



On the Analysis of Porous Media Dynamics using a DUNE-PANDAS Interface

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Outline

- Introduction
- Theory of Porous Media
- Numerical Treatment
- Interface
- Numerical Example
- Summary & Outlook

Introduction

TPM

Numerical
Treatment

Interface

Numerical
Example

Summary
& Outlook



Introduction

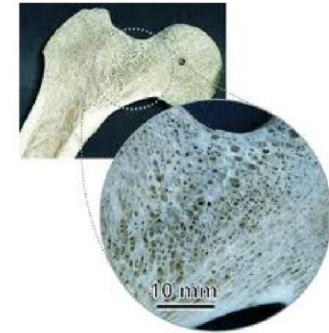
- Porous media can be found in different branches of engineering



foams in mechanical engineering



soil and concrete in civil engineering



soft and hard tissue in biological engineering

- Solid skeleton can undergo large deformations



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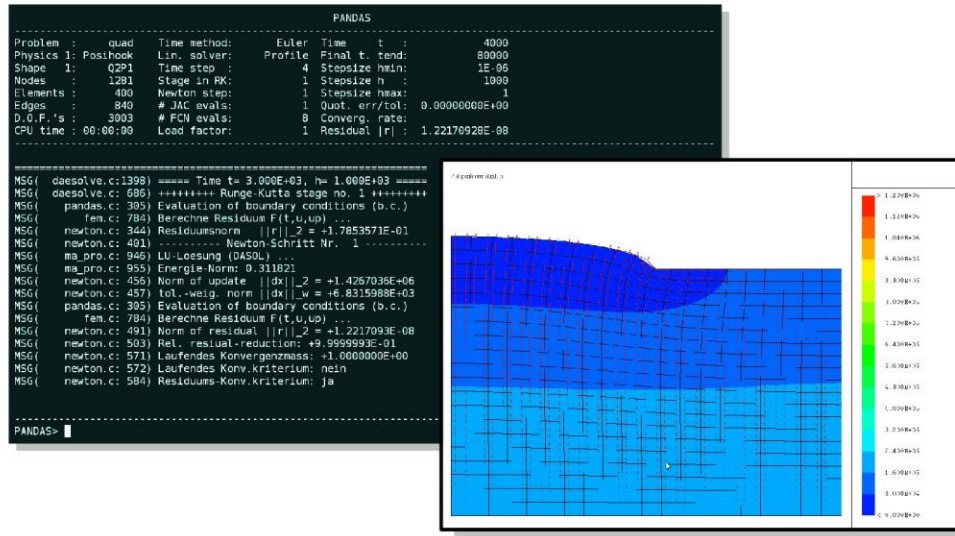
➤ **Goal:**

- Simulating the interaction between the deformable solid skeleton and the pore fluid in large-scale problems

➤ **Method:**

- Description of the problem by the Theory of Porous Media (TPM)
- Discretisation by the Finite Element Method within the framework of PANDAS^[1]

- Motivation
- TPM
- Numerical Treatment
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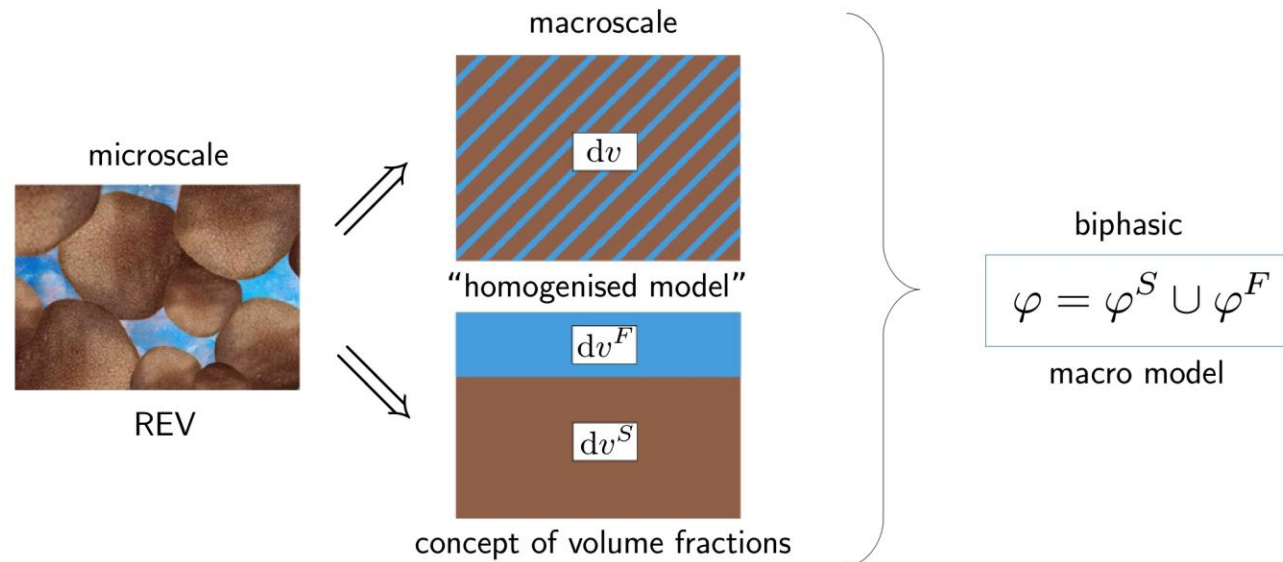
- ⇒ as a purely sequential code, PANDAS has limited capabilities
- ⇒ parallelisation of PANDAS by use of a DUNE-PANDAS interface

