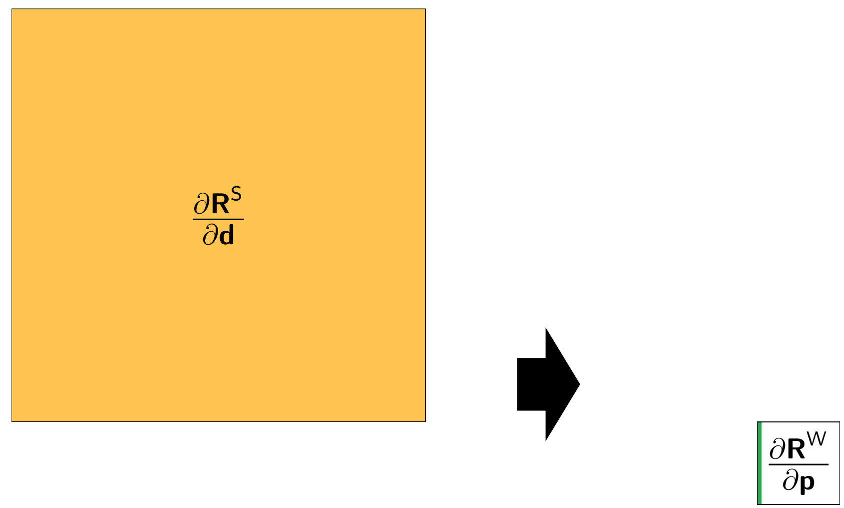
Mechanics



Validation with MRI



Inverse analysis



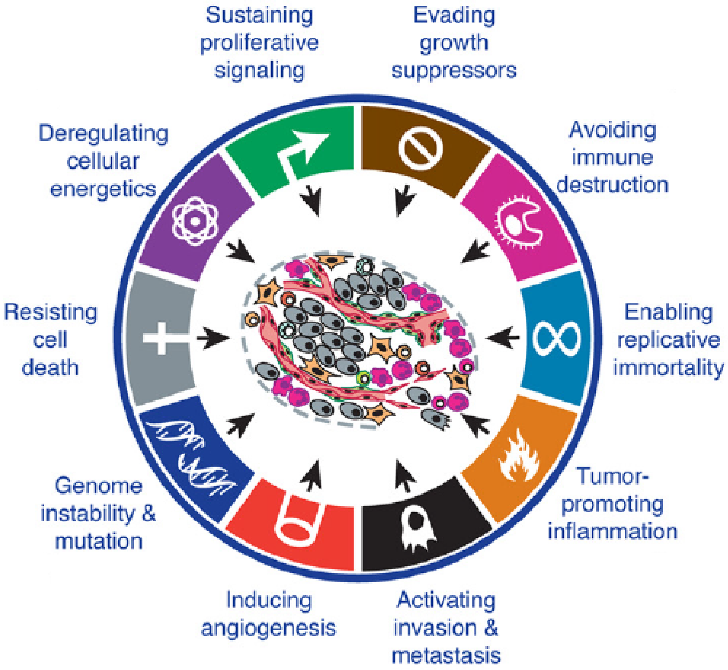
Coupeld model order reduction

Oncology – tumor growth – drug delivery – nanomedicine

J. Kremheller, A.-T. Vuong, L. Yoshihara, B. Schrefler (TUM-IAS)

Motivation

- Cancer is the second leading cause of death with 8 million deaths annually (WHO)
- The disease is so complex that only an interdisciplinary approach combining experts from all physical and natural sciences with physicians may advance our understanding
- However, nearly all cancer types share a common type of characteristics coined “hallmarks of cancer” [Hanahan and Weinberg]



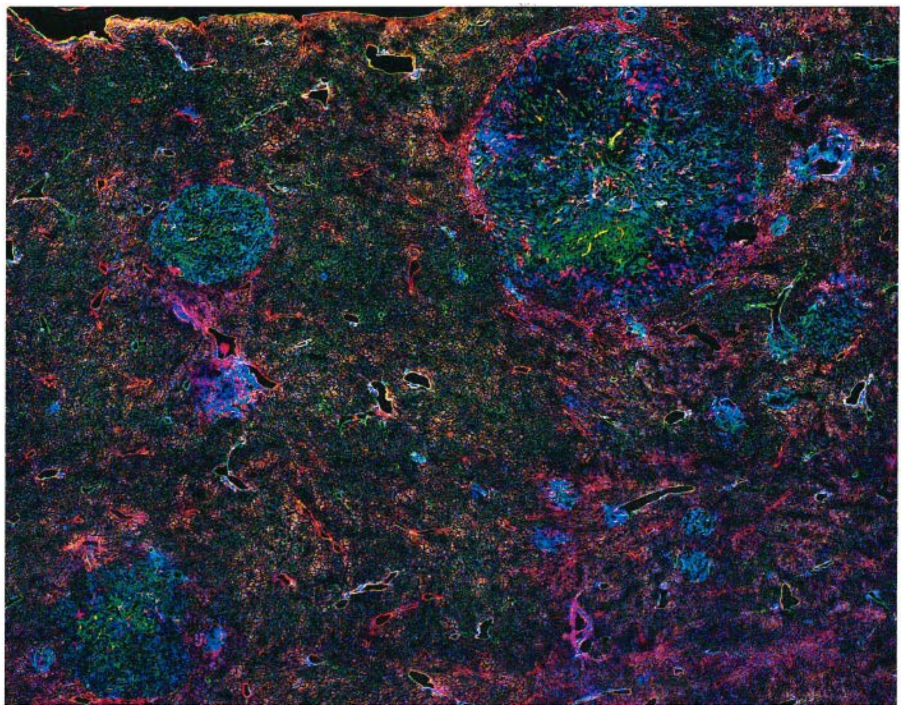
What does physics have to do with cancer?

A physics-based model of cancer

- reduce the complexity of cancer to its underlying physical principles
- cancer is viewed as “a disease of multiscale mass transport deregulation involving the biological barriers that separate different body compartments” [Michor et al.]

Examples of the role of physics in cancer progression

- ECM stiffness affects tumor growth and metastasis
- Increased interstitial pressure inhibits efficient drug delivery into tumors
- Non-genetic (physical) heterogeneity



Unpublished data (courtesy of HMRI)

Our multiphase tumor growth model

Evolution equation for angiogenesis:

$$\frac{\partial \varepsilon^v}{\partial t}\Big|_{\boldsymbol{X}} + \varepsilon^v \boldsymbol{\nabla} \cdot \boldsymbol{v}^s - \boldsymbol{\nabla} \cdot (D^v \boldsymbol{\nabla} \varepsilon^v) + \boldsymbol{\nabla} \cdot \left(\varepsilon^v \varepsilon S^l \chi \left(\omega^{TAF\bar{l}}\right) \boldsymbol{\nabla} \omega^{TAF\bar{l}}\right) = 0$$

Balance of mass of fluid phases:

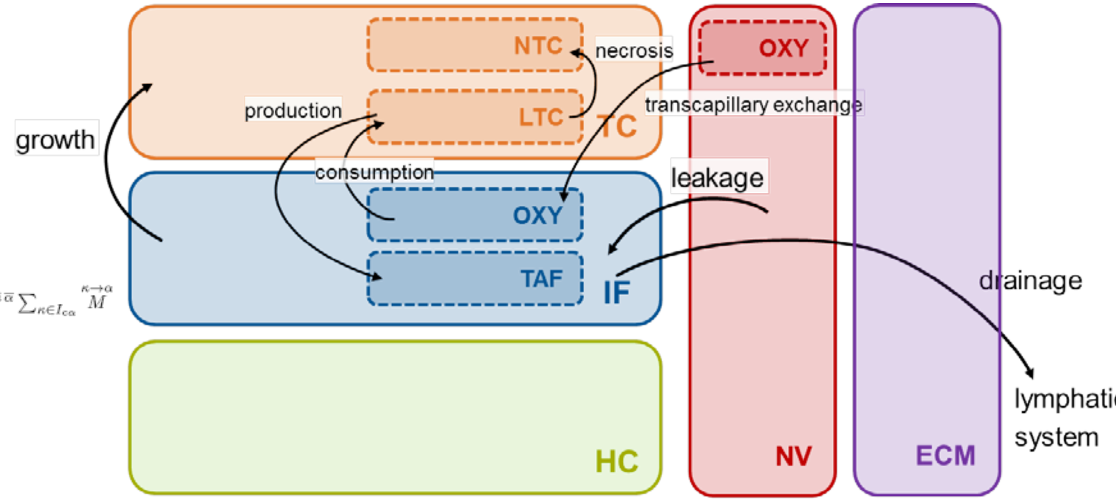
$$\varepsilon \sum_{\beta=1}^{n_{\text{fld}}} \frac{\partial S^\alpha}{\partial \psi^\beta} \frac{\partial \psi^\beta}{\partial t}\Big|_{\boldsymbol{X}} - S^\alpha \frac{\partial \varepsilon^v}{\partial t}\Big|_{\boldsymbol{X}} + S^\alpha (1-\varepsilon^v) \boldsymbol{\nabla} \cdot \boldsymbol{v}^s - \boldsymbol{\nabla} \cdot \left(\frac{k^\alpha_{rel} \boldsymbol{k}}{\mu_\alpha} \sum_{\beta=1}^{n_{\text{fld}}} \frac{\partial p^\alpha}{\partial \psi^\beta} \boldsymbol{\nabla} \psi^\beta\right) = \frac{\sum_{\kappa \in I_{c\alpha}} \overset{\kappa\to\alpha}{M}}{\rho^\alpha}$$

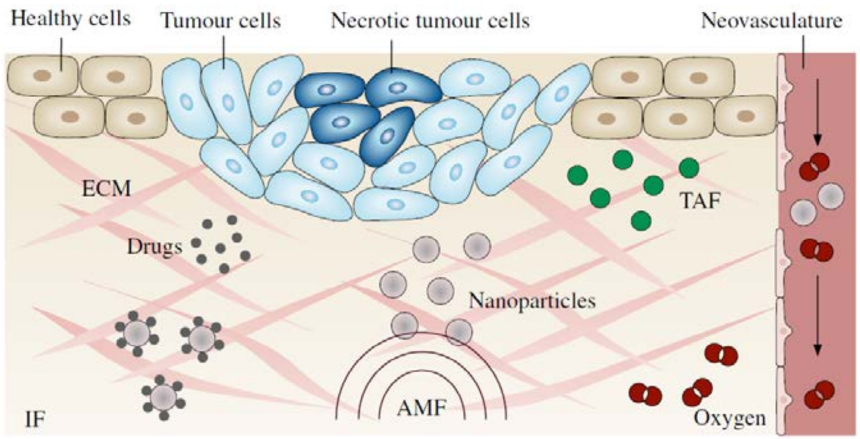
Balance of mass of species

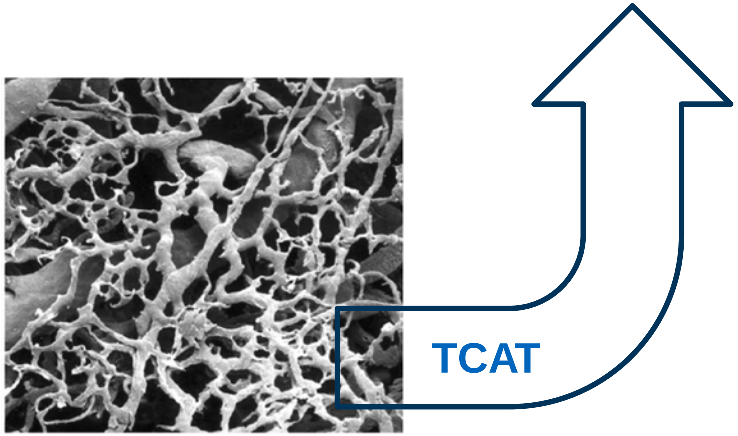
$$\rho^\alpha \varepsilon^\alpha \frac{\partial \omega^{i\bar{\alpha}}}{\partial t}\Big|_{\boldsymbol{X}} - \rho^\alpha \frac{k^\alpha_{rel} \boldsymbol{k}}{\mu_\alpha} \boldsymbol{\nabla} p^\alpha \cdot \boldsymbol{\nabla} \omega^{i\bar{\alpha}} - \boldsymbol{\nabla} \cdot \left(\rho^\alpha \varepsilon^\alpha D^{i\alpha}_{\text{eff}} \boldsymbol{\nabla} \omega^{i\bar{\alpha}}\right) = \sum_{\kappa \in I_{c\alpha}} \overset{i\kappa\to i\alpha}{M} + \varepsilon^\alpha r^{i\alpha} - \omega^{i\bar{\alpha}} \sum_{\kappa \in I_{c\alpha}} \overset{\kappa\to\alpha}{M}$$

Balance of linear momentum

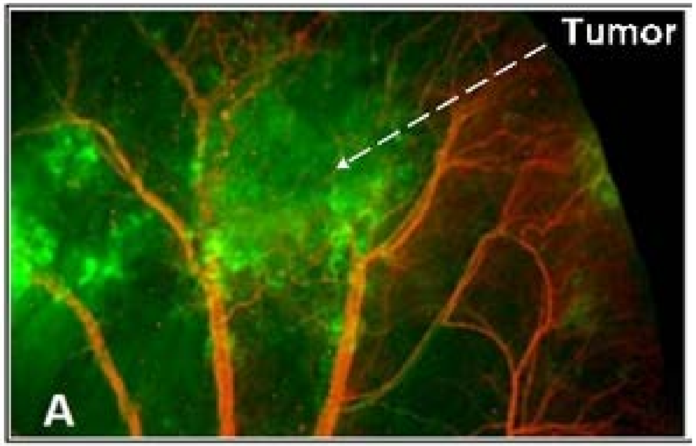
$$\nabla_0 \cdot \left(\boldsymbol{F} \cdot \boldsymbol{S}^s_{\text{eff}} - \boldsymbol{F} \cdot J \boldsymbol{F}^{-1} \cdot \boldsymbol{F}^{-T} p^s\right) = \boldsymbol{0} \qquad \text{in } \Omega_0 \times [t_0, t_E]$$



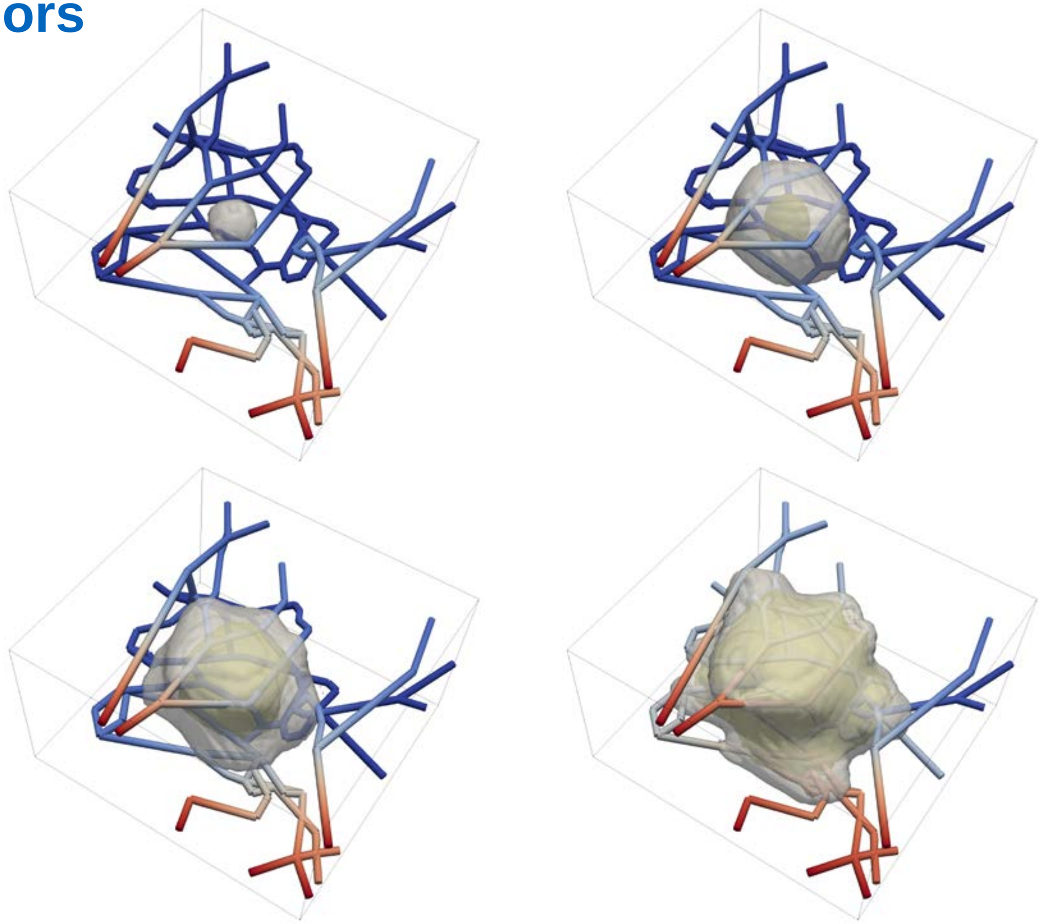




A novel method for the interaction of complex vascular networks with tumors

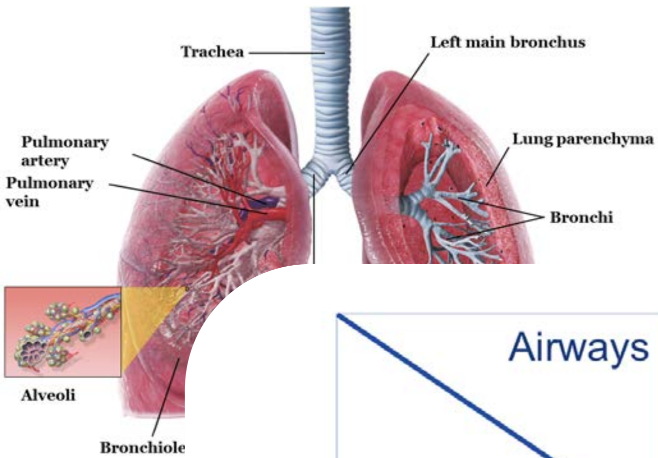


[Kalchenko et al.]



The respiratory system

C. Roth, M. Ismail, A. Birzle, S. Rausch, L. Yoshihara



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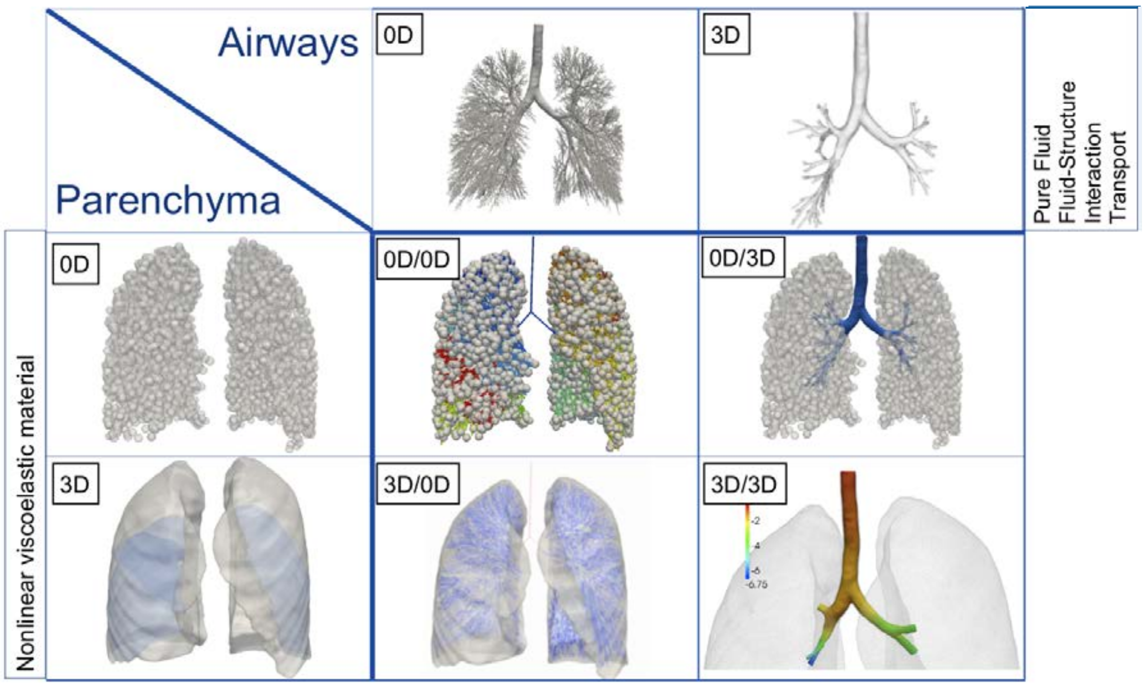
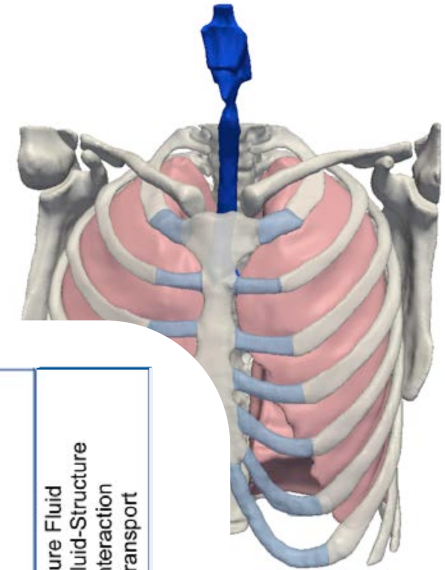
menschliche Körp
[5] Picture adapte
detail of alveoli ar

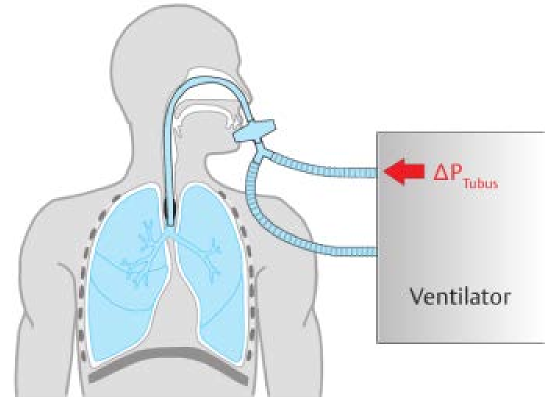




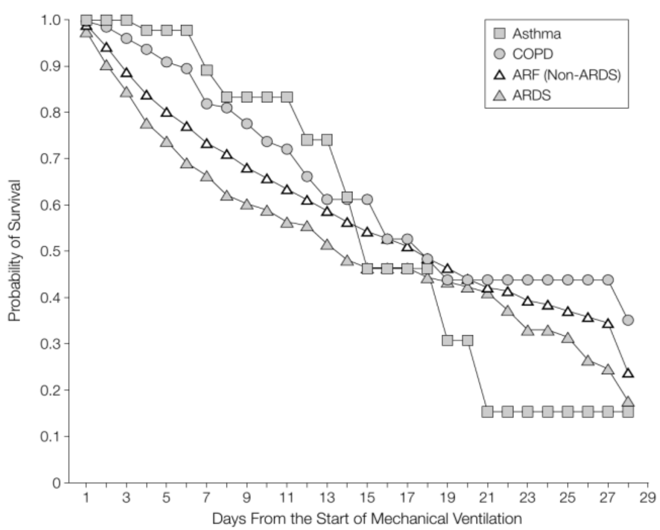
Motivation: VILI – protective ventilation

American Lung Association:
Deaths due to lung diseases are increasing

Acute Respiratory Distress Syndrome (ARDS):
- 7% of all ICU patients
- 16% of all mechanically ventilated patients



(Rathgeber 2010)



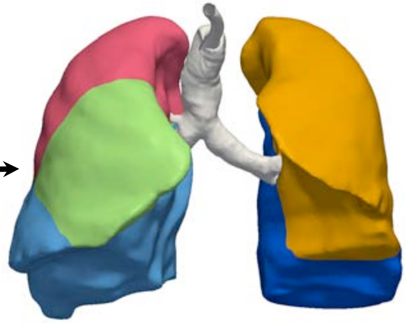
	ICU Mortality, % (95% Confidence Interval) Factors Developing
Barotrauma	50 (42-58)
ARDS	63 (56-70)
Pneumonia	38 (35-41)
Sepsis	55 (51-58)
Shock	61 (58-64)
Renal failure	61 (58-74)
Hepatic failure	69 (63-74)
Coagulopathy	61 (56-65)
Metabolic acidosis	59 (53-65)
Respiratory acidosis	37 (32-43)

(Esteban et al. 2002)

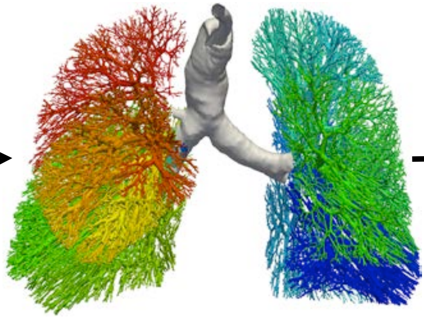
Comprehensive Computational Lung Model

CT/MRI scan

Segmentation



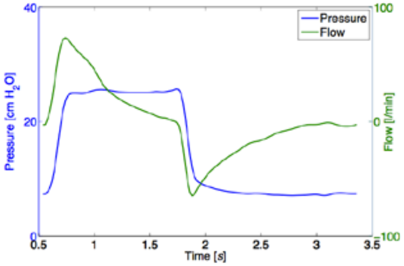
Tree-growing [1,2]



$$C\frac{dP_{in}}{dt} + Q_{out} - Q_{in} = 0$$

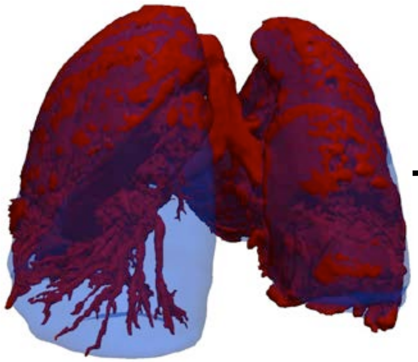
$$I\frac{dQ_{out}}{dt} + RQ_{out} + P_{out} - P_{in} = 0$$

Lung tissue [3]

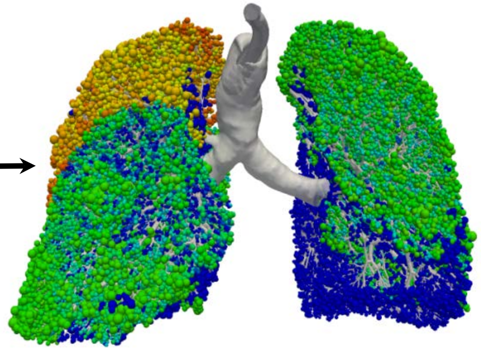


$$P = \frac{V_0}{V} * \frac{\kappa}{\beta} * \left(1 - \left(\frac{V_0}{V}\right)^{\beta}\right)$$

Collapsed Lung Regions



Computational Lung Model

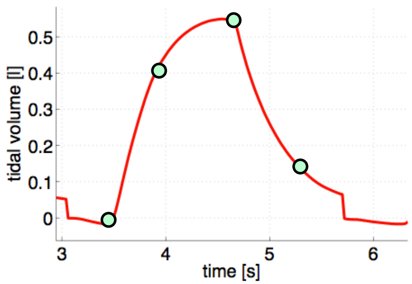


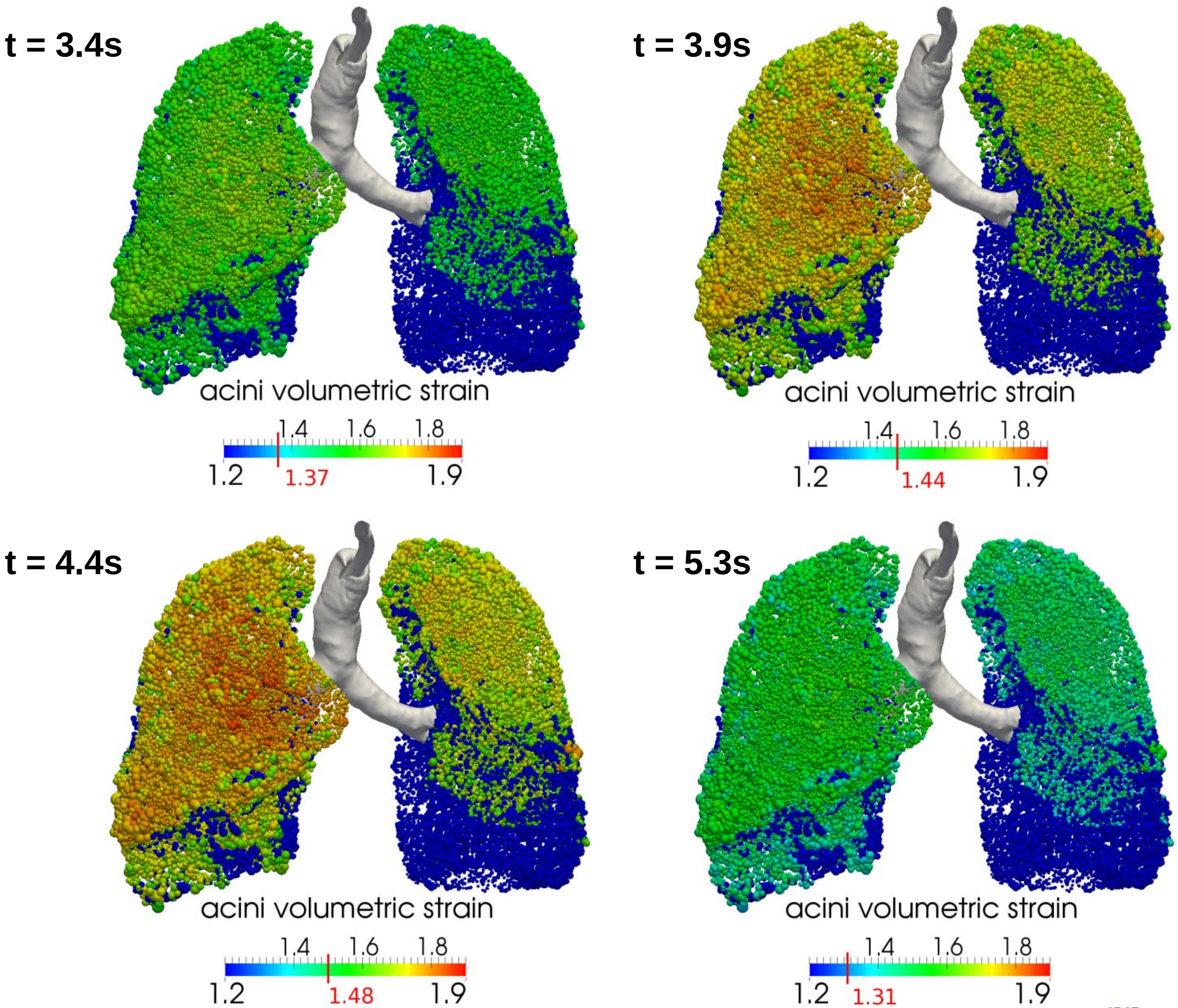
Allows computation of **regional ventilation** for **any prescribed ventilation protocol**

[1] Ismail M, Comerford A, Wall WA, *Int J Numer Meth Biomed Engng*, **29:**1285-1305, 2013
[2] Weibel, E., *The Pathway for Oxygen*, Harvard University Press: Cambridge, MA, 1984
[3] Ogden R, *J Mech Phys Solids*, **22:**541-553, 1974

Results - local quantities

Single breath evaluation





Electrical Impedance Tomography (EIT)

About EIT

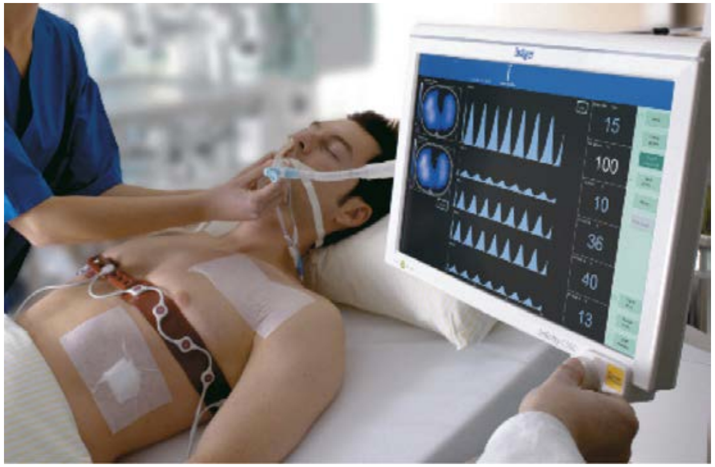
Medical imaging technique based on tissue resistivity (CT: tissue density)

Non-invasive

Radiation-free

Low spatial but high temporal resolution (50Hz)

Long-term imaging possible



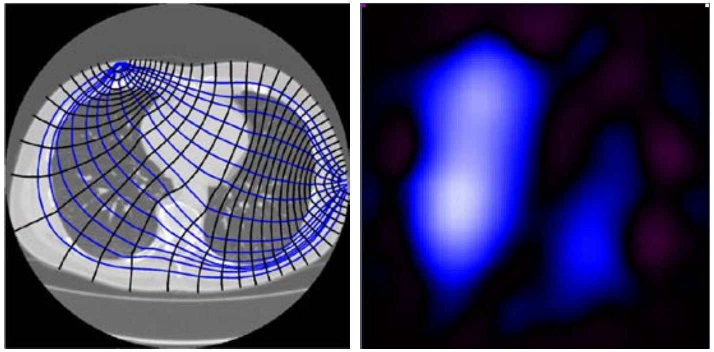


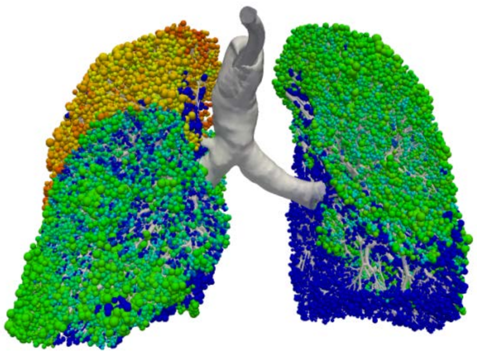
Table 1. Typical values of tissue resistivity at a frequency of about 10 kHz.

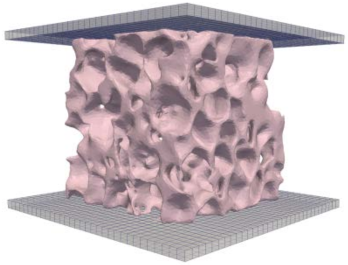
Muscle	2–4 Ω m
Fat	20 Ω m
Lungs	10 Ω m (this changes with respiration)
Blood	1.6 Ω m
Bone	>40 Ω m

[1] Table taken from: B. H. Brown (2003), *Journal of Medical Engineering & Technology*, **27**:97-108
[2] Image taken from: EIDORS: *Electrical Impedance Tomography and Diffuse Optical Tomography Reconstruction Software, http://eidors3d.sourceforge.net/*

Computational Model & EIT

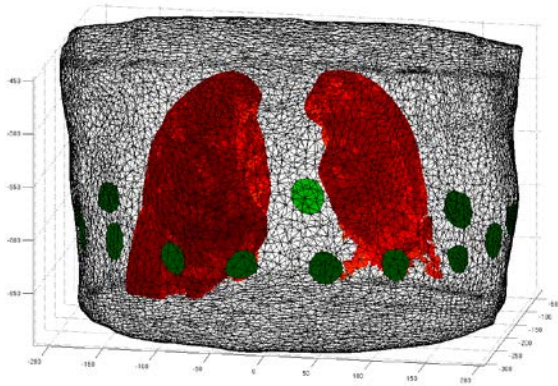
Local air content





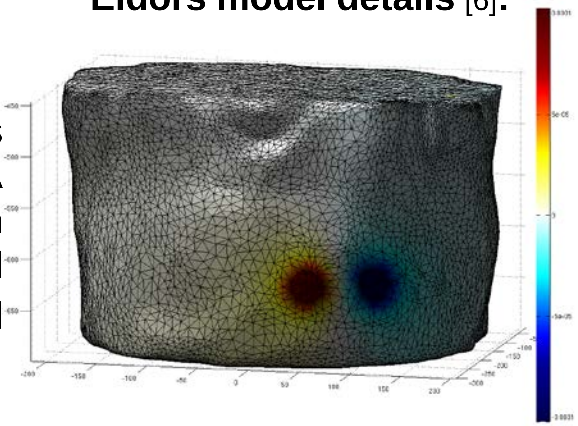
$$\bar{\rho}_{\text{eff}} = \frac{\bar{\tau}}{\sigma_{\text{Alv}}} \left(\frac{V_{air}}{V_{tissue}} + 1 \right)$$

Mapped Conductivities [5]

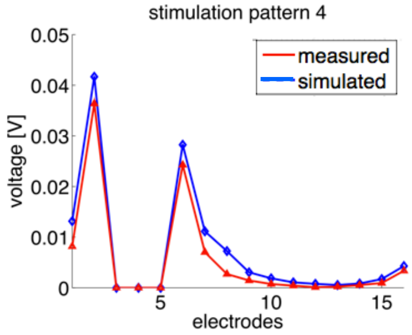


Eidors model details [6]**:**

16 electrodes
current: 10mA
adjacent stimulation
background
resistivity: 4Ohm*m [7]



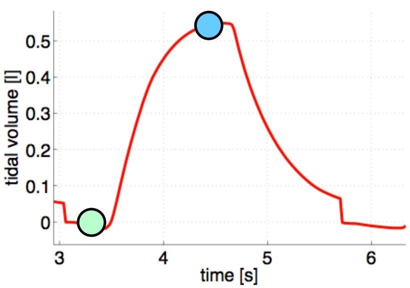
Raw Measurements



[5] Roth CJ, Ehrl A, Becher T, Frerichs I, et *al*., *Physiol Meas*, **36**:1211-26, 2015
[6] Adler A, Lionheart WRB, *Physiol Meas*, **27:**S25, 2006
[7] Brown BH, *J Med Eng Technol*, **27**:97-108, 2003

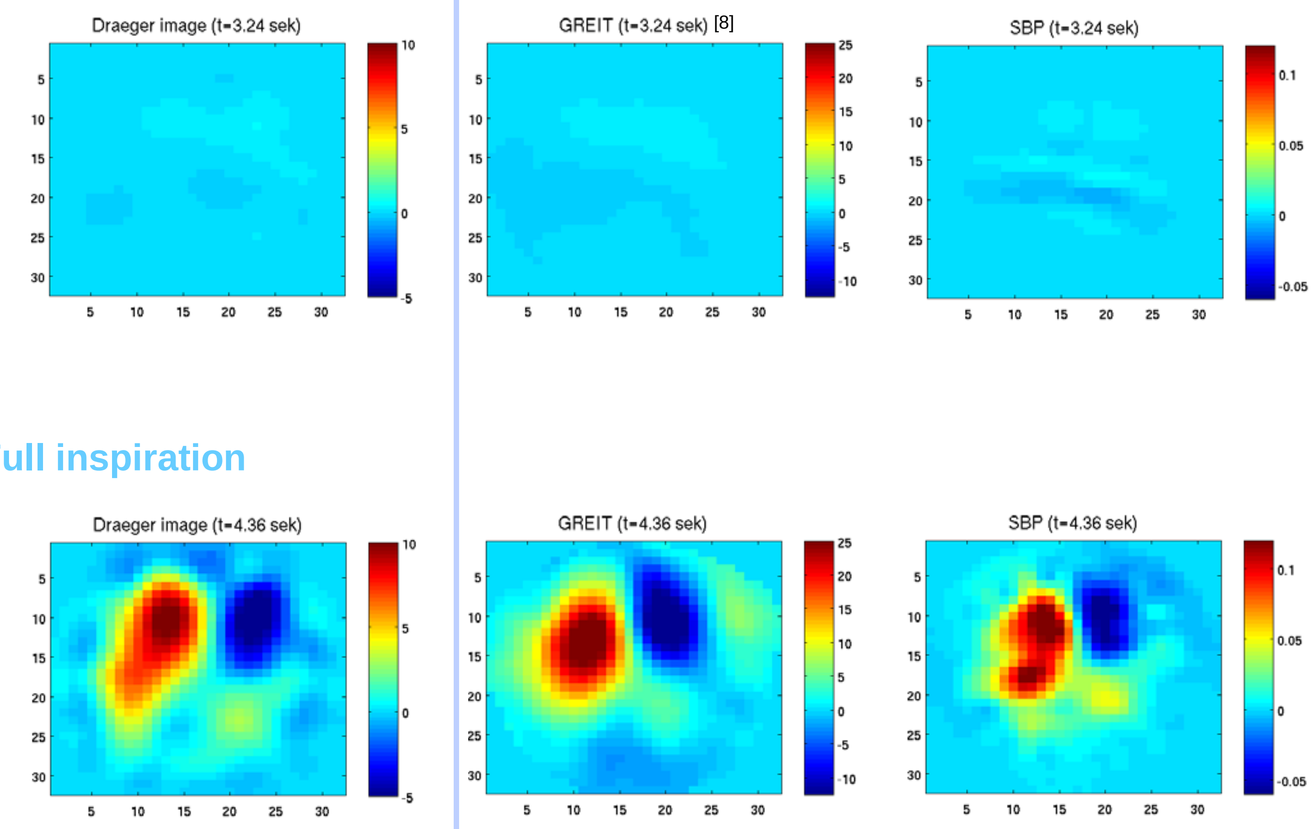
Results - local EIT image

Single breath evaluation



Reference state

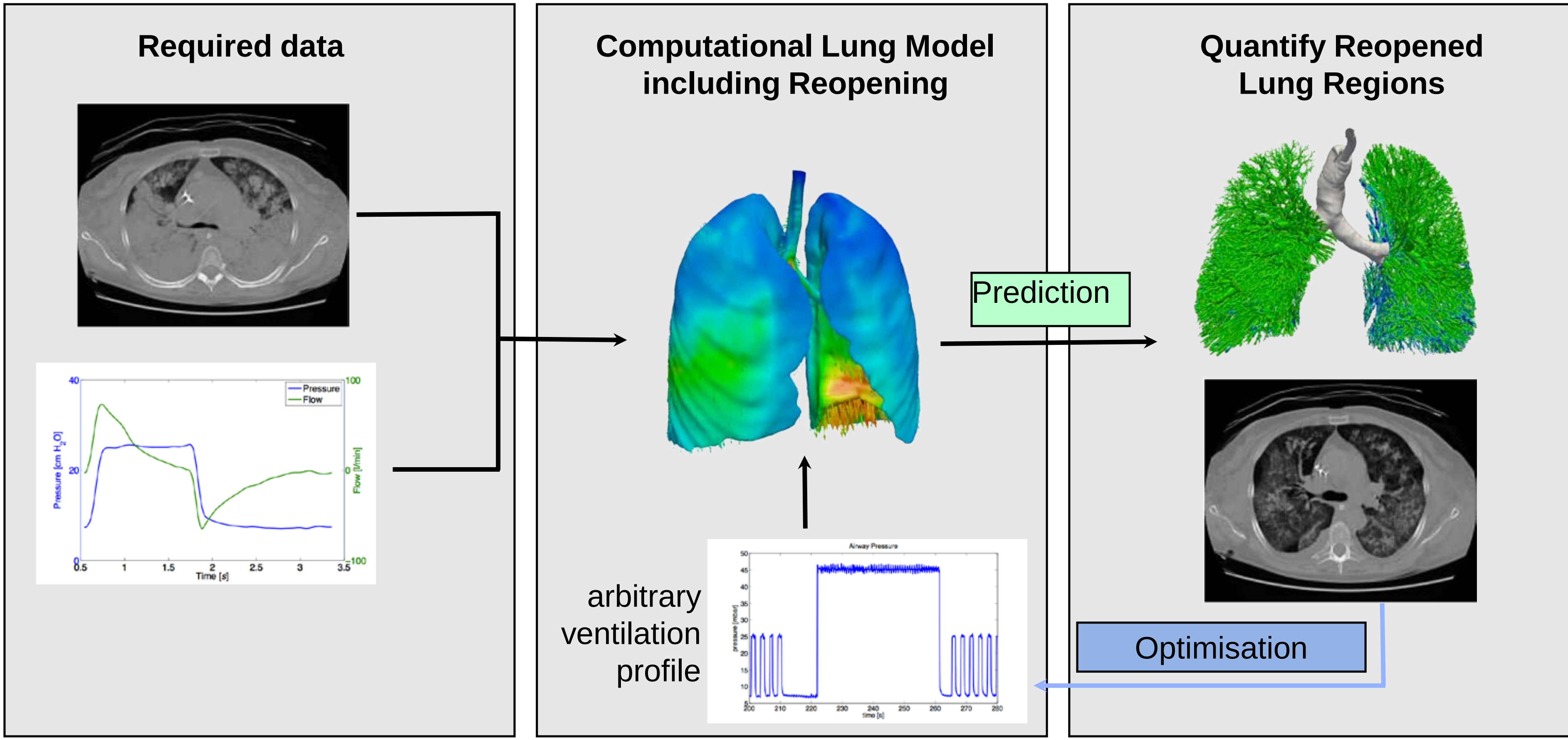
Full inspiration



Computational

[8] Adler A, Arnold JH, Bayford R, et *al.*, *Physiol Meas*, **30:**S35, 2009
[9] Roth CJ et *al.*, *in preparation*

Outlook


Required data
Pressure
Flow
Time [s]
Computational Lung Model
including Reopening
arbitrary
ventilation
profile
Prediction
Quantify Reopened
Lung Regions
Optimisation

EBENBUILD

Team


Dr. Kei Müller


Dr. Jonas Biehler


Karl Wichmann


Dr. Peter Sieb


Dr. Lena Yoshihara


Carolin Geitner


Prof. Wolfgang Wall

Clinical partners


Dr. Kossmann
MRI


Dr. Becher
UKSH


Prof. Weiler
UKSH


Prof. Koch
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ESF
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Zusammen. Zukunft. Gestalten.

Europäische Union

Das Vorhaben AescuLab wird im Rahmen des EXIST-Programms durch das Bundeministerium für Wirtschaft und Energie und den Europäischen Sozialfonds gefördert.

Bayesian Multi-Fidelity Monte Carlo

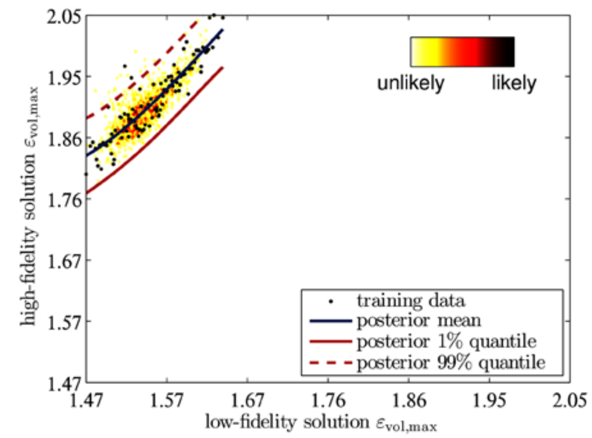
J. Biehler

High-fidelity model:

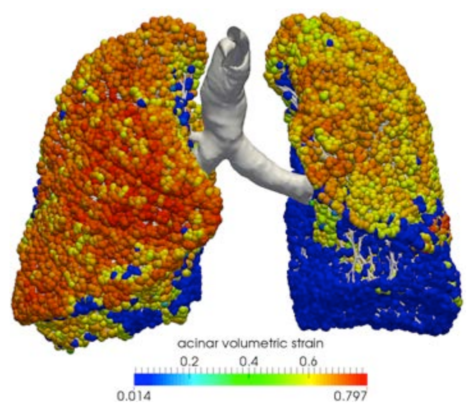
- 17 generations
- Computational cost 98 CPU h

Low-fidelity model:

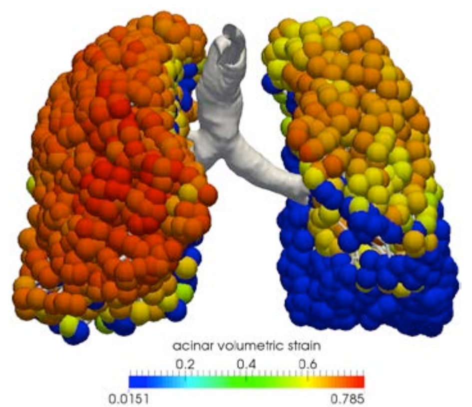
- 12 generations, reduced load
- Computational cost 0.35 CPU h



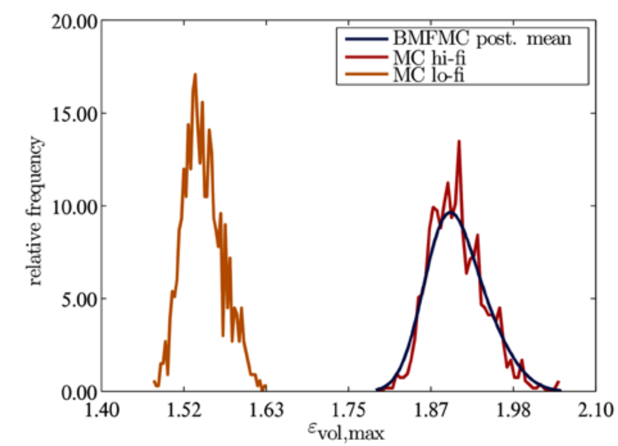
Relationship between models



High-fidelity model



Low-fidelity model



Estimated densities

Code development: Adapted to hardware

Complex simulation software BACI in C++ programming language

- Focus of research activities at LNM: *Application motivated fundamental research* – specific implementation, combining a sophisticated code with a broad spectrum of further software packages for infrastructure (e.g. Trilinos, with Sandia National Laboratories)
- C++ compiler translates application code into **optimized machine code for hardware** at LRZ (SuperMUC, SuperMUC-NG) → Current computer architecture allows to use a unified C++ code without system-specific solutions
- Our code fully supports **vector instructions** of SuperMUC/SuperMUC-NG (AVX, AVX-512) via abstract "SIMD vector" data types and template programming
- **Parallelization** with MPI
- **Code tuning** in collaboration with experts from LRZ
  - Joint work with CFD group (Momme Allalen)
  - Several successful KONWIHR projects
  - Identification of suitable algorithms
  - Continuous performance analysis and improvement
  - Preparatory work for SuperMUC-NG (AVX-512, MPI+X)

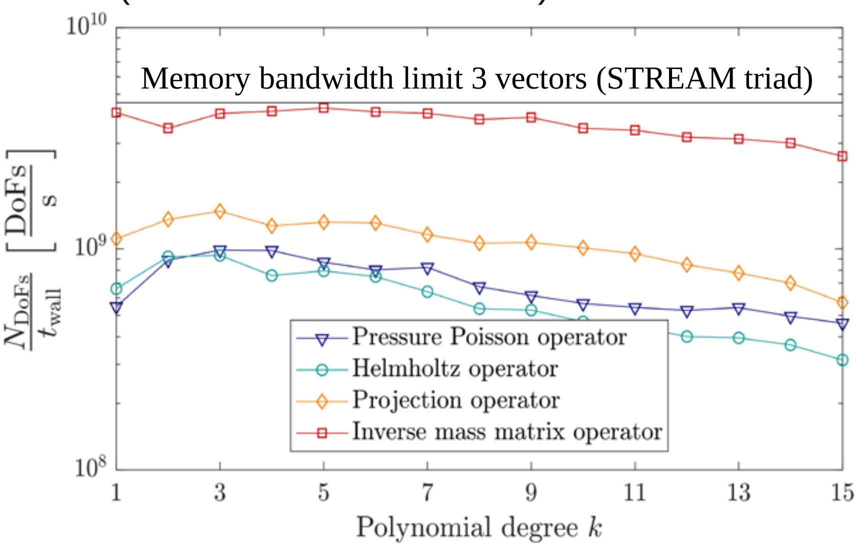
Code design: Optimal performance on SuperMUC

M. Kronbichler, B. Krank, N. Fehn

Node-level performance

Efficient use of hardware components within a node

Algorithm choice: arithmetic is relatively cheap compared to access from main memory (RAM) → prefer repeated calculations of integrals for matrix-vector products rather than storing a big matrix (matrix-free linear solvers)

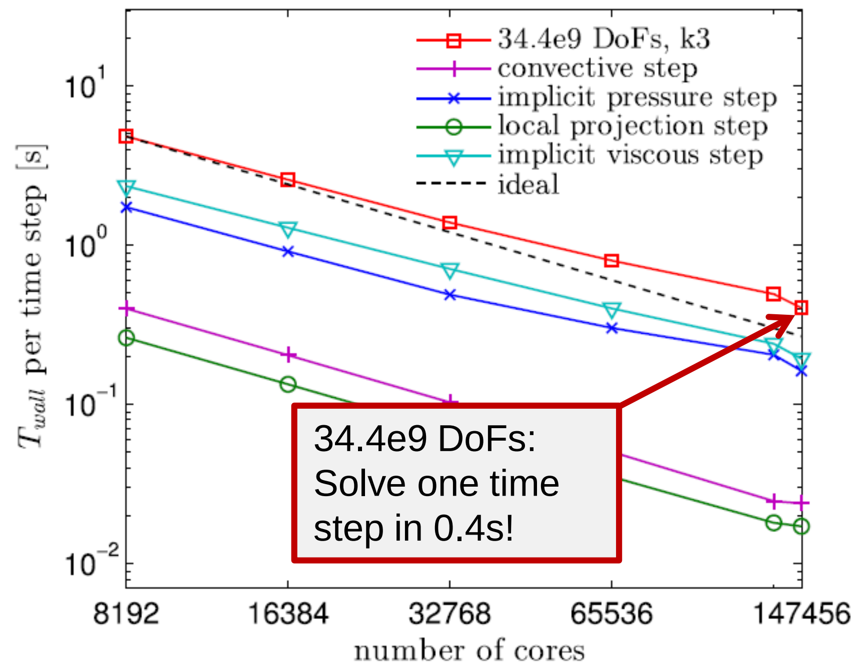


SuperMUC Phase 2 (28 cores, Intel Haswell)

Strong scaling on up to 147.457 cores

Analyze reduction of compute time with increasing resources

Parallelized with MPI



SuperMUC Phase 1

Research Software Sustainability

A.-T. Vuong, M. Kronbichler

4C – BACI

„Foresee"
***C**omprehensive **C**omputational **C**ommunity **C**ode*

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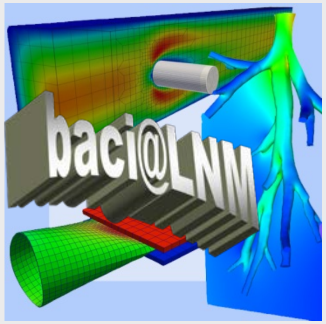

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Helmholtz-Zentrum
Geesthacht
Zentrum für Material- und Küstenforschung

(plus AG Schulz a.o.)

Perspectives

Requirements on hardware infrastructure

- Mix of arithmetic compute power, memory bandwidth and network latency are all important for optimal performance with our code
- It is important to be able to use standard programming in C++ with long-term functionality (10+ years)
- Main adaptations done for SuperMUC-NG: Select algorithms which compute more and access less memory, given the relatively low memory bandwidth per node (high machine balance Flop/Byte); optimal use of caches
- Ideal architecture for our needs beyond SuperMUC-NG…
  - 2-20 GB fast memory per node (ideally > 1 TB/s)
  - Unified address space
  - Fast transfer between main memory and high bandwidth memory
  - Typical network as in SuperMUC/SuperMUC-NG sufficient
  - Performance on up to 1,000 nodes most important
- Ideal infrastructure for us…
  - Possibilities for automated performance testing (e.g. Linux cluster)
  - Continue successful collaboration with LRZ experts

Lehrstuhl für Numerische Mechanik

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„Application-motivated fundamental research“ in Computational Mechanics

„Theoria cum Praxi“

…

„commune bonum“

G.W. Leibniz

Thank you for your attention!

Questions?

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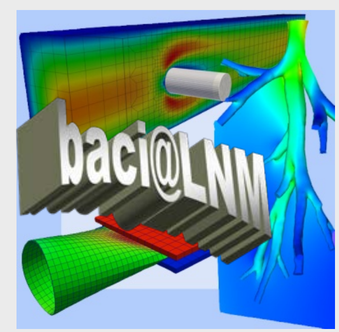

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