Towards a Multi-physics Material Toolbox for LS-DYNA

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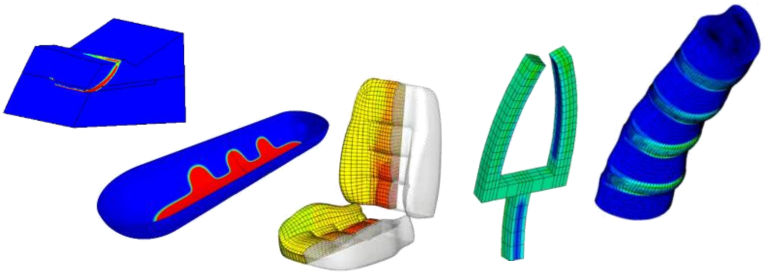
Introduction
Theory
Numerical Treatment
Simulation
Application Examples
Summary & Future Aspects



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SimTech Cluster of Excellence
Universität Stuttgart Germany
Institut für Mechanik Prof. Dr.-Ing. W. Ehlers

Introduction

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▷ **Coupled problems**

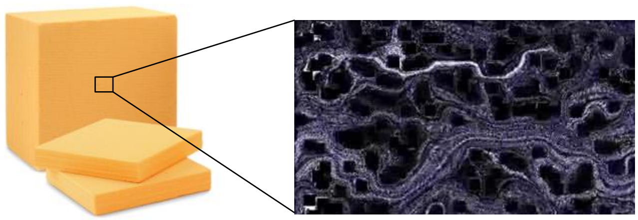
- Inherent mutual interaction between different systems
- Distinguished into surface- and volume-coupled problems
- Surface-coupled problems (distinct coupling surface)

aeroelastic fluttering

- Volume-coupled problem (no distinct coupling interface)

thermoelasticity

▷ What are multi-physics materials?



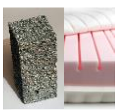
foam porous-media flow

→ the microstructural surface-coupled problems is more conveniently described through a macroscopic volume-coupled approach if the microstructure is

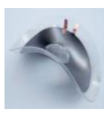
- unkown (e. g. in geomechanical problems)
- or very complex (e. g. in biomechanical problems)

→ in **multi-physics material** the macroscopic behaviour is driven by multiple mutual interacting microstructural physical phenomena

▷ Application examples


foams

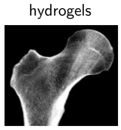

hydrogels


electroactive polymers


soils


geothermal plants


cartilage


bone


wood


fibre-reinforced plastics


lithium-ion batteries

▷ Objectives

- Simulation of multi-physics materials through LS-DYNA

▷ Solution approach

- Using a macroscopic modelling framework → volume-coupled multi-field materials
- Finite-element-based spatial discretisation
- Implementation of the material model into PANDAS[1]
- LS-DYNA/PANDAS co-simulation based on the user-defined element subroutine
  → large-scale simulations, complex initial-boundary-value problems

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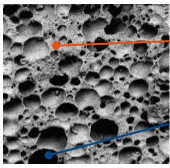
Theoretical Fundamentals

▷ **Theory of Porous Media** [*Bowen, de Boer, Ehlers, Lewis & Schrefler*]

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



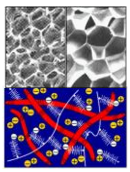
solid skeleton: φ^S
e. g. soil, polymer, cartilage

pore fluid: $\varphi^F = \bigcup_\beta \varphi^\beta$
e. g. water, air, interstitial fluid

← fluid mixture $\varphi^\beta = \bigcup_\gamma \varphi^\gamma$
e. g.: solution, vaporised water

- **Homogenisation process of multiphasic porous media**

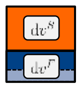
Representative Elementary Volume (REV)



of the underlying microscale

macroscale

"homogenised model"



micro-to-macro transition

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

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

$$n^{\alpha} := \frac{1}{V_m} \int_{V^\alpha} \mathrm{d}v_m^\alpha$$

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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.:	$\mathbf{0} \;=\; \mathbf{I} \times \mathbf{T} \quad \to \quad \mathbf{T} = \mathbf{T}^T$
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

$$\sum_\alpha \hat\rho^\alpha \;=\; 0$$
$$\sum_\alpha \hat{\mathbf{s}}^\alpha \;=\; \mathbf{0} \quad \text{with} \quad \hat{\mathbf{s}}^\alpha = \hat{\mathbf{p}}^\alpha + \hat\rho^\alpha \overset{\prime}{\mathbf{x}}_\alpha$$
$$\sum_\alpha \hat{\mathbf{h}}^\alpha \;=\; \mathbf{0} \quad \text{with} \quad \hat{\mathbf{h}}^\alpha = \hat{\mathbf{m}}^\alpha + \mathbf{x} \times \hat{\mathbf{s}}^\alpha$$
$$\sum_\alpha \hat e^\alpha \;=\; 0 \quad \text{with} \quad \hat e^\alpha = \hat\varepsilon^\alpha + \hat{\mathbf{p}}^\alpha \cdot \overset{\prime}{\mathbf{x}}_\alpha + \hat\rho^\alpha (\varepsilon^\alpha + \tfrac{1}{2} \overset{\prime}{\mathbf{x}}_\alpha \cdot \overset{\prime}{\mathbf{x}}_\alpha)$$
$$\sum_\alpha \hat\eta^\alpha \;\geq\; 0 \quad \text{with} \quad \hat\eta^\alpha = \hat\zeta^\alpha + \hat\rho^\alpha \eta^\alpha$$

Relations between total and partial quantities

$$\rho \mathbf{b} = \sum_\alpha \rho^\alpha \mathbf{b}^\alpha$$
$$\mathbf{T} = \sum_{\alpha=1}^k (\mathbf{T}^\alpha - \rho^\alpha \mathbf{d}_\alpha \otimes \mathbf{d}_\alpha)$$
$$\rho \varepsilon = \sum_\alpha \rho^\alpha (\varepsilon^\alpha + \tfrac{1}{2} \mathbf{d}_\alpha \cdot \mathbf{d}_\alpha)$$
$$\mathbf{q} = \sum_\alpha \{\mathbf{q}^\alpha - (\mathbf{T}^\alpha)^T \mathbf{d}_\alpha + \rho^\alpha \varepsilon^\alpha \mathbf{d}_\alpha + \tfrac{1}{2} \rho^\alpha (\mathbf{d}_\alpha \cdot \mathbf{d}_\alpha) \mathbf{d}_\alpha\}$$
$$\rho r = \sum_\alpha \rho^\alpha (r^\alpha + \mathbf{b}^\alpha \cdot \mathbf{d}_\alpha)$$
$$\rho \eta = \sum_\alpha \rho^\alpha \eta^\alpha$$

- **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* $\to$ depends on the investigated modelling approach

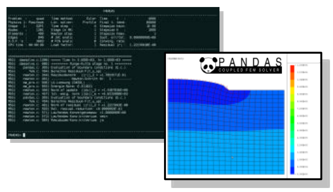
Numerical Treatment

▷ Discretisation

- Spatial discretisation: mixed finite elements (FE) [*Taylor & Hood* 1973]
  → satisfy LBB condition
- Temporal discretisation, e. g.
  - implicit *Euler* or *Newmark* scheme [*Newmark* 1959]
  - explicit methods (e. g. central-difference method, forward *Euler* method)

▷ Solution Procedure

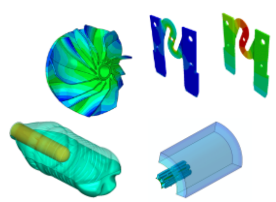
- Material-model implementation into the in-house FE code PANDAS[1]
  - coupled multi-field solver
  - object-oriented C code
  - monolithic solution strategy
  - sequential code
  - command-lines interface
  - pre- and post-processing via third party tools (e. g. Cubit, Tecplot)



[1]**P**orous media **A**daptive **N**on-linear finite-element solver based on **D**ifferential **A**lgebraic **S**ystem (www.get-pandas.com)

▷ LS-DYNA/PANDAS co-simulation

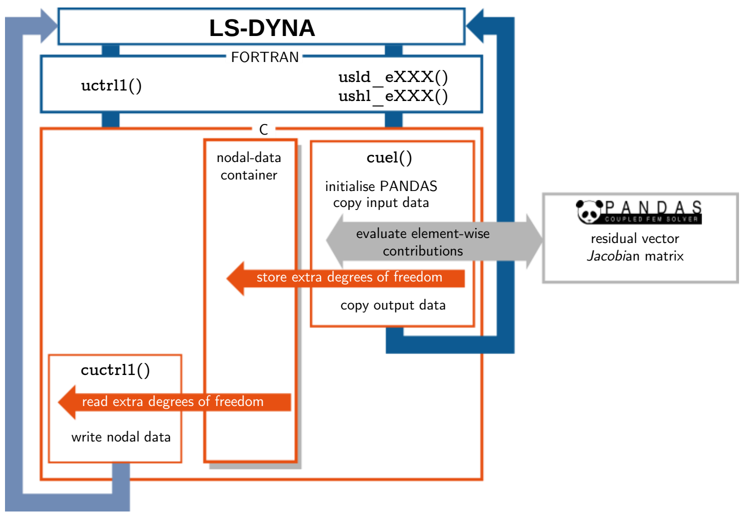
- widely used in industry and research
- comprehensive numerical-modelling capabilities
- large-scale simulations (parallelisation)
- customisation via user-defined subroutines
- ...