^[1] Porous media **A**daptive **N**on-linear finite element solver based on **D**ifferential **A**lgebraic **S**ystems



Theory of Porous Media (TPM)

➤ **Homogenisation:** micro-to-macro transition [Bowen, de Boer, Ehlers]



• **Concept of volume fractions:**

$$\sum_{\alpha} n^{\alpha} = \sum_{\alpha} \frac{dv^{\alpha}}{dv} = 1 \quad \text{with } \alpha = \{S, F\}$$

• **Density relations:**

$$\left. \begin{aligned} \rho^{\alpha R} &= \frac{dm^{\alpha}}{dv^{\alpha}} \\ \rho^{\alpha} &= \frac{dm^{\alpha}}{dv} \end{aligned} \right\} \rho^{\alpha} = n^{\alpha} \rho^{\alpha R}$$

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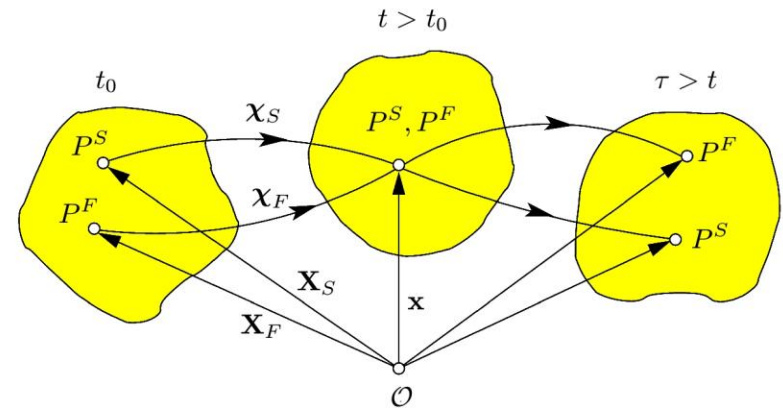
➤ Mixture Kinematics

- Superimposed continua with individual states of motion

$$\mathbf{x} = \chi_\alpha(\mathbf{X}, t)$$

$$\implies \dot{\mathbf{x}}_\alpha = \frac{d\chi_\alpha(\mathbf{X}_\alpha, t)}{dt},$$

$$\ddot{\mathbf{x}}_\alpha = \frac{d^2\chi_\alpha(\mathbf{X}_\alpha, t)}{dt^2}$$



- Motion of the solid skeleton (*Lagrangean*)

$$\text{Displacement: } \mathbf{u}_S = \mathbf{x} - \mathbf{X}_S$$

$$\text{Velocity: } \mathbf{v}_S = \dot{\mathbf{x}}_S = (\mathbf{u}_S)'_S$$

$$\text{Acceleration: } (\mathbf{v}_S)'_S = \ddot{\mathbf{x}}_S = (\mathbf{u}_S)''_S$$

- Motion of the pore fluid (modified *Eulerian*)

$$\text{Velocity: } \mathbf{v}_F = \dot{\mathbf{x}}_F$$

$$\text{Acceleration: } (\mathbf{v}_F)'_F = (\mathbf{v}_F)'_S + \text{grad } \mathbf{v}_F (\mathbf{v}_F - \mathbf{v}_S)$$

$$\text{Seepage velocity: } \mathbf{w}_F = \mathbf{v}_F - \mathbf{v}_S$$



➤ Incompressible binary porous media model

• Assumptions:

- * binary model

$$\alpha = \{S, F\}$$

- * no mass production

$$\hat{\rho}^S = \hat{\rho}^F = 0$$

- * incompressible constituents

$$(\rho^{SR})'_S = (\rho^{FR})'_S = 0$$

- * equal body forces (gravitation)

$$\mathbf{b}^S = \mathbf{b}^F = \mathbf{b}$$

- * fully saturated soil

$$n^S + n^F = 1$$

- * iso-thermal conditions

$$\Theta^S = \Theta^F = \Theta = \text{const.}$$

• Incompressible binary porous media balance equations

- * total momentum balance (solid and pore fluid):

$$\rho^S (\mathbf{v}_S)'_S + \rho^F [(\mathbf{v}_F)'_S + (\text{grad } \mathbf{v}_F) \mathbf{w}_F] = \text{div} (\mathbf{T}^S + \mathbf{T}^F) + (\rho^S + \rho^F) \mathbf{b} + \underbrace{\hat{\mathbf{s}}^S + \hat{\mathbf{s}}^F}_{=0}$$

- * fluid momentum balance:

$$\rho^F (\mathbf{v}_F)'_S + \rho^F (\text{grad } \mathbf{v}_F) \mathbf{w}_F = \text{div } \mathbf{T}^F + \rho^F \mathbf{b} + \hat{\mathbf{s}}^F$$

- * total volume balance (solid and pore fluid):

$$0 = \text{div} [(\mathbf{u}_S)'_S + n^F \mathbf{w}_F]$$

where: $\mathbf{T}^S/\mathbf{T}^F$: partial Cauchy stress tensors (solid/fluid)

$\hat{\mathbf{s}}^S/\hat{\mathbf{s}}^F$: momentum productions (solid/fluid), with $\hat{\mathbf{s}}^\alpha = \hat{\mathbf{p}}^\alpha + \hat{\rho}^\alpha \dot{\mathbf{x}}_\alpha$

\mathbf{b} : body force



➤ Constitutive Setting

- **Principle of effective stress** [*Terzaghi 1925; Skempton 1960; Ehlers 1993*]

$$\mathbf{T}^S = \mathbf{T}_E^S - n^S p \mathbf{I}$$

$$\mathbf{T}^F = \mathbf{T}_E^F - n^F p \mathbf{I}$$

$$\hat{\mathbf{p}}^F = \hat{\mathbf{p}}_E^F + p \text{grad } n^F$$

$$\text{with: } \mathbf{T}_E^F \approx \mathbf{0}$$

- **Fluid constituent** (isotropic, lingering fluid condition)

$$\hat{\mathbf{p}}_E^F = - \frac{(n^F)^2 \gamma^{FR}}{k^F} \mathbf{w}_F$$

$$\text{where: } \gamma^{FR} : \text{specific weight of the pore fluid}$$

$$k^F : \text{Darcy permeability}$$

- **Solid constituent** (elasto-viscoplastic, small deformations)

* decomposition of the strain tensor:

$$\boldsymbol{\varepsilon}_S = \boldsymbol{\varepsilon}_{Se} + \boldsymbol{\varepsilon}_{Sp}$$

* solid extra stress (generalised Hookean law):

$$\mathbf{T}_E^S = 2\mu^S \boldsymbol{\varepsilon}_{Se} + \lambda^S (\boldsymbol{\varepsilon}_{Se} \cdot \mathbf{I}) \mathbf{I} \quad \text{where: } \mu^S, \lambda^S : \text{Lamé constants}$$

* elastic strain tensor (small strains)

$$\boldsymbol{\varepsilon}_{Se} = \frac{1}{2} (\text{grad } \mathbf{u}_S + \text{grad}^T \mathbf{u}_S) - \boldsymbol{\varepsilon}_{Sp}$$



* single-surface yield criterion [Ehlers 1993]:

$$F = \Phi^{1/2} + \beta I + \epsilon I^2 - \kappa$$

$$\Phi = \mathbb{II}^D (1 + \gamma \vartheta)^m + \frac{1}{2} \alpha I^2 + \delta^2 I^4$$

$$\vartheta = \mathbb{III}^D / (\mathbb{II}^D)^{3/2}$$

principal invariants: $I, \mathbb{II}^D, \mathbb{III}^D$ of \mathbf{T}_E^S

* parameters of the yield surface:

$$\text{hydrostatic plane: } \mathbf{s}_h = (\delta, \epsilon, \beta, \alpha, \kappa)^T$$

$$\text{deviatoric plane: } \mathbf{s}_d = (\gamma, m)^T$$

* plastic potential [Ehlers & Mahnkopf 1999]:

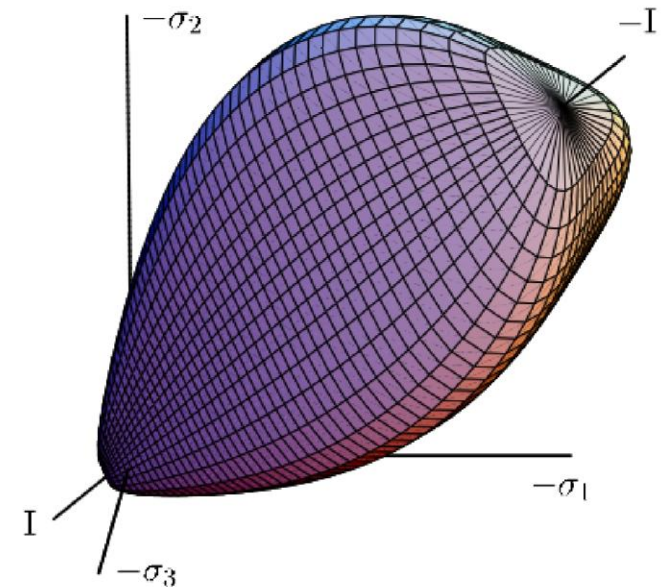
$$G = \sqrt{\psi_1 \mathbb{II}^D + \frac{1}{2} \alpha I^2 + \delta^2 I^4} + \psi_2 \beta I + \epsilon I^2$$

* flow rule and plastic multiplier:

$$(\boldsymbol{\varepsilon}_{Sp})'_S = \Lambda \frac{\partial G}{\partial \mathbf{T}_E^S}$$

visco-plasticity [Perzyna 1966]:

$$\Lambda = \frac{1}{\eta} \left\langle \frac{F}{\sigma_0} \right\rangle^r$$





Numerical Treatment

➤ Variational Approach based on the *Bubnov-Galerkin* Method

- **Strong formulations:**

- * solid displacement-velocity relation (order reduction):

$$(\mathbf{u}_S)'_S = \mathbf{v}_S$$

- * total momentum balance:

$$\rho^S (\mathbf{v}_S)'_S + \rho^F [(\mathbf{v}_F)'_S + (\text{grad } \mathbf{v}_F) \mathbf{w}_F] = \text{div} (\mathbf{T}_E^S - p \mathbf{I}) + (\rho^S + \rho^F) \mathbf{b}$$

- * fluid momentum balance:

$$\rho^F (\mathbf{v}_F)'_S + \rho^F (\text{grad } \mathbf{v}_F) \mathbf{w}_F = \text{div} (-n^F p \mathbf{I}) + \rho^F \mathbf{b} - \frac{(n^F)^2 \gamma^{FR}}{k^F} \mathbf{w}_F + p \text{grad } n^F$$

- * total volume balance:

$$0 = \text{div} \left(\mathbf{v}_S + \underbrace{\frac{k^F}{\gamma^{FR}} \{ \rho^{FR} [\mathbf{b} - (\mathbf{v}_F)'_S - (\text{grad } \mathbf{v}_F) \mathbf{w}_F] - \text{grad } p \}}_{n^F \mathbf{w}_F} \right)$$

- **Primary variables:**

$$\mathbf{u}_S, \quad \mathbf{v}_S, \quad \mathbf{v}_F, \quad p$$



- **Weak formulations**

* displacement-velocity relation (test function $\delta \mathbf{u}_S$):

$$\mathcal{G}_{\mathbf{v}_S} = \int_{\Omega} \delta \mathbf{u}_S \cdot [(\mathbf{u}_S)'_S - \mathbf{v}_S] dv = 0$$

* total momentum balance (test function $\delta \mathbf{u}_S$):

$$\begin{aligned} \mathcal{G}_{\mathbf{u}_S} = & \int_{\Omega} \delta \mathbf{u}_S \cdot \{ \rho^S [(\mathbf{v}_S)'_S - \mathbf{b}] + \rho^F [(\mathbf{v}_F)'_S + (\text{grad } \mathbf{v}_F) \mathbf{w}_F - \mathbf{b}] \} dv + \\ & + \int_{\Omega} \text{grad } \delta \mathbf{u}_S \cdot (\mathbf{T}_E^S - p \mathbf{I}) dv + \int_{\Gamma_{\bar{\mathbf{t}}}^S} \delta \mathbf{u}_S \cdot \underbrace{(\mathbf{T}_E^S - p \mathbf{I}) \mathbf{n}}_{\bar{\mathbf{t}}} da = 0 \end{aligned}$$

* fluid momentum balance (test function $\delta \mathbf{v}_F$):

$$\begin{aligned} \mathcal{G}_{\mathbf{v}_F} = & \int_{\Omega} \delta \mathbf{v}_F \cdot [\rho^F (\mathbf{v}_F)'_S + (\text{grad } \mathbf{v}_F) \mathbf{w}_F - \mathbf{b}] dv + \int_{\Omega} \delta \mathbf{v}_F \cdot [\frac{(n^F)^2 \gamma^{FR}}{k^F} \mathbf{w}_F - p \text{grad } n^F] dv + \\ & + \int_{\Omega} \text{div } \delta \mathbf{v}_F (-n^F p) dv + \int_{\Gamma_{\bar{\mathbf{t}}}^F} \delta \mathbf{v}_F \cdot \underbrace{(-n^F p \mathbf{I}) \mathbf{n}}_{\bar{\mathbf{t}}^F} da = 0 \end{aligned}$$

* total volume balance (test function δp)

$$\begin{aligned} \mathcal{G}_p = & \int_{\Omega} \delta p \text{div } \mathbf{v}_S dv - \int_{\Omega} \text{grad } \delta p \cdot \frac{k^F}{\gamma^{FR}} \{ \text{grad } p - \rho^{FR} [\mathbf{b} - (\mathbf{v}_F)'_S - (\text{grad } \mathbf{v}_F) \mathbf{w}_F] \} dv + \\ & + \int_{\Gamma_{\bar{\mathbf{v}}}} \delta p \underbrace{n^F \mathbf{w}_F \cdot \mathbf{n}}_{\bar{\mathbf{v}}} da = 0 \end{aligned}$$



➤ Spatial Discretisation

- **Approximation of the unknown fields within small but finite subdomains**

* trial function: $\mathbf{u}(\mathbf{x}, t) \approx \mathbf{u}^h(\mathbf{x}, t) = \bar{\mathbf{u}}^h(\mathbf{x}, t) + \sum_{i=1}^N \Phi^i(\mathbf{x}) \hat{\mathbf{u}}^i(t)$

* test function: $\delta \mathbf{u}(\mathbf{x}) \approx \delta \mathbf{u}^h(\mathbf{x}) = \sum_{i=1}^N \Phi^i(\mathbf{x}) \delta \hat{\mathbf{u}}^i$

with: $\Phi^i(\mathbf{x})$: matrix containing the shape functions
 $\hat{\mathbf{u}}^i(t) / \delta \hat{\mathbf{u}}^i$: vector containing the nodal degrees of freedom

- **Approximation of the integral of the weak forms**

$$\int_{\Omega^e} \mathbf{g}(\mathbf{x}, t) dv \approx \sum_{p=1}^{\bar{P}} w_p \mathbf{g}(\mathbf{x}_p, t) \quad \text{with: } w_p \quad : \text{ weight of an integration point}$$

$$\bar{P} \quad : \text{ number of integration points of an element}$$

- **Semi-discrete initial-boundary-value problem**

$$\mathbf{F}^h(t, \mathbf{u}, \mathbf{u}', \mathbf{q}, \mathbf{q}') = \begin{bmatrix} \mathcal{G}^h(t, \mathbf{u}, \mathbf{u}', \mathbf{q}) \\ \mathcal{L}^h(t, \mathbf{q}, \mathbf{q}', \mathbf{u}) \end{bmatrix} = \begin{bmatrix} \mathbf{M}\mathbf{u}' + \mathbf{K}(\mathbf{u}, \mathbf{q}) - \mathbf{f} \\ \mathbf{A}\mathbf{q}' + \mathbf{G}(\mathbf{q}, \mathbf{u}) \end{bmatrix} \stackrel{!}{=} \mathbf{0}$$

with: $\mathbf{u} = [(\hat{\mathbf{u}}_S^1, \hat{\mathbf{v}}_S^1, \hat{\mathbf{v}}_F^1, \hat{\mathbf{p}}^1), \dots, (\hat{\mathbf{u}}_S^N, \hat{\mathbf{v}}_S^N, \hat{\mathbf{v}}_F^N, \hat{\mathbf{p}}^N)]^T$

$\mathbf{q} = [(\boldsymbol{\varepsilon}_{Sp}^1, \Lambda^1), \dots, (\boldsymbol{\varepsilon}_{Sp}^P, \Lambda^P)]^T$



➤ Solution Strategy

- Splitting the overall Differential-Algebraic System of Equations (DAE) into a local and a global system

$$F^h(t, \mathbf{u}, \mathbf{u}', \mathbf{q}, \mathbf{q}') = \begin{bmatrix} \mathcal{G}^h(t, \mathbf{u}, \mathbf{u}', \mathbf{q}) \\ \mathcal{L}^h(t, \mathbf{u}, \mathbf{q}, \mathbf{q}') \end{bmatrix} = \begin{bmatrix} \boxed{M\mathbf{u}' + \mathbf{K}(\mathbf{u}, \mathbf{q}) - \mathbf{f}} \\ \boxed{A\mathbf{q}' + \mathbf{G}(\mathbf{q}, \mathbf{u})} \end{bmatrix} \stackrel{!}{=} \mathbf{0}$$

global system
local system

- Structure of the global system of equations

$$\mathcal{G}^h = \underbrace{\begin{bmatrix} \mathbf{I} & 0 & 0 & 0 \\ 0 & M_{22} & M_{23} & 0 \\ 0 & 0 & M_{33} & 0 \\ 0 & 0 & M_{43} & 0 \end{bmatrix}}_M \underbrace{\begin{bmatrix} \dot{\mathbf{u}}_S \\ \dot{\mathbf{v}}_S \\ \dot{\mathbf{v}}_F \\ \dot{\mathbf{p}} \end{bmatrix}}_{\mathbf{u}'} + \underbrace{\begin{bmatrix} 0 & -\mathbf{I} & 0 & 0 \\ \mathbf{K}_{21} & \mathbf{K}_{22} & \mathbf{K}_{23} & \mathbf{K}_{24} \\ 0 & \mathbf{K}_{32} & \mathbf{K}_{33} & \mathbf{K}_{34} \\ 0 & \mathbf{K}_{42} & \mathbf{K}_{43} & \mathbf{K}_{44} \end{bmatrix}}_K \underbrace{\begin{bmatrix} \mathbf{u}_S \\ \mathbf{v}_S \\ \mathbf{v}_F \\ \mathbf{p} \end{bmatrix}}_{\mathbf{u}} - \underbrace{\begin{bmatrix} 0 \\ \mathbf{b}_1 + \mathbf{f}_{S+F} \\ \mathbf{b}_2 + \mathbf{f}_F \\ \mathbf{b}_3 + \mathbf{f}_p \end{bmatrix}}_f \stackrel{!}{=} \mathbf{0}$$

- Structure of the local system of equations (element level)

$$\mathcal{L}^h = A\mathbf{q}' + G(\mathbf{q}, \mathbf{u}) = \begin{bmatrix} (\boldsymbol{\varepsilon}_{Sp})' \\ 0 \end{bmatrix} - \begin{bmatrix} \Lambda \frac{\partial G}{\partial \mathbf{T}_E^S} \\ \frac{1}{\eta} \left\langle \frac{F(\mathbf{T}_E^S)}{\sigma_0} \right\rangle^r - \Lambda \end{bmatrix} \stackrel{!}{=} \mathbf{0}$$

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➤ Temporal Discretisation

• Temporal discretisation of the **local system** of equations

* backward Euler (implicit):

$$\mathcal{L}_n^h(t_n, \mathbf{q}_n, \mathbf{q}'_n, \mathbf{u}_n) = \mathbf{A} \mathbf{q}'_n + \mathbf{G}(\mathbf{q}_n, \mathbf{u}_n) = \mathbf{0} \quad \text{with: } \mathbf{q}'_n \approx \frac{\mathbf{q}_n - \mathbf{q}_{n-1}}{\Delta t_n} = \frac{\Delta \mathbf{q}_n}{\Delta t_n}$$

$$\mathbf{q}_n \approx \mathbf{q}_{n-1} + \Delta \mathbf{q}_n$$

$$\implies \mathcal{L}_n^h(t_n, \mathbf{q}_{n-1} + \Delta \mathbf{q}_n, \frac{1}{\Delta t_n} \Delta \mathbf{q}_n, \mathbf{u}_{n-1} + \Delta \mathbf{u}_n) \stackrel{!}{=} \mathbf{0}$$

$$\implies \text{solve for } \Delta \mathbf{q}_n \text{ while } \Delta \mathbf{u}_n \text{ is kept constant}$$

$$\implies \text{update: } \mathbf{q}_n = \mathbf{q}_{n-1} + \Delta \mathbf{q}_n$$

• Temporal discretisation of the **global system** of equations

* backward Euler (implicit):

$$\mathcal{G}_n^h(t_n, \mathbf{u}_n, \mathbf{u}'_n, \mathbf{q}_n) = \mathbf{M} \mathbf{u}'_n + \mathbf{K} \mathbf{u}_n - \mathbf{f}_n = \mathbf{0} \quad \text{with: } \mathbf{u}'_n \approx \frac{\mathbf{u}_n - \mathbf{u}_{n-1}}{\Delta t_n} = \frac{\Delta \mathbf{u}_n}{\Delta t_n}$$

$$\mathbf{u}_n \approx \mathbf{u}_{n-1} + \Delta \mathbf{u}_n$$

$$\implies \mathcal{G}_n^h(t_n, \mathbf{u}_{n-1} + \Delta \mathbf{u}_n, \frac{1}{\Delta t_n} \Delta \mathbf{u}_n, \mathbf{q}_{n-1} + \Delta \mathbf{q}_n) \stackrel{!}{=} \mathbf{0}$$

$$\implies \text{solve for } \Delta \mathbf{u}_n \text{ while } \Delta \mathbf{q}_n \text{ is kept constant}$$

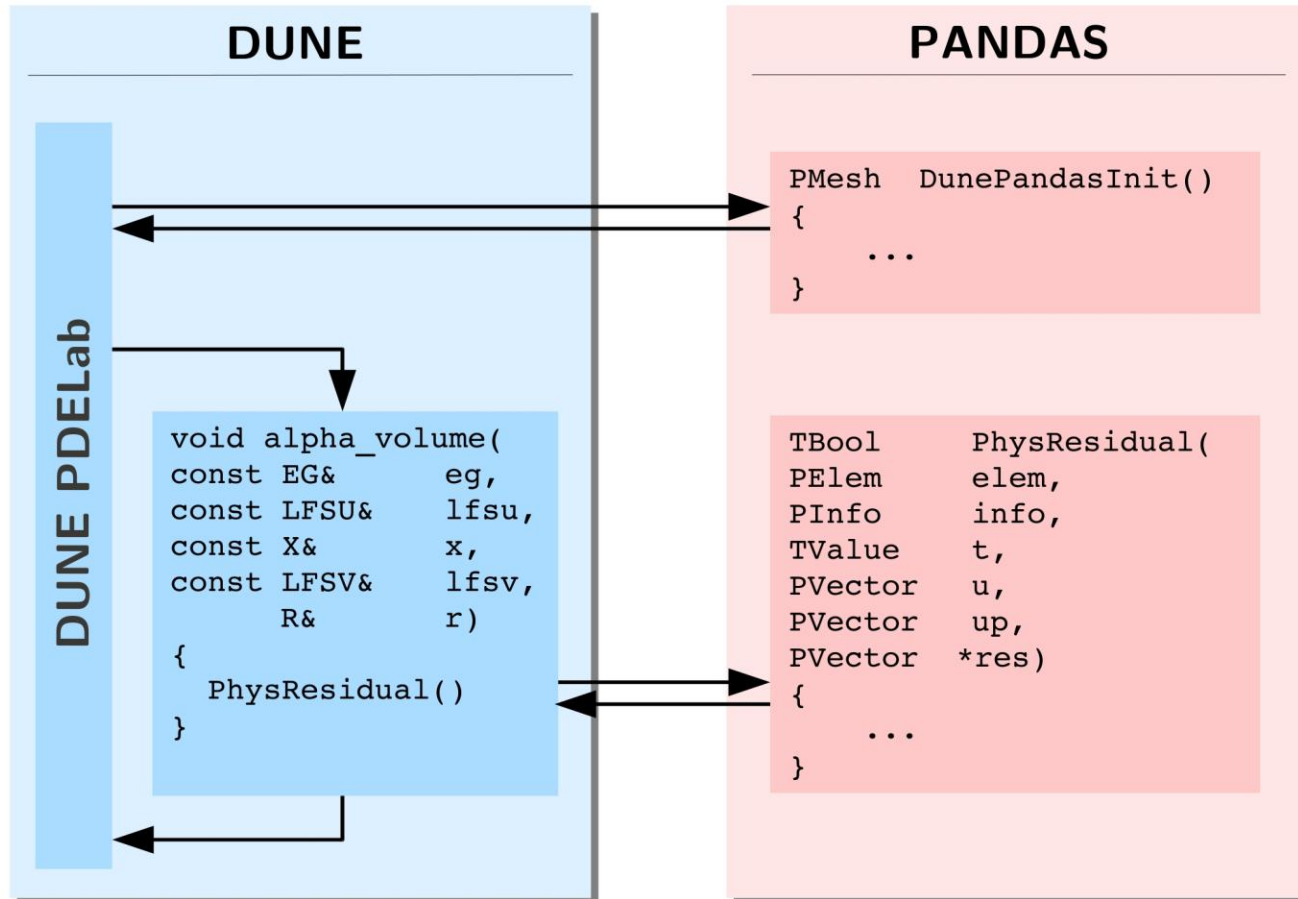
$$\implies \text{update: } \mathbf{u}_n = \mathbf{u}_{n-1} + \Delta \mathbf{u}_n$$



Interface

➤ DUNE-PANDAS-Interface Workflow

* intersection of DUNE and PANDAS is the local operator of DUNE PDELab



⇒⇒ functionality of `alpha_volume()` will be replaced by `PhysResidual()`

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➤ Data transfer

* data containers of `alpha_volume()` and `PhysResidual()`

eg: pointer on grid entity

lfsu: pointer on trial functions
of local function space

lfsv: pointer on test functions
of local function space

t: value of current time

x: pointer on...
1) current solution
(local operator)
2) time derivative of current sol.
(time local operator)

r: pointer on internal
response (residual)

elem: pointer on element

nodal coordinates,
trial- and test functions,
history variables (q_{n-1}),
secondary variables

t: value of current time

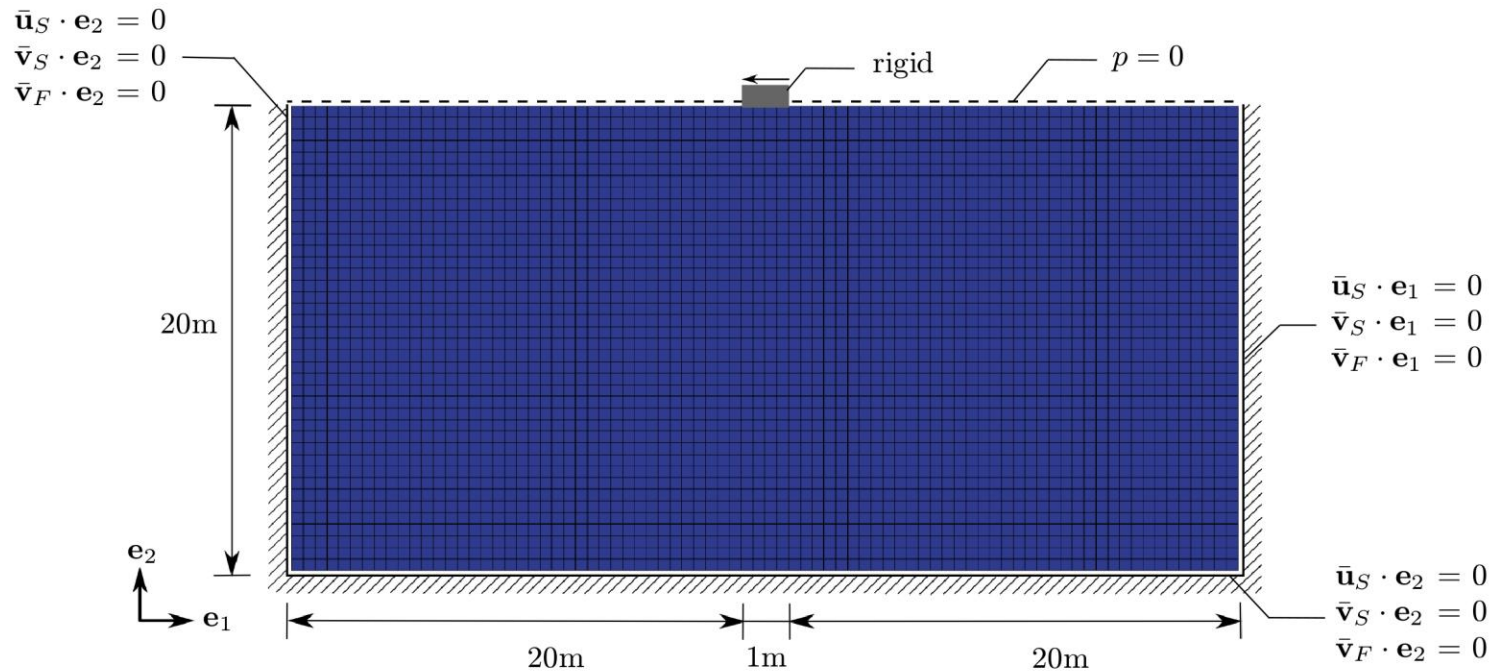
u: pointer on cur. solution (u_n)

up: pointer on time derivative
of current solution (u'_n)

res: pointer on internal
response (residual)

Numerical Example

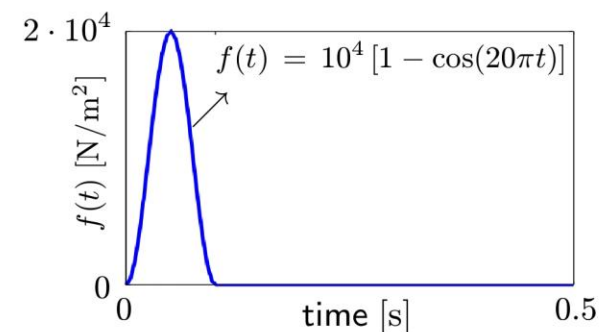
➤ Two-dimensional Elastic Shear-Wave Propagation



• Parameters:

