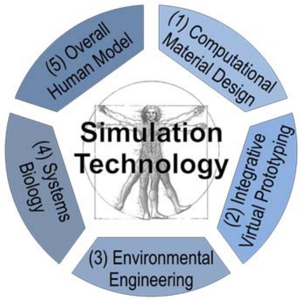
Simulation Technology Applied to Coupled Problems in Continuum Mechanics



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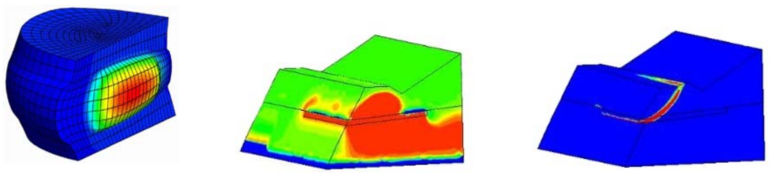
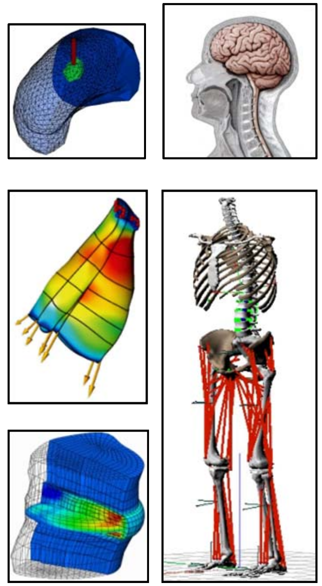


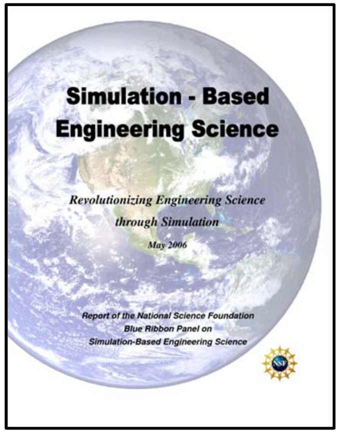


11. LS-DYNA Forum 2012
Maritim Hotel Ulm, 9.-10. Oktober 2012

- **Simulation Technology**
- **TPM & Coupled Problems**
- **Geotechnical Engineering**
- **Biomechanical Engineering**
- **Conclusions & Outlook**

Simulation Technology: Motivation & Recognition

- Simulation Technology involves …
  - ✓ "… challenges in ***multi-scale, multi-physics modelling, model validation and verification, handling large data, visualisation, and CSE***."
  - ✓ "… a further challenge is the education of the ***next generation of engineers and scientists*** in the theory and practices of SBES."



- Recognition by the ***World Technology Evaluation Center*** Simulation-Based Engineering and Science 2009:
  - ✓ "… ***pockets of excellence exist in Europe and Asia*** *that are more advanced than US groups, and* ***Europe is leading in training the next generation of engineering simulation experts***."
  - ✓ "... ***examples*** *of pockets* ***of excellence*** *in engineering simulation* ***include*** *… the* ***University of Stuttgart***."

Simulation Technology
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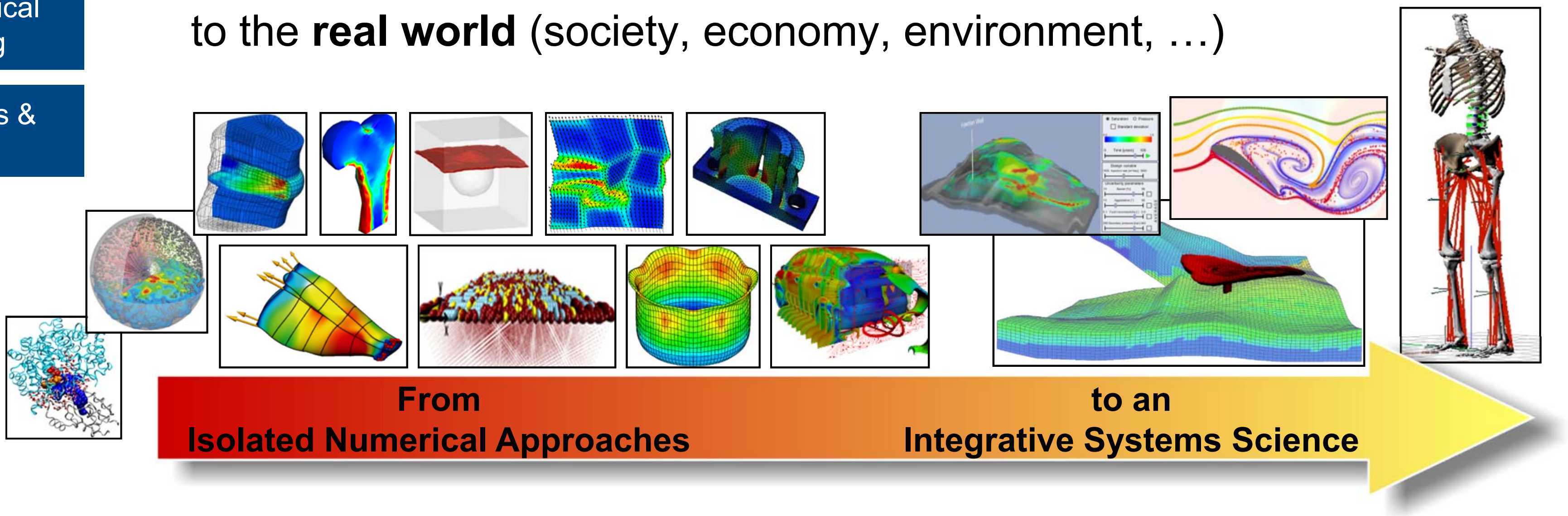
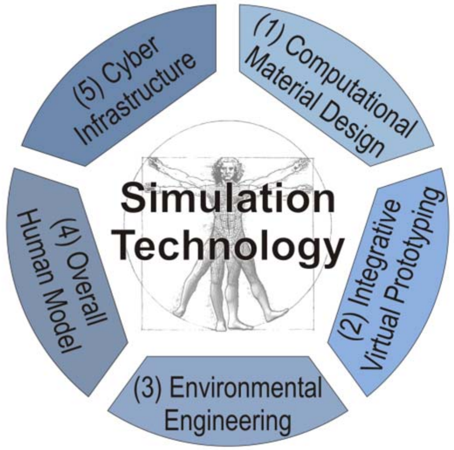
SimTech and the Integrative Systems Science

- To combine a wide range of scientific disciplines into an **interdisciplinary effort to address new problem classes** which cannot be dealt with otherwise
- To **integrate disciplinary methods** into a new context giving rise to entirely **new solution strategies**
- To **form a new scientific field** by establishing a core of know how, a pool of techniques, a terminology, … and a curriculum
- To **reach out** from the **virtual world** (models and simulation) to the **real world** (society, economy, environment, …)



SimTech Visions – from 2012 on



From Empirical Material Description towards Computational Material Design

Towards Integrative Virtual Prototyping

Towards Interactive Environmental Engineering

Towards an Integrated Overall Human Model

Beyond a Simulation Cyber Infrastructure

Research Areas (RA)

- Our disciplinary core competences

A Molecular and Particle Simulations

B Advanced Mechanics of Multi-scale and Multi-field Problems

C Analysis, Design and Optimisation of Systems

D Numerical and Computational Mathematics

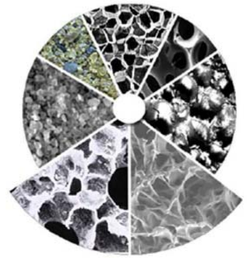
E Integrated Data Management and Interactive Visualisation

F Hybrid High-performance Computing Systems and Simulation Software Engineering

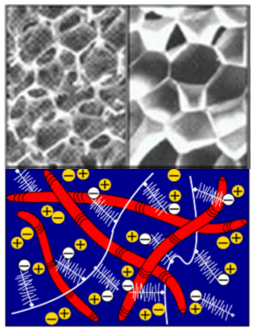
G Integrative Platform of Reflection and Contextualisation

Theory of Porous Media and Coupled Problems

- Theoretical (mathematical) and numerical modelling of saturated and partially saturated porous solid material
- Macroscopic modelling based on a (virtual) homogenisation process of multiphasic porous media



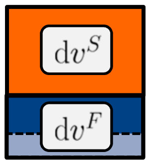
Representative Elementary Volume (REV)



of the underlying microscale

macroscale

"homogenised model"



volume fractions

micro-to-macro transition

$$\rho^{\alpha R} := \frac{1}{V_m^\alpha} \int_{V^\alpha} \rho_m^\alpha \, dv_m^\alpha$$

$$\rho^\alpha := \frac{1}{V_m} \int_{V^\alpha} \rho_m^\alpha \, dv_m^\alpha$$

$$n^\alpha := \frac{1}{V_m} \int_{V^\alpha} dv_m^\alpha$$

Multi-component and multi-physical models: $\varphi = \bigcup_\alpha \varphi^\alpha$

Fundamentals of the Theory of Porous Media

[*Bowen* 1980, *Lewis & Schrefler* 1998, *Ehlers* 1989, 1993, 2002, 2009]

- **Saturated solid skeleton with (multi-component) pore fluid(s)**

solid skeleton	pore fluid(s)	fluid mixture
φ^S	$\varphi^F = \bigcup_\beta \varphi^\beta$	$\varphi^\beta = \bigcup_\gamma \varphi^\gamma$
e.g.: soil, ECM, cartilage (including fixed charges)	e.g.: water, air, blood, interstitial fluid	e.g.: solvent, therapeutic agent, charged ions