- Convenient environment for user-programmable elements in PANDAS
- Extension of LS-DYNA-material-model library by PANDAS material models
  → **transfer of research results in a production environment**

- **Co-simulation approach**
  - based on the user-defined element subroutines usld_eXXX() and ushl_eXXX()
  - PANDAS is linked as a library to LS-DYNA
    →PANDAS subroutines replace user-element functionality
  - exploit extra degrees of freedom to hold additional field variables during simulation
  - exploit temporary text file and uctrl1() for the post-processing of the additional field variables

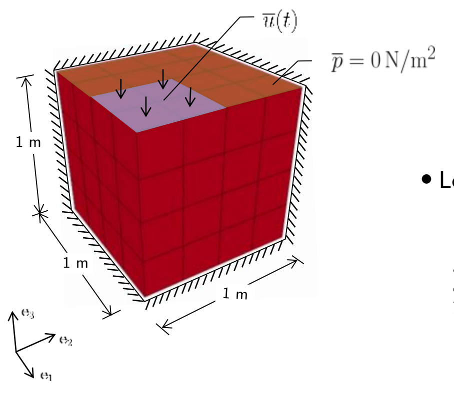
- Co-simulation workflow



Simulation

▷ Compression of a fluid-saturated foam

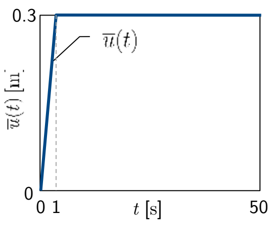
- Geometry, boundary conditions



- Material parameters

Parameter	Value	Unit
μ^S	26	$\mathrm{kN/m^2}$
λ_S	40	$\mathrm{kN/m^2}$
ρ^{SR}	2700	$\mathrm{kg/m^3}$
ρ^{FR}	1000	$\mathrm{kg/m^3}$
n^S_{0S}	0.6	
k^F	10^{-3}	$\mathrm{m/s}$

- Loading



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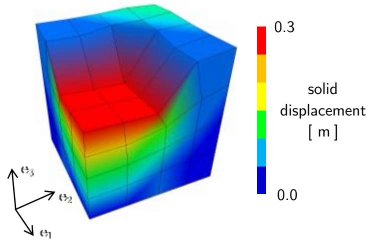
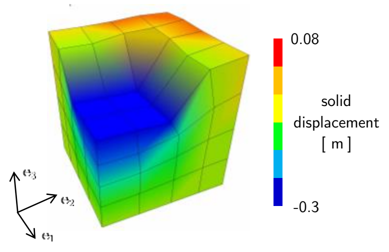
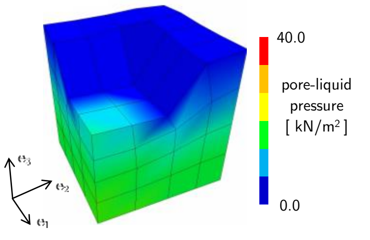
- Results
  - magnitude of solid displacement



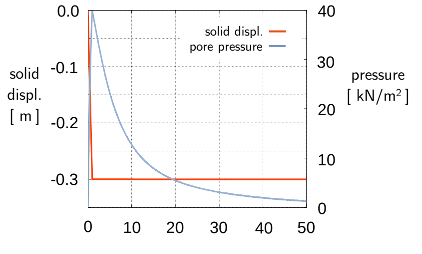
  - solid displacement in direction e_3



  - pore-liquid pressure



  - evolution of the pore-liquid pressure and in solid displacement in e_3



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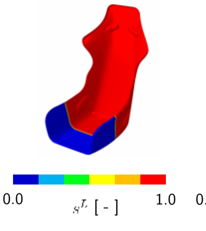
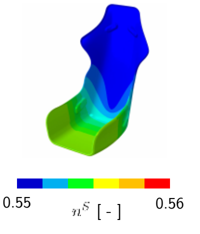
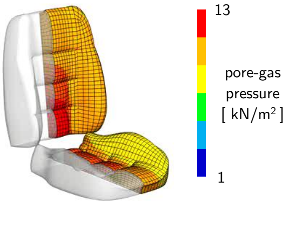
Further Application Scenarios

▷ **Vacuum-assisted resin transfer moulding**



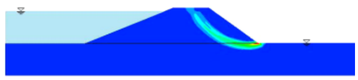


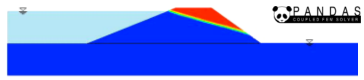
▷ **Impact on a car-seat cushion** [*Markert* 2005]



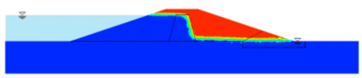
▷ Embankment failure

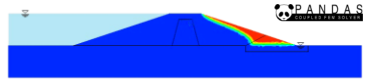
- Flow through an embankment


accumulated plastic strains


pore-liquid saturation

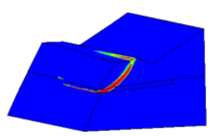
- Flow through an embankment with seal and filter

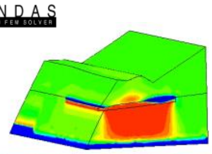

pore-liquid saturation


pore-liquid saturation

▷ Slope Failure [*Wieners* et *al.* 2005]

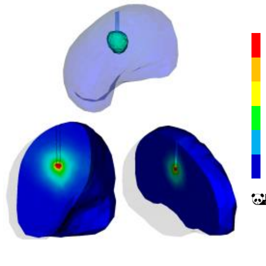
M++/ PANDAS


0.05 accumulated plastic strain [-] 0.15

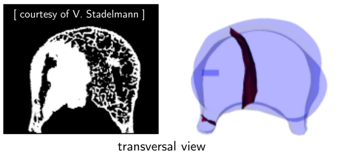

0.1 pore-liquid saturation [-] 0.194

▷ Biomaterials (e. g. bone, cartilage, skin)

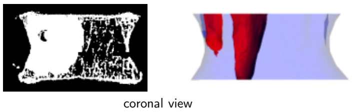
- Drug infusion
  [*Ehlers & Wagner* 2015]



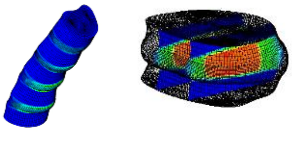
- Vertebroplasty (vertebral enforcement)
  [*Bleiler* et *al.* 2015]



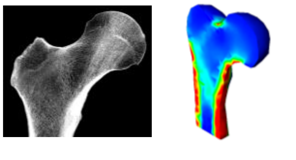
transversal view


coronal view

- Human intervertebral disc (IVD)
  [*Ehlers* et *al.* 2009]

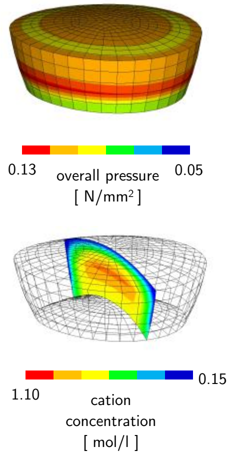


- Bone remodelling
  [*Krause* et *al.* 2009]

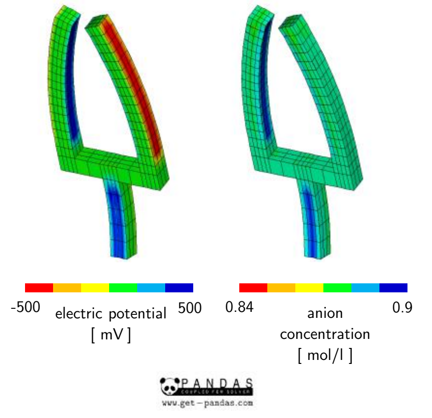


▷ Electro-chemically active media

- Swelling of a hydrogel disc [*Acartürk* 2008]



- Electro-active polymer gripper (EAP) [*Acartürk* 2008]



Towards a Multi-physics Material Toolbox for LS-DYNA

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▷ Summary

- Modelling of multi-phasic materials through the TPM
- Numerical implementation into the PANDAS FE software
- Straight forward transfer of research into industrial applications via LS-DYNA/PANDAS co-simulation approach

▷ Future Aspects

- Visualisation of dependent variables (e. g. stresses, seepage velocities)
- Modelling framework applicable to further multi-physics materials, e. g. lithium-ion batteries, fuel cells
- ...

→ many potential application scenario within industrial applications