- **Basic variables of the (extended) Theory of Porous Media**

- Volume fractions, saturations

$$n^\alpha = \frac{\mathrm{d}v^\alpha}{\mathrm{d}v}\,, \qquad s^\beta = \frac{n^\beta}{n^F}$$

$$n^F = \textstyle\sum_\beta n^\beta$$: porosity

- Volumetrical constraints

$$\textstyle\sum_\alpha n^\alpha = 1\,, \qquad \sum_\beta s^\beta = 1$$

- Material and partial densities

$$\rho^{\alpha R} = \frac{\mathrm{d}m^\alpha}{\mathrm{d}v^\alpha}\,, \quad \rho^\alpha = \frac{\mathrm{d}m^\alpha}{\mathrm{d}v} \quad \rightarrow \quad \rho^\alpha = n^\alpha \rho^{\alpha R}$$

- Miscible components and concentrations

$$\rho^\gamma = n^F \rho_F^\gamma\,, \quad \text{where} \quad \rho_F^\gamma = c_m^\gamma\, M_m^\gamma$$

$$c_m^\gamma = \frac{\mathrm{d}n_m^\gamma}{\mathrm{d}v^F}\,, \quad \text{with} \quad \begin{cases} M_m^\gamma & : \text{molar mass} \\ n_m^\gamma & : \text{number of moles} \\ \rho^{FR} = \sum_\gamma \rho_F^\gamma & \end{cases}$$

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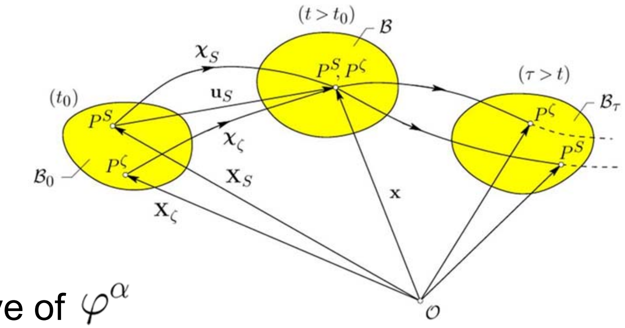
Kinematics of porous materials



- Motion of φ^α

$$\mathbf{x} = \boldsymbol{\chi}_\alpha(\mathbf{X}_\alpha,\, t)$$
$$\mathbf{X}_\alpha = \boldsymbol{\chi}_\alpha^{-1}(\mathbf{x},\, t)$$

- Individual velocity of φ^α

$$\overset{\prime}{\mathbf{x}}_\alpha = \frac{\mathrm{d}\boldsymbol{\chi}_\alpha(\mathbf{X}_\alpha,\, t)}{\mathrm{d}t}\,,$$

$(\,\cdot\,)'_\alpha$: material time derivative of φ^α

- *Lagrange*an description of φ^S

$\mathbf{u}_S = \mathbf{x} - \mathbf{X}_S$: solid displacements

- Modified *Euler*ian description of φ^β

$\mathbf{w}_\beta = \overset{\prime}{\mathbf{x}}_\beta - \overset{\prime}{\mathbf{x}}_S$: seepage velocities

- Pore-diffusion velocity of pore-fluid components φ^γ in φ^β

$\mathbf{d}_{\gamma\beta} = \mathbf{w}_\gamma - \mathbf{w}_\beta = \overset{\prime}{\mathbf{x}}_\gamma - \overset{\prime}{\mathbf{x}}_\beta\,,$ where $\mathbf{d}_{\gamma\beta}$: pore-diffusion velocities

- Material deformation gradient, inverse and Jacobian

$$\mathbf{F}_\alpha = \frac{\partial\boldsymbol{\chi}_\alpha(\mathbf{X}_\alpha, t)}{\partial\mathbf{X}_\alpha} = \mathrm{Grad}_\alpha\,\mathbf{x}\,,\quad \mathbf{F}_\alpha^{-1} = \frac{\partial\boldsymbol{\chi}_\alpha^{-1}(\mathbf{x}, t)}{\partial\mathbf{x}} = \mathrm{grad}\,\mathbf{X}_\alpha\,,\quad \det\mathbf{F}_\alpha = J_\alpha > 0$$

- Non-linear deformation and strain measures using $\mathbf{F}_\alpha = \mathbf{R}_\alpha\,\mathbf{U}_\alpha = \mathbf{V}_\alpha\,\mathbf{R}_\alpha$

$$\mathbf{C}_\alpha = \mathbf{F}_\alpha^T\,\mathbf{F}_\alpha = \mathbf{U}_\alpha\,\mathbf{U}_\alpha\,,\qquad \mathbf{E}_\alpha = \tfrac{1}{2}\,(\mathbf{F}_\alpha^T\,\mathbf{F}_\alpha - \mathbf{I}) = \tfrac{1}{2}\,(\mathbf{U}_\alpha\,\mathbf{U}_\alpha - \mathbf{I})$$
$$\mathbf{B}_\alpha = \mathbf{F}_\alpha\,\mathbf{F}_\alpha^T = \mathbf{V}_\alpha\,\mathbf{V}_\alpha\,,\qquad \mathbf{K}_\alpha = \tfrac{1}{2}\,(\mathbf{F}_\alpha\,\mathbf{F}_\alpha^T - \mathbf{I}) = \tfrac{1}{2}\,(\mathbf{V}_\alpha\,\mathbf{V}_\alpha - \mathbf{I})$$

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Material independent balance equations

Balance relations for the overall aggregate

mass:	$\dot{\rho} + \rho \operatorname{div} \dot{\mathbf{x}} = 0$
momentum:	$\rho \ddot{\mathbf{x}} = \operatorname{div} \mathbf{T} + \rho \mathbf{b}$
m. o. m.:	$\mathbf{0} = \mathbf{I} \times \mathbf{T} \quad \rightarrow \quad \mathbf{T} = \mathbf{T}^T$
energy:	$\rho \dot{\varepsilon} = \mathbf{T} \cdot \mathbf{L} - \operatorname{div} \mathbf{q} + \rho r$
entropy:	$\rho \dot{\eta} \geq \operatorname{div} \boldsymbol{\phi}_\eta + \sigma_\eta = \operatorname{div}(-\frac{1}{\theta} \mathbf{q}) + \frac{1}{\theta} \rho r$

Balance relations for the particular constituents

mass:	$(\rho^\alpha)'_\alpha + \rho^\alpha \operatorname{div} \overset{\prime}{\mathbf{x}}_\alpha = \hat{\rho}^\alpha$
momentum:	$\rho^\alpha \overset{\prime\prime}{\mathbf{x}}_\alpha = \operatorname{div} \mathbf{T}^\alpha + \rho^\alpha \mathbf{b}^\alpha + \hat{\mathbf{p}}^\alpha$
m. o. m.:	$\mathbf{0} = \mathbf{I} \times \mathbf{T}^\alpha + \hat{\mathbf{m}}^\alpha$
energy:	$\rho^\alpha (\varepsilon^\alpha)'_\alpha = \mathbf{T}^\alpha \cdot \mathbf{L}_\alpha - \operatorname{div} \mathbf{q}^\alpha + \rho^\alpha r^\alpha + \hat{\varepsilon}^\alpha$
entropy:	$\rho^\alpha (\eta^\alpha)'_\alpha = \operatorname{div}(-\frac{1}{\theta^\alpha} \mathbf{q}^\alpha) + \frac{1}{\theta^\alpha} \rho^\alpha r^\alpha + \hat{\zeta}^\alpha$

Resulting constraints and relations

Specific constraints for total and direct production terms

$$\textstyle\sum_\alpha \hat{\rho}^\alpha = 0$$

$$\textstyle\sum_\alpha \hat{\mathbf{s}}^\alpha = \mathbf{0} \quad \text{with} \quad \hat{\mathbf{s}}^\alpha = \hat{\mathbf{p}}^\alpha + \hat{\rho}^\alpha \overset{\prime}{\mathbf{x}}_\alpha$$

$$\textstyle\sum_\alpha \hat{\mathbf{h}}^\alpha = \mathbf{0} \quad \text{with} \quad \hat{\mathbf{h}}^\alpha = \hat{\mathbf{m}}^\alpha + \mathbf{x} \times \hat{\mathbf{s}}^\alpha$$

$$\textstyle\sum_\alpha \hat{e}^\alpha = 0 \quad \text{with} \quad \hat{e}^\alpha = \hat{\varepsilon}^\alpha + \hat{\mathbf{p}}^\alpha \cdot \overset{\prime}{\mathbf{x}}_\alpha + \hat{\rho}^\alpha (\varepsilon^\alpha + \frac{1}{2} \overset{\prime}{\mathbf{x}}_\alpha \cdot \overset{\prime}{\mathbf{x}}_\alpha)$$

$$\textstyle\sum_\alpha \hat{\eta}^\alpha \geq 0 \quad \text{with} \quad \hat{\eta}^\alpha = \hat{\zeta}^\alpha + \hat{\rho}^\alpha \eta^\alpha$$

Relations between total and partial quantities

$$\rho \mathbf{b} = \textstyle\sum_\alpha \rho^\alpha \mathbf{b}^\alpha$$

$$\mathbf{T} = \textstyle\sum_{\alpha=1}^k (\mathbf{T}^\alpha - \rho^\alpha \mathbf{d}_\alpha \otimes \mathbf{d}_\alpha)$$

$$\rho \varepsilon = \textstyle\sum_\alpha \rho^\alpha (\varepsilon^\alpha + \frac{1}{2} \mathbf{d}_\alpha \cdot \mathbf{d}_\alpha)$$

$$\mathbf{q} = \textstyle\sum_\alpha \{\mathbf{q}^\alpha - (\mathbf{T}^\alpha)^T \mathbf{d}_\alpha + \rho^\alpha \varepsilon^\alpha \mathbf{d}_\alpha + \frac{1}{2} \rho^\alpha (\mathbf{d}_\alpha \cdot \mathbf{d}_\alpha) \mathbf{d}_\alpha\}$$

$$\rho r = \textstyle\sum_\alpha \rho^\alpha (r^\alpha + \mathbf{b}^\alpha \cdot \mathbf{d}_\alpha)$$

$$\rho \eta = \textstyle\sum_\alpha \rho^\alpha \eta^\alpha$$

Constitutive equations

- Required to account for the *closure problem* and to describe the *physical response* of multiphasic materials
- Derived from the *entropy inequality* in order to satisfy *thermodynamical consistency* $\rightarrow$ depends on the investigated modelling approach

Show Cases for Selected Coupled Problems

from **Geotechnical** and **Biomechanical** Applications

Embankments & Slope failure

- Triphasic modelling approach (partially saturated soil, liquid, gas)
- Elasto-(visco)plastic solid skeleton
- Quasi-static processes


Earthquake & Vibrations

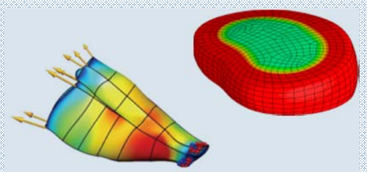
- Biphasic modelling approach
- Elasto-(visco)plastic solid
- Dynamic processes
- Abaqus-PANDAS Interface


Swelling Phenomena

- Biphasic, multi-component model approach
- Charged hydrated porous microstructure
- Chemical and electrical active

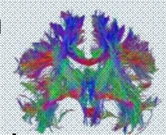
Lumbar Spine

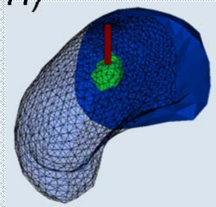
- Integrated overall model
- Coupling discrete mechanics (MKS) with a multiphasic continuum-biomechanical model of the IVD and a multi-physical muscle




Brain Tumour Treatment

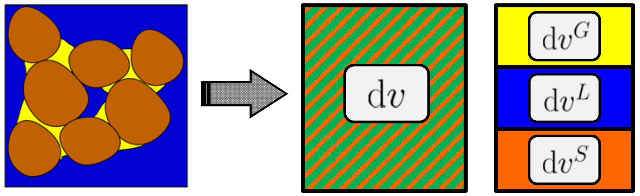
- Ternary, multi-component modelling approach
- Anisotropic tissue characteristics
- Utilisation of medical imaging data (DTI)





Geotechnical Engineering: Modelling Approach

- Fully coupled triphasic model based on the TPM



REV of the microscale

"homogenised model" on the macroscale

Multi-physical modelling approach

$$\varphi = \bigcup_\alpha \varphi^\alpha, \quad \alpha \in \{S,\ L,\ G\}$$

- Elasto-(visco)plastic solid skeleton φ^S
- Materially incompressible pore liquid φ^L
- Materially compressible pore gas φ^G

- Set of governing balance relations (quasi-static, no mass exchanges)
  - Solid skeleton:

$$\left.\begin{aligned} \mathbf{0} &= \operatorname{div} \mathbf{T}^S + n^S \rho^{SR} \mathbf{g} - \hat{\mathbf{p}}^F \\ 0 &= (n^S)'_S + n^S \operatorname{div}(\mathbf{u}_S)'_S \end{aligned}\right\} \quad \text{where: } \left\{\begin{aligned} \hat{\mathbf{p}}^F &= \hat{\mathbf{p}}^L + \hat{\mathbf{p}}^G \\ n^S &= n^S_{0S}\,(1 - \operatorname{div} \mathbf{u}_S) \end{aligned}\right.$$

  - Pore liquid:

$$\mathbf{0} = \operatorname{div} \mathbf{T}^L + n^L \rho^{LR} \mathbf{g} + \hat{\mathbf{p}}^L \quad \text{where: } n^L = s^L(1 - n^S)$$

$$0 = (n^L)'_S + n^L \operatorname{div}(\mathbf{u}_S)'_S + \operatorname{div}(n^L \mathbf{w}_L)$$

  - Pore gas:

$$\mathbf{0} = \operatorname{div} \mathbf{T}^G + n^G \rho^{GR} \mathbf{g} + \hat{\mathbf{p}}^G \quad \text{where: } n^G = (1 - s^L)(1 - n^S)$$

$$0 = n^G (\rho^{GR})'_S + \rho^{GR} (n^G)'_S + n^G \rho^{GR} \operatorname{div}(\mathbf{u}_S)'_S + \operatorname{div}(n^G \rho^{GR} \mathbf{w}_G)$$

  - Primary variables of IBVP

$$\mathbf{u}_S,\ p^{LR},\ p^{GR}$$

  - Constitutive equations required for

$$\mathbf{T}^\alpha,\ \hat{\mathbf{p}}^\beta,\ \rho^{GR},\ s^L$$

Simulation Technology

TPM & Coupled Problems

Geotechnical Engineering

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Conclusions & Outlook

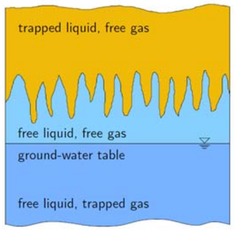
Geotechnical Engineering: Constitutive Settings

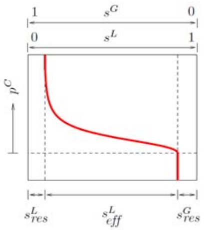
- Principle of effective stresses

$$\begin{aligned} \mathbf{T}^S &= -n^S p\,\mathbf{I} + \mathbf{T}^S_E \\ \mathbf{T}^\beta &= -n^\beta p^{\beta R}\,\mathbf{I} + \mathbf{T}^\beta_E \\ \hat{\mathbf{p}}^\beta &= p^{\beta R}\,\mathrm{grad}\, n^\beta + \hat{\mathbf{p}}^\beta_E \end{aligned}$$

$$p = s^L p^{LR} + (1 - s^L)\, p^{GR}$$

- Capillary pressure and saturations





$$p^C := p^{GR} - p^{LR}$$

$$s^L_{eff} = \frac{s^L - s^L_{res}}{1 - s^L_{res} - s^G_{res}}$$

$$s^L_{eff}(p^C) := [1 + (\alpha\, p^C)^j]^{-h}$$

- The fluid constituents
  - Preliminary assumptions

    $\mathbf{T}^\beta_E \approx \mathbf{0}$ (dim. analysis)

    $$\hat{\mathbf{p}}^\beta_E = -(n^\beta)^2 \gamma^{\beta R} (\mathbf{K}^\beta_r)^{-1} \mathbf{w}_\beta$$

    where $\mathbf{K}^\beta_r = \kappa^\beta_r(s^\beta)\mathbf{K}^\beta(n^S)$

  - Darcy-type equations

    $$n^\beta \mathbf{w}_\beta = -\frac{\mathbf{K}^\beta_r}{\gamma^{\beta R}}(\mathrm{grad}\, p^{\beta R} - \rho^{\beta R}\,\mathbf{b})$$

  - Ideal gas law (Boyle-Mariotte)

    $$\rho^{GR} = \frac{p_0 + p^{GR}}{\bar{R}^G \Theta}$$

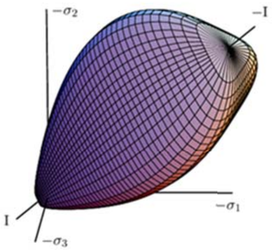
    where $\bar{R}^G \Theta = \text{const.}$

- The elasto-(visco)plastic solid skeleton
  - Decomposition of the strain tensor

    $$\boldsymbol{\varepsilon}_S = \tfrac{1}{2}(\mathrm{Grad}_S \mathbf{u}_S + \mathrm{Grad}^T_S \mathbf{u}_S) =: \boldsymbol{\varepsilon}_{Se} + \boldsymbol{\varepsilon}_{Sp}$$

  - Effective stress of the skeleton

    $$\mathbf{T}^S_E = 2\,\mu^S \boldsymbol{\varepsilon}_{Se} + \lambda^S (\boldsymbol{\varepsilon}_{Se} \cdot \mathbf{I})\,\mathbf{I}$$



  - Single-surface yield criterion

    $$\begin{aligned} F &= \Phi^{1/2} + \beta\, \mathrm{I} + \varepsilon\, \mathrm{I}^2 - \kappa \\ \Phi &= \mathrm{I\!I}^D (1 + \gamma \vartheta)^m + \tfrac{1}{2}\alpha\, \mathrm{I}^2 + \delta^2\, \mathrm{I}^4 \\ \vartheta &= \mathrm{I\!I\!I}^D / (\mathrm{I\!I}^D)^{3/2} \end{aligned}$$

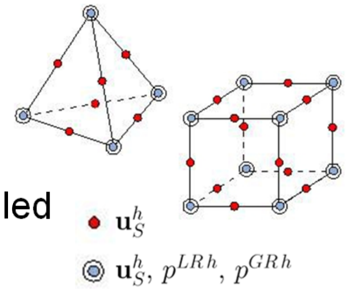
    principal invariants I, $\mathrm{I\!I}^D$, $\mathrm{I\!I\!I}^D$ of $\mathbf{T}^S_E$

  - Plastic potential $G = \sqrt{\psi_1\, \mathrm{I\!I}^D + \tfrac{1}{2}\alpha\, \mathrm{I}^2 + \delta^2\, \mathrm{I}^4} + \psi_2\, \mathrm{I} + \varepsilon\, \mathrm{I}^2$
  - Evolution equation and plastic multiplier

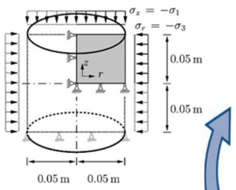
    $$(\boldsymbol{\varepsilon}_{Sp})'_S = \Lambda \frac{\partial G}{\partial \mathbf{T}^S_E}, \qquad \Lambda = \frac{1}{\eta}\left\langle \frac{F(\mathbf{T}^S_E)}{\sigma_0} \right\rangle^r$$

Geotechnical Engineering: Simulation Procedure

- Mixed finite-element formulation in PANDAS
  - **Weak formulations** of the coupled governing balance equations
  - Simultaneous approximation of all primary unknowns → **monolytical solution** of the strongly coupled problem
  - Quadratic approximation of the solid displacement and linear approximations for the pore-fluid pressures → LBB condition is fulfilled
  - These elements are known as ***Taylor-Hood* elements** (in 3-dim. fully integrated with 27 *Gauss* points)
  - **Temporal discretisation** with an **implicit** *Euler* time-integration scheme



- Numerical prediction and validation of real geotechnical applications
  - Triaxial test



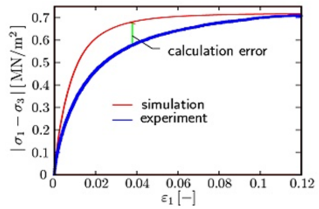
Continuum Mechanics
Theory of Porous Media

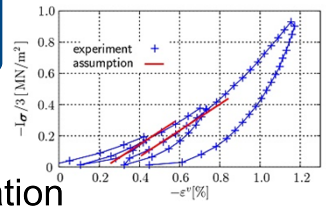
Simulation

Verification/Validation Experiments
Triaxial / Slope-failure Tests

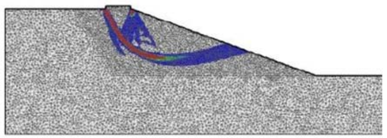
Parameter Identification
Nonlinear Optimisation

- Comparison of experimental and simulation data



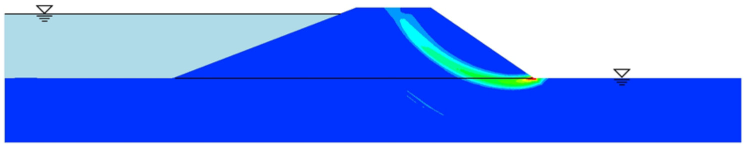


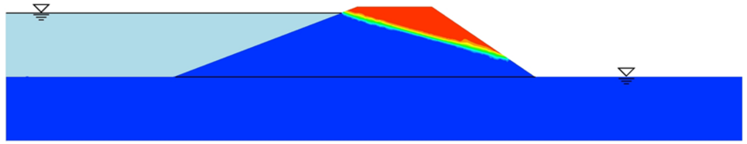
- Inverse problem
- Least-squares minimisation



Show Case: Embankments and Slope Failure

- Flow through a deformable embankment

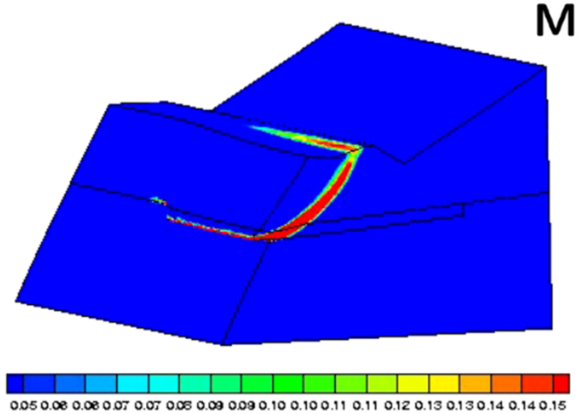


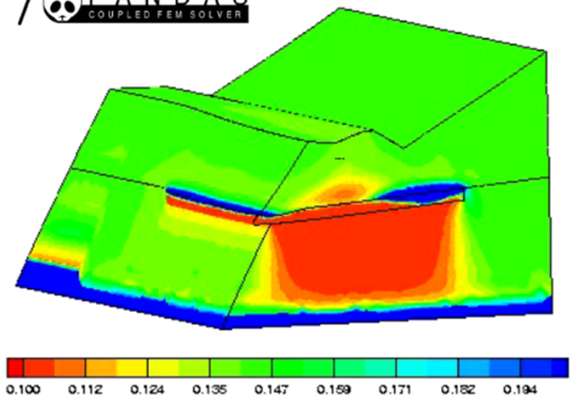


- Accumulated plastic strains
- Liquid saturation

- Slope failure of a natural railroad dam due to a heavy rainfall event (Joint work with C. Wieners)

M++ / PANDAS COUPLED FEM SOLVER

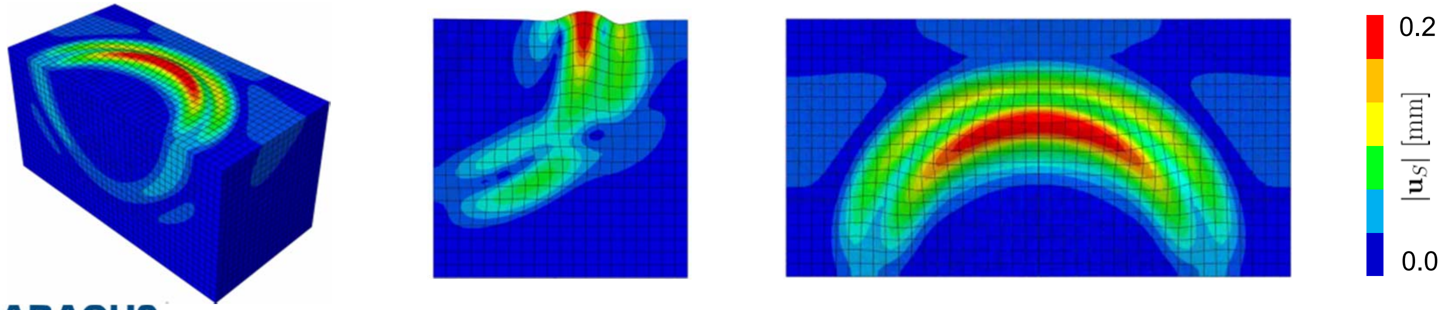




Elements	DOF	Integration points	Internal variables	CPU	Comp. time [h]
2 562 048	11 208 869	38 430 720	968 454 144	88	1070:22

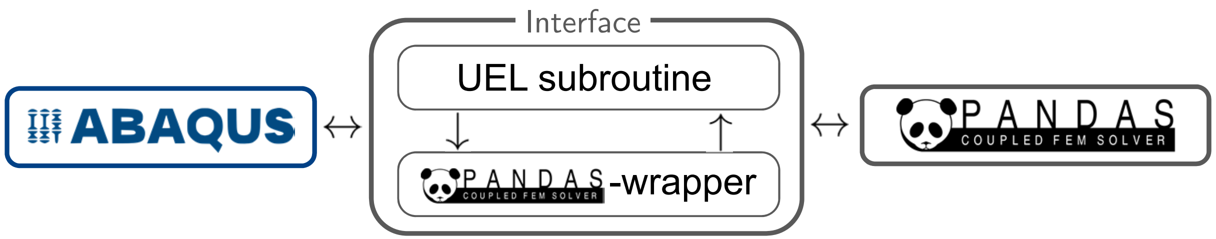
Show Case: Dynamic Problems (Earthquake)

- **3-dimensional wave propagation** (dynamic, biphasic, elastic solid)



- Parallel computation on 4 CPU with approx. 300,000 DOF

- **Abaqus-PANDAS Interface**
  - Based on the user-defined element subroutine (UEL) of Abaqus
  - FE package PANDAS is linked into a shared library
  - Tasks of the UEL are accomplished by PANDAS subroutines
  - Python scripts for the pre- and post-processing

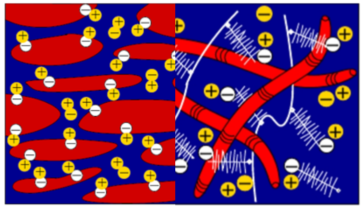


Chemically Active Media: Modelling Approach

- Natural materials show often a charged hydrated porous microstructure
- Materials respond to changes in chemical and electrical conditions

offshore platform

hydrogel mixture



REV of the microstructure

$$\varphi = (\varphi^S \cup \varphi^{fc}) \cup \varphi^F$$
$$\varphi^F = \varphi^L \cup \varphi^+ \cup \varphi^-$$

- Macroscopic multiphasic modelling approach
  - Solid skeleton: $\alpha = S$ (incl. fixed charges φ^{fc})
  - Ionised pore liquid: $\alpha = F = \sum \beta$
  - with liquid solvent: $\beta = L$
  - and charged ions: $\beta = \gamma = +, -$

  $\rightarrow$ real fluid mixture embedded in the TPM approach

- Possible simplifications
  - complete or general swelling model: $\gamma = +, -$
  - explicit exploitation of electroneutrality condition: $\gamma = +$
  - solutes (mobile ions) are assumed to diffuse rapidly: $\gamma = \emptyset$

Chemically Active Media: Constitutive Settings

- Isothermal and chemically inert
- constraints by saturation and electroneutrality
- Chemical potentials and osmotic pressures

$$\mu_m^\beta = \frac{\partial \Psi_F^F}{\partial c_m^\beta} = \frac{\partial \Psi_F^\beta}{\partial c_m^\beta} = \mu_{0m}^\beta + R\,\theta \ln c_m^\beta$$

$$\pi^\beta = c_m^\beta\, \mu_m^\beta - \Psi_F^\beta = R\,\theta\, c_m^\beta\,,$$

$$\pi = \sum_\beta \pi^\beta = R\,\theta \sum_\beta c_m^\beta$$

- Extended Darcy law

$$n^F \mathbf{w}_F = -\frac{\mathbf{K}^F}{\gamma^{FR}} \left(\operatorname{grad} \mathcal{P} \;-\; \rho^{FR}\,\mathbf{b} \;-\; z^{fc} c_m^{fc}\, F \operatorname{grad} \mathcal{E} \right)$$

- Extended Nernst-Planck equation

$$n^F c_m^\gamma \mathbf{d}_{\gamma F} = -\frac{\mathbf{D}^\gamma}{R\theta} \left(R\theta \operatorname{grad}\, c_m^\gamma + z^\gamma c_m^\gamma\, F \operatorname{grad} \mathcal{E} \right)$$

- Poisson equation (PE)

$$\operatorname{div}\,\operatorname{grad} \mathcal{E} \;=\; \frac{n^F F}{\epsilon^F} \left(\sum_\gamma z^\gamma c_m^\gamma + z^{fc} c_m^{fc} \right)$$

- Partial and overall Cauchy stresses

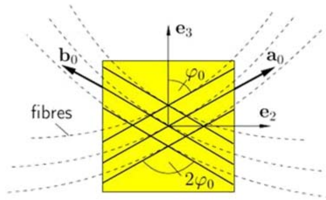
$$\begin{aligned}
\mathbf{T}^S &= -n^S(\mathcal{P}+\pi)\,\mathbf{I} - \rho_e^{fc}\,\mathcal{E}\,\mathbf{I} + \mathbf{T}^S_{E\,mech.}\\
\mathbf{T}^L &= -(n^L\mathcal{P} + n^F\pi^L)\,\mathbf{I} + \mathbf{T}^L_{E\,mech.}\\
\mathbf{T}^\gamma &= -(n^\gamma\mathcal{P} + n^F\pi^\gamma)\,\mathbf{I} - \rho_e^\gamma\,\mathcal{E}\,\mathbf{I} + \mathbf{T}^\gamma_{E\,mech.}\\
\mathbf{T}^F &= \textstyle\sum_\beta \mathbf{T}^\beta = -n^F(\mathcal{P}+\pi)\,\mathbf{I} - \sum_\gamma \rho_e^\gamma\,\mathcal{E}\,\mathbf{I} + \mathbf{T}^F_{E\,mech.}\\
\mathbf{T} &= -p\,\mathbf{I} + \mathbf{T}^S_{E\,mech.} \quad \text{where} \quad p = \mathcal{P} + \pi
\end{aligned}$$

- Momentum productions

$$\begin{aligned}
\hat{\mathbf{p}}^L &= \mathcal{P} \operatorname{grad} n^L + \pi^L \operatorname{grad} n^F + \hat{\mathbf{p}}^L_{E,\,mech.}\\
\hat{\mathbf{p}}^\gamma &= \mathcal{P} \operatorname{grad} n^\gamma + \pi^\gamma \operatorname{grad} n^F + \mathcal{E} \operatorname{grad}(\rho_e^\gamma) + \hat{\mathbf{p}}^\gamma_{E,\,mech.}\\
\hat{\mathbf{p}}^F &= \mathcal{P} \operatorname{grad} n^F + \pi \operatorname{grad} n^F + \mathcal{E} \textstyle\sum_\gamma \operatorname{grad}(\rho_e^\gamma) + \hat{\mathbf{p}}^F_{E,\,mech.}
\end{aligned}$$

- Anisotropic finite-elastic solid constituent

$$\mathbf{T}^S_E = \mathbf{T}^S_{E,\,iso} + \mathbf{T}^S_{E,\,aniso}$$



$$\mathbf{T}^S_{E,\,iso} = \frac{\mu^S}{J_S}(\mathbf{B}_S - \mathbf{I}) + \lambda^S (1 - n^S_{0S})^2 \left(\frac{1}{1-n^S_{0S}} - \frac{1}{J_S - n^S_{0S}}\right)\mathbf{I}$$

$$\begin{aligned}
\mathbf{T}^S_{E,\,aniso} = \frac{\tilde{\mu}^S_1}{J_S}\big[& I_4^{-1}(I_4^{\tilde{\gamma}^S_1/2} - 1)\,(\mathbf{F}_S\,\mathbf{a}_0 \otimes \mathbf{F}_S\,\mathbf{a}_0) +\\
& I_6^{-1}(I_6^{\tilde{\gamma}^S_1/2} - 1)\,(\mathbf{F}_S\,\mathbf{b}_0 \otimes \mathbf{F}_S\,\mathbf{b}_0)\big]
\end{aligned}$$

Simulation Technology

TPM & Coupled Problems

Geotechnical Engineering

Biomechanical Engineering

Conclusions & Outlook

Chemically Active Media: Numerical Treatment

- Electric and electrochemical relations as initial boundary conditions
  - Donnan equation [Donnan 1911]

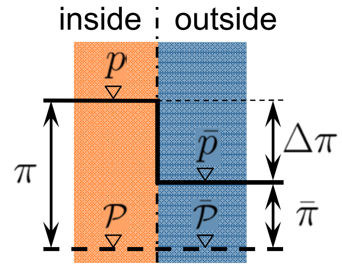
$$c_m^\gamma(\mathbf{u}_S,\, \bar{c}_m^\gamma) \;=\; \frac{1}{2\,|z^\gamma|}\Big(\sqrt{(\,z^{fc}\,c_m^{fc}\,)^2 - 4\,z^+z^-\,(\bar{c}_m^\gamma)^2} \;-\; z^{fc}\,c_m^{fc}\Big)$$

  - Osmotic pressure [Vanthoff 1886]

$$p\,(c_m^\gamma,\, \bar{c}_m^\gamma,\, \bar{p}\,) \;=\; \bar{p} + R\theta\,\big[(c_m^+ + c_m^-) \;-\; (\bar{c}_m^+ + \bar{c}_m^-)\big]$$

  - Nernst potential [Nernst 1888]:

$$\mathcal{E}\,(c_m^\gamma,\, \bar{c}_m^\gamma,\, \bar{\mathcal{E}}) \;=\; \bar{\mathcal{E}} \;+\; \frac{R\theta}{z^\gamma F}\,\ln\Big(\frac{\bar{c}_m^\gamma}{c_m^\gamma}\Big)$$



$(\bar{\cdot})$: prescribed external quantities

→ **Deformation-dependent boundary conditions**

- Governing weak formulations (primary variables $\mathbf{u}_S$, p , c_m^γ , $\mathcal{E}$)
  (with weakly fulfilled boundary conditions for p , c_m^γ , $\mathcal{E}$)

- MB of φ

$$\int_\Omega (\mathbf{T}^S_{E\,mech.} - p\,\mathbf{I}) \cdot \mathrm{grad}\;\delta\mathbf{u}_S\,\mathrm{d}v \;-\; \int_\Omega (\rho^S + \rho^F)\,\mathbf{b}\cdot\delta\mathbf{u}_S\,\mathrm{d}v = \int_{\Gamma_t} \bar{\mathbf{t}}\cdot\delta\mathbf{u}_S\,\mathrm{d}a$$

- VB of φ^F

$$\int_\Omega n^F\mathbf{w}_F\cdot\mathrm{grad}\,\delta p\,\mathrm{d}v - \int_\Omega \mathrm{div}\,(\mathbf{u}_S)'_S\,\delta p\,\mathrm{d}v + \int_{\Gamma_p}\epsilon\big[p - \bar{p} - R\theta\sum_\gamma(c_m^\gamma - \bar{c}_m^\gamma)\big]\,\delta p\,\mathrm{d}a \;=\; \int_{\Gamma_q}\bar{q}\,\delta p\,\mathrm{d}a$$

- CB of φ^γ

$$\int_\Omega n^F c_m^\gamma\mathbf{w}_\gamma\cdot\mathrm{grad}\,\delta c_m^\gamma\,\mathrm{d}v \;-\; \int_\Omega\big[\,n^F(c_m^\gamma)'_S + c_m^\gamma\,\mathrm{div}\,(\mathbf{u}_S)'_S\,\big]\,\delta c_m^\gamma\,\mathrm{d}v \;+$$

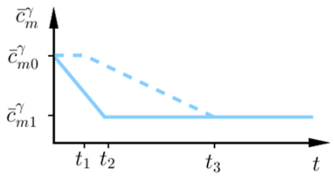
$$+\int_{\Gamma_{c_m^\gamma}}\epsilon\,\Big[c_m^\gamma - \frac{1}{2\,|z^\gamma|}\Big(\sqrt{(\,z^{fc}\,c_m^{fc}\,)^2 - 4\,z^+z^-\,(\,\bar{c}_m^\gamma\,)^2} - z^{fc}\,c_m^{fc}\Big)\Big]\delta c_m^\gamma\,\mathrm{d}a \;=\; \int_{\Gamma_{\bar{j}^\gamma}}\bar{j}^\gamma\,\delta c^\gamma\,\mathrm{d}a$$

- Poisson equation

$$\int_\Omega \mathrm{grad}\,\mathcal{E}\cdot\mathrm{grad}\,\delta\mathcal{E}\,\mathrm{d}v \;-\; \int_\Omega\frac{n^F F}{\epsilon^F}\Big(\sum_\gamma z^\gamma c_m^\gamma + z^{fc}c_m^{fc}\Big)\,\delta\mathcal{E}\,\mathrm{d}v + \int_{\Gamma_\xi}\epsilon\Big(\mathcal{E} - \bar{\mathcal{E}} - \frac{R\theta}{z^+F}\,\ln\frac{\bar{c}_m^+}{c_m^+}\Big)\,\delta\mathcal{E}\,\mathrm{d}a \;=\; \int_{\Gamma_{\bar{e}}}\bar{e}\,\delta\mathcal{E}\,\mathrm{d}a$$

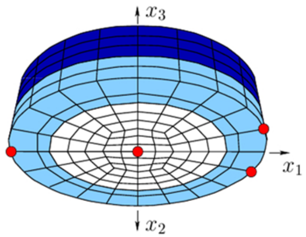
Show Case: Swelling of a Hydrogel Disc

- Chemical loading, geometry & mesh



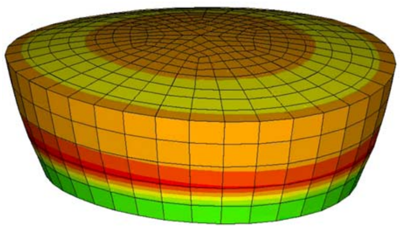
$r/R \times h = 1.5/1.7 \times 1.0\,\mathrm{mm}^3$

chemical loading path (solid line)
chemical loading path (dashed line)
transition zone

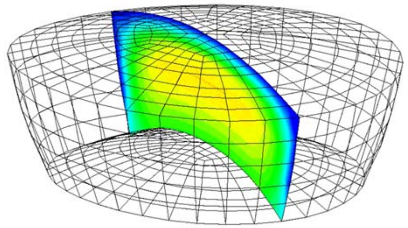


$\bar{c}_{m0}^\gamma = 2.5\,\mathrm{mol/l}$, $\bar{c}_{m1}^\gamma = 2.4\,\mathrm{mol/l}$,
$c_{m0S}^{fc} = 0.3\,\mathrm{eq/l}$, $t_1 = 145\,\mathrm{s}$,
$t_2 = 175\,\mathrm{s}$, $t_3 = 495\,\mathrm{s}$

- Simulation results



overall pressure

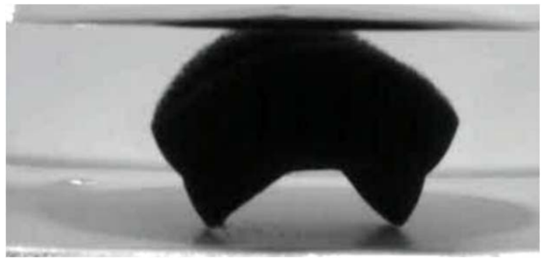


cation concentration

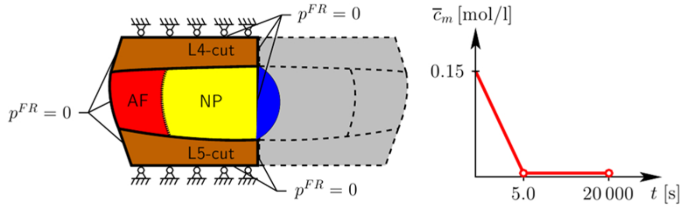
p: 0.13 0.09 0.05 $[\mathrm{N/mm}^2]$

c_m^+: 1.10 0.60 0.15 [mol/l]

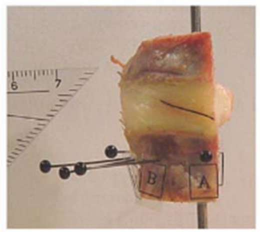
- Movie of an experiment
  [by courtesy of J. Huyghe]



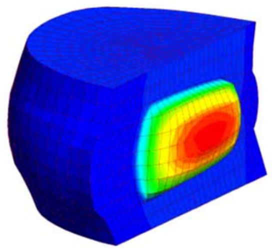
- Intervertebral Disc



Swelling of the nucleus pulposus ex vivo



[picture by courtesy of G. Holzapfel]



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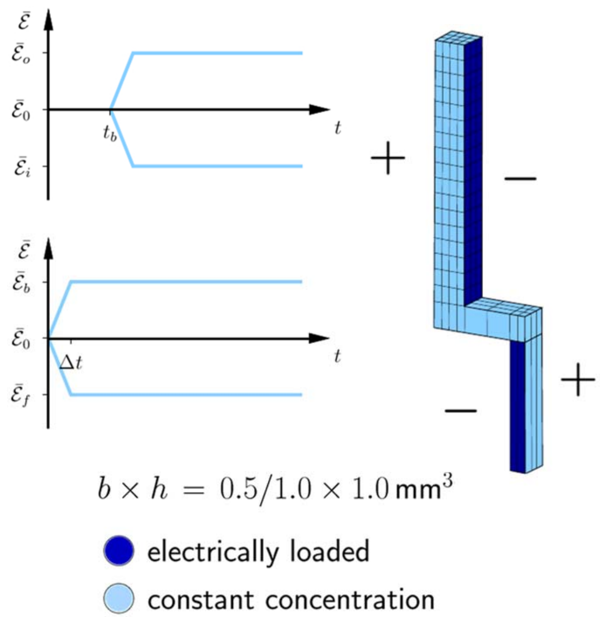
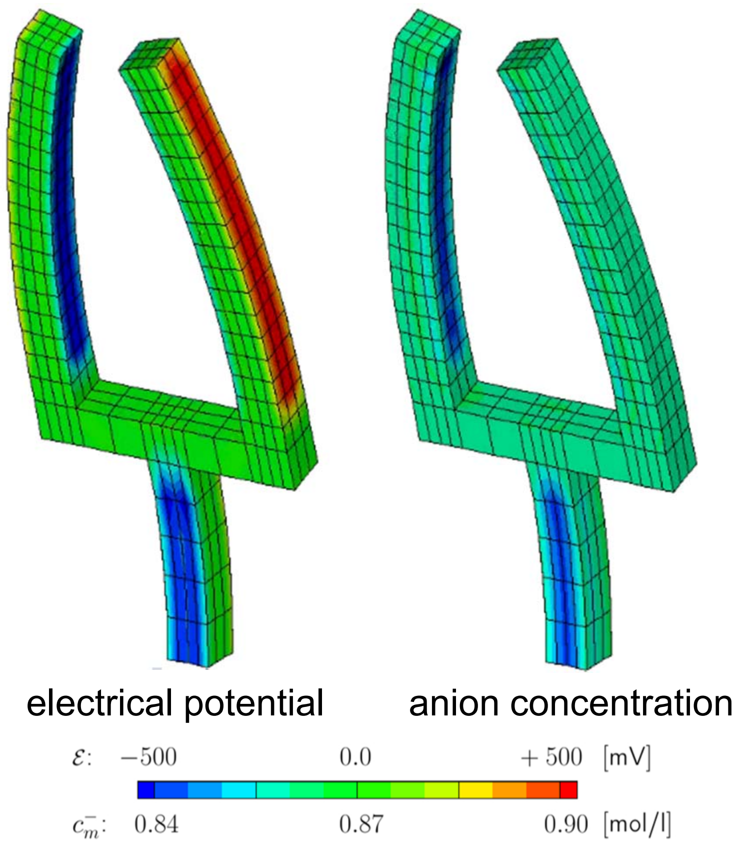
Show Case: Electroactive Polymer Gripper

- Electrical loading, simulation parameters, geometry and mesh



$$\bar{\mathcal{E}}_o/\bar{\mathcal{E}}_i = \pm 500\,\mathrm{mV}\,, \quad \bar{\mathcal{E}}_b/\bar{\mathcal{E}}_f = \pm 425\,\mathrm{mV}\,,$$
$$t_b = 450\,\mathrm{s}\,, \quad \Delta t = 4\,\mathrm{s}\,,$$
$$\mu^S = 0.14\,\mathrm{N/mm}^2\,, \quad \lambda^S = 0.02\,\mathrm{N/mm}^2\,,$$
$$\bar{c}_m^{\gamma} = 1.0\,\mathrm{mol/l}\,, \quad c_{m0S}^{fc} = 0.3\,\mathrm{eq/l}$$

- Simulation results



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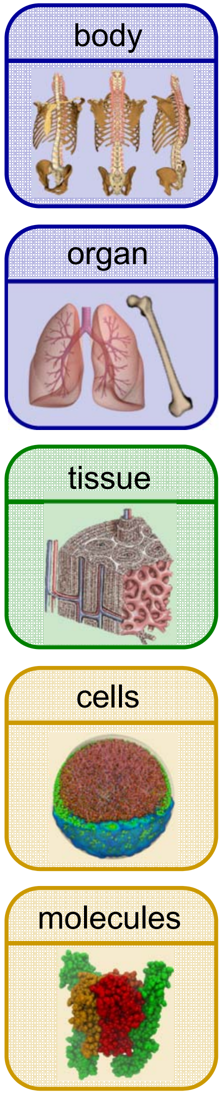
Integrated Overall Human Model



Discrete Biomechanics:

- Sports and movement science
- Multi-body Systems, Robotics, etc.

Continuum Biomechanics:

- Solid Mechanics
- Fluid Mechanics
- Fluid-Structure Interaction
- Theory of Porous Media
- Multi-phase Flow
- Multi-component Transport

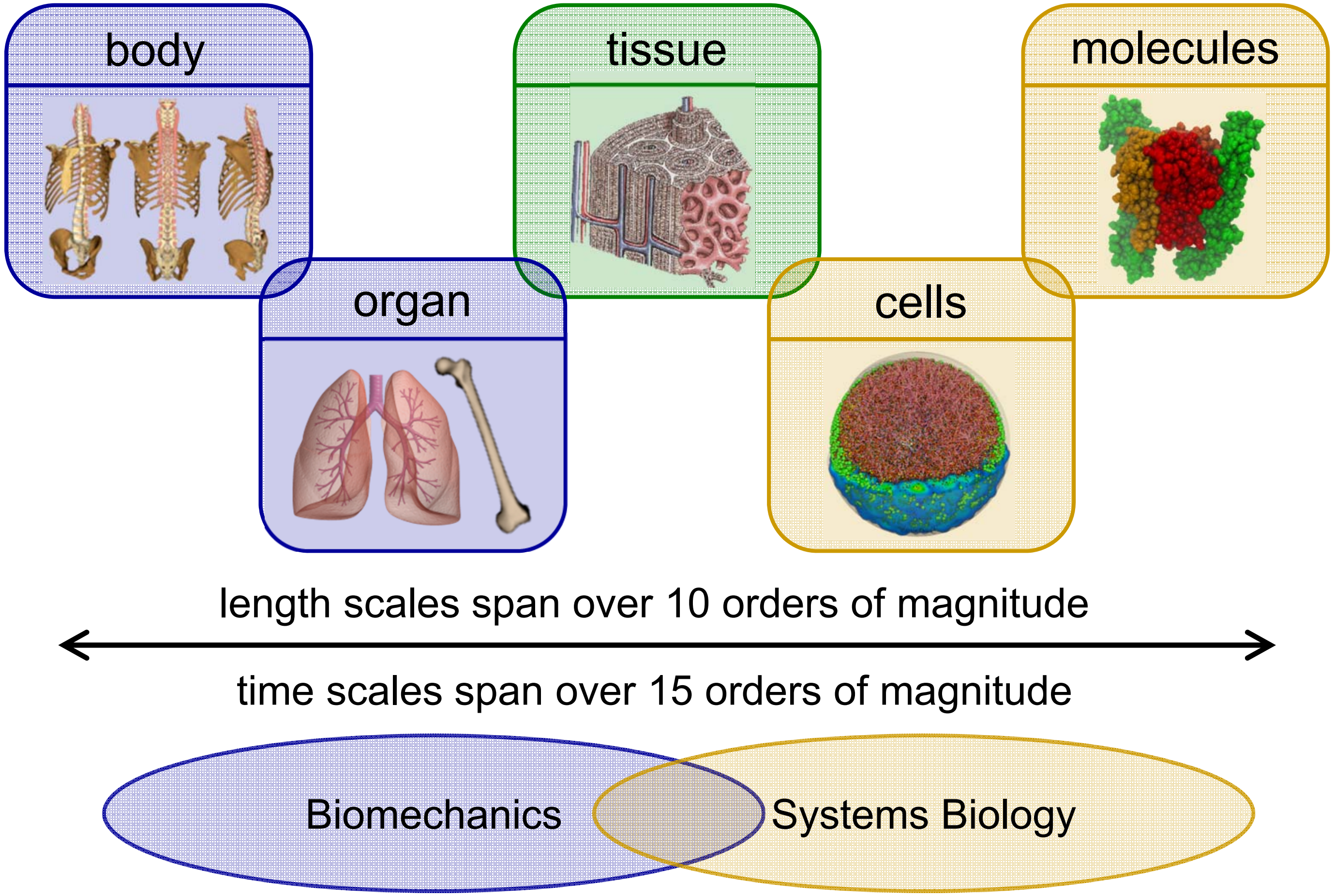
Systems Biology:

- Chemical Reaction Kinetics
- Signal Transduction Pathways
- Heterogeneous Cell Populations
- Statistical Methods

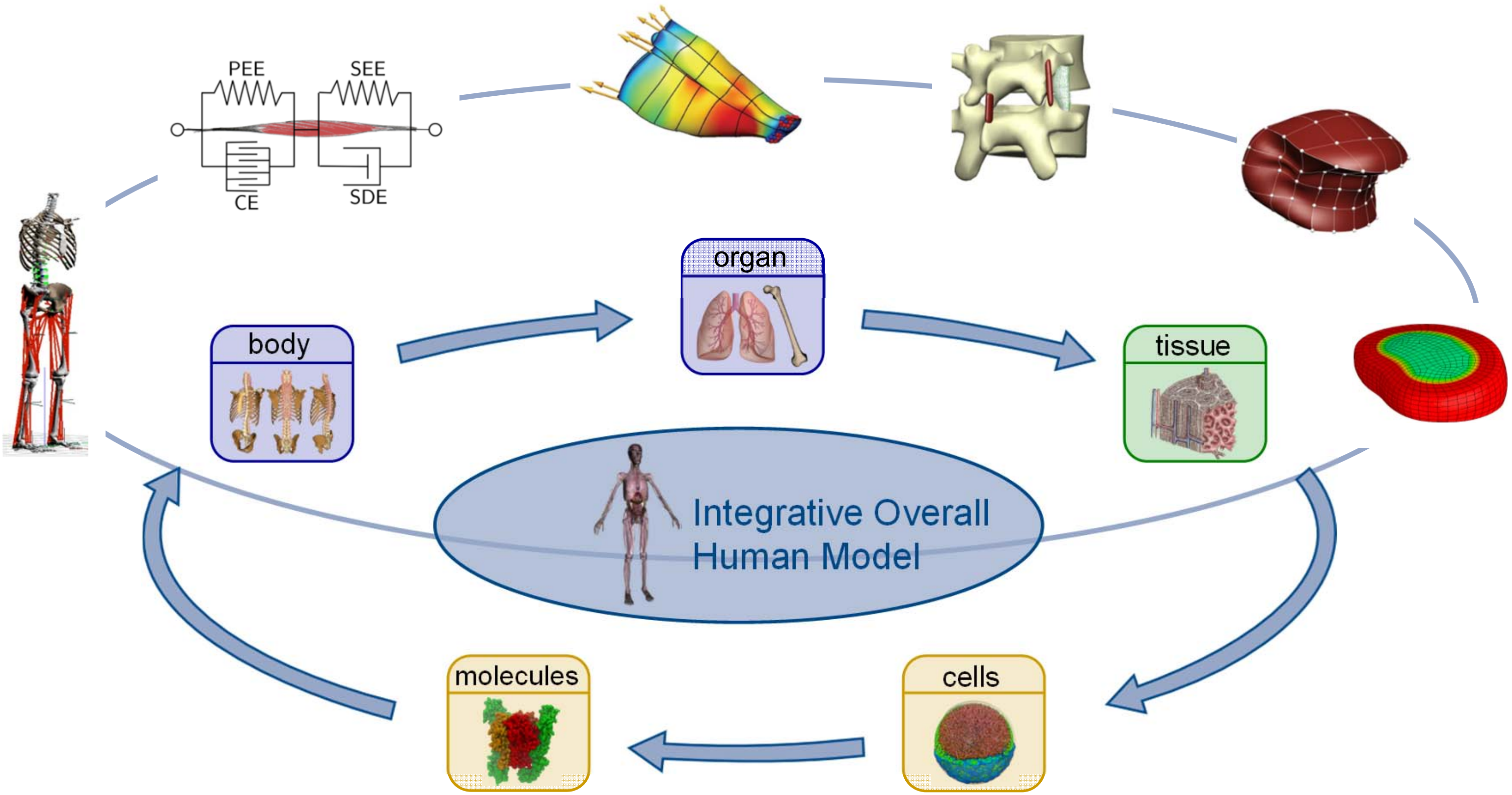
Molecular Biology, Biochemistry:

- Molecular Dynamics
- Phenomics, Genomics

Integrated Overall Human Model



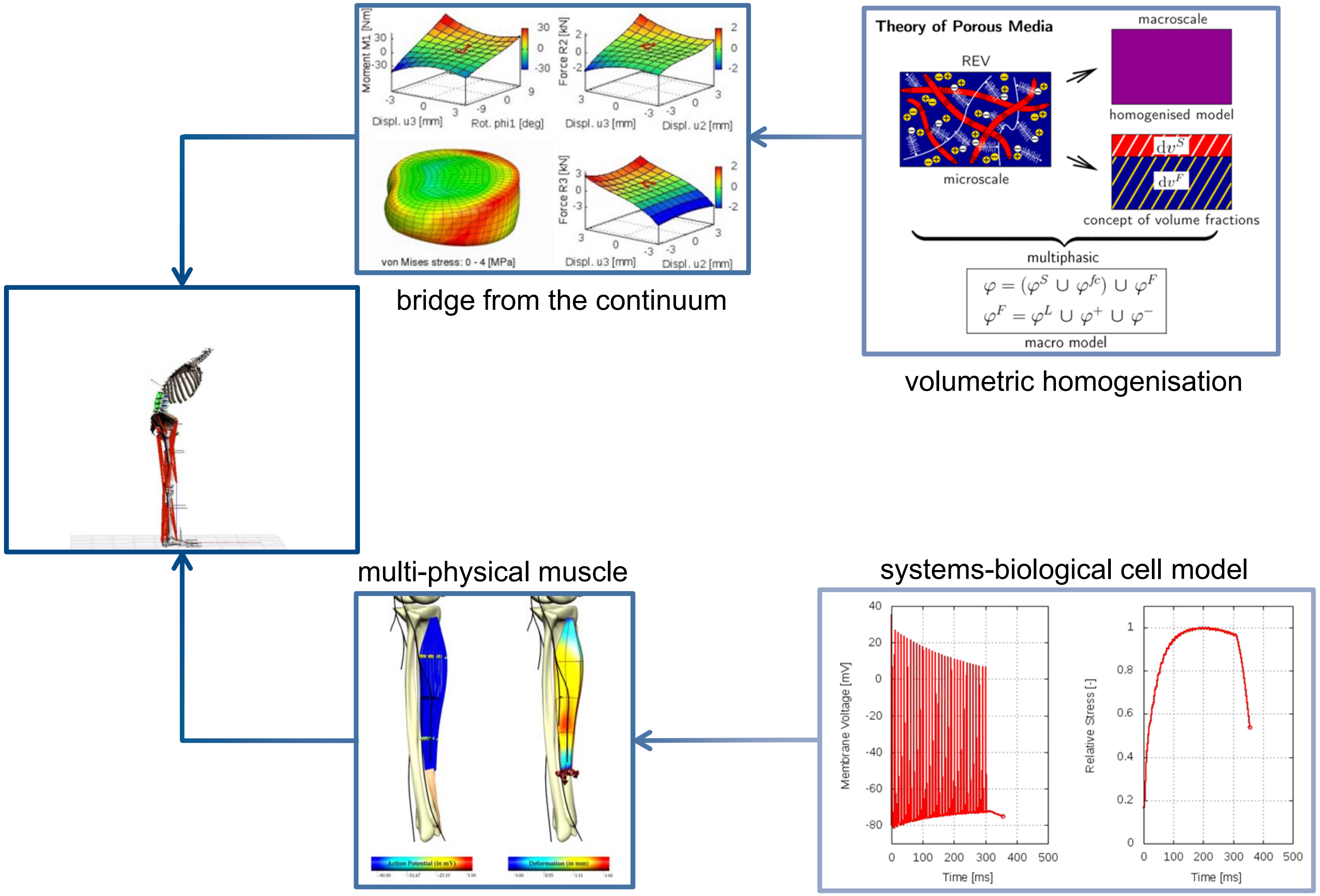
Integrated Overall Human Model



- **The Integrative Overall Human Model** is a toolbox of multi-physical models ranging from the molecular to the full body scale. It provides bridging information on the coupled driving quantities to generate a custom model for a specific application.

Show Case: Lumbar Spine

- Multi-scale simulation of the dynamic loads on the lumbar spine



Show Case: Lumbar Spine

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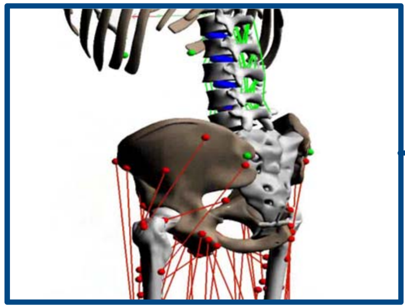
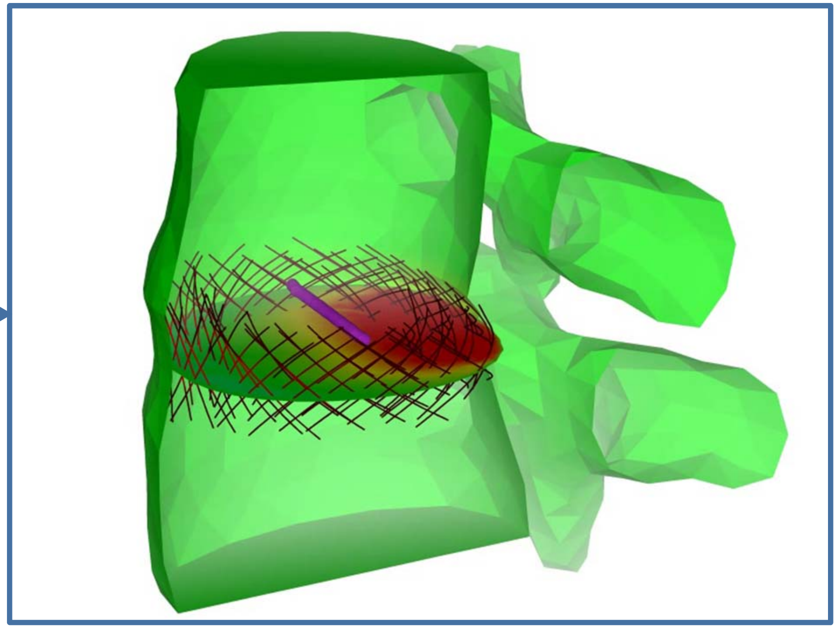


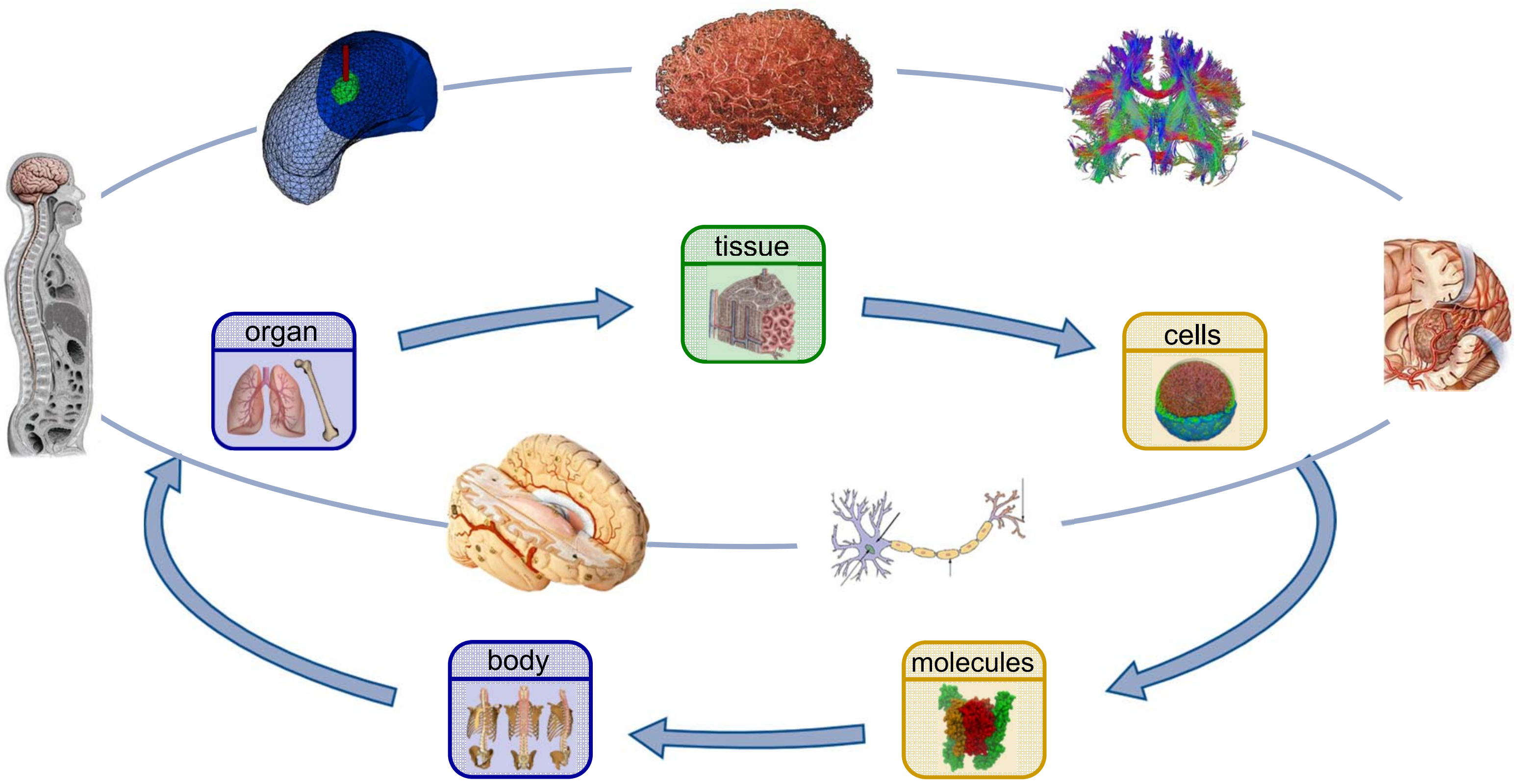
application of dynamic loading conditions



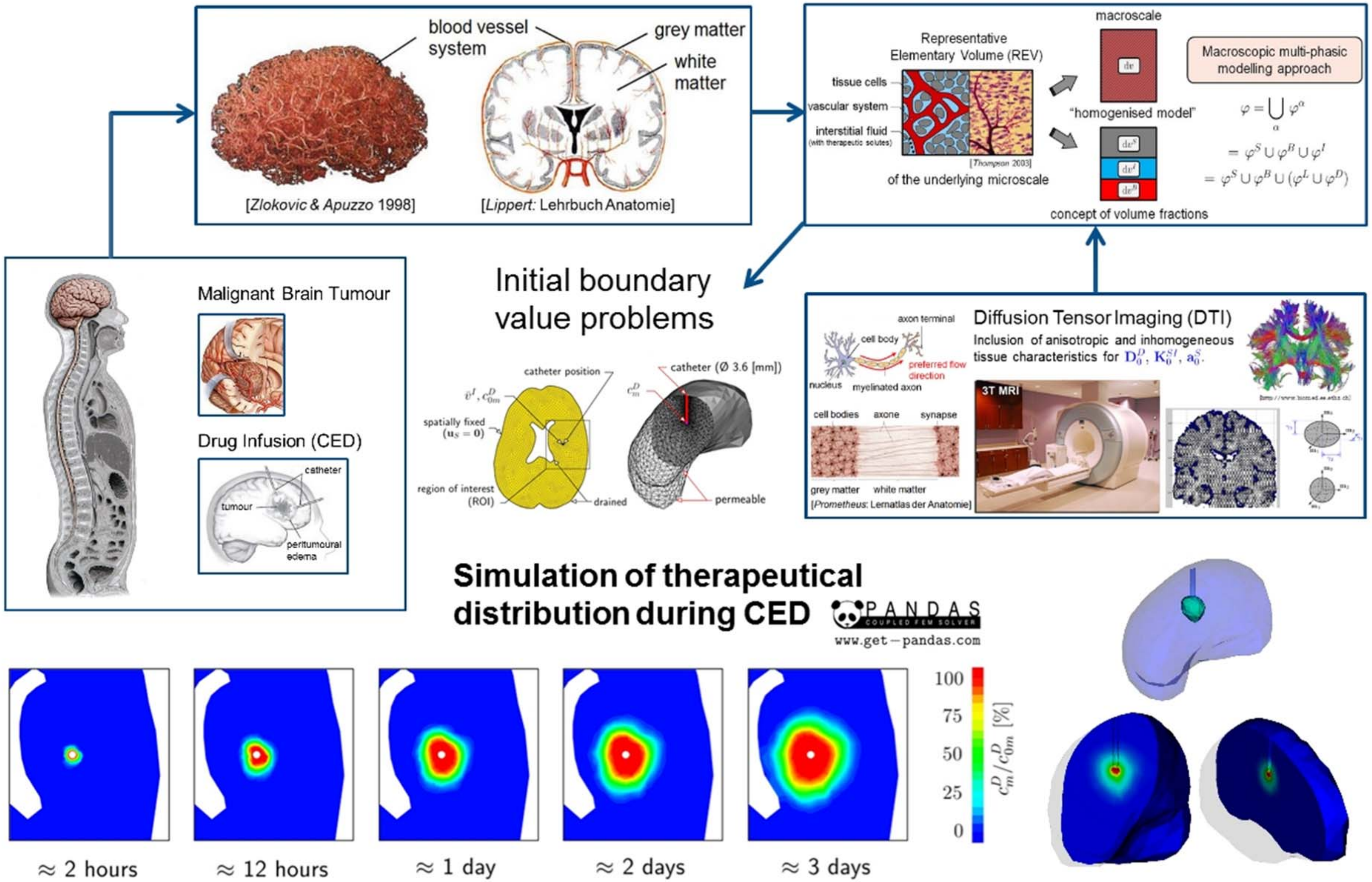
to recover local stresses and strains

Show Case: Human Brain Tissue

- Addressing coupled biomechanical problems that span from the organ over the tissue to the cellular scale.



Show Case: Human Brain Tissue



Simulation Technology Applied to Coupled Problems in Continuum Mechanics

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Stuttgart Research Centre for
Simulation Technology
www.simtech.uni-stuttgart.de

Structural elements of Simulation Technology

- Generating an unique research and education infrastructure
- Performing internationally visible research with high impact
- Establishing a trans-disciplinary working research community

Scientific elements of Simulation Technology

- Addressing strongly coupled problems in various applications of highly complex multiphasic and multicomponent materials
- Vision of an integrative systems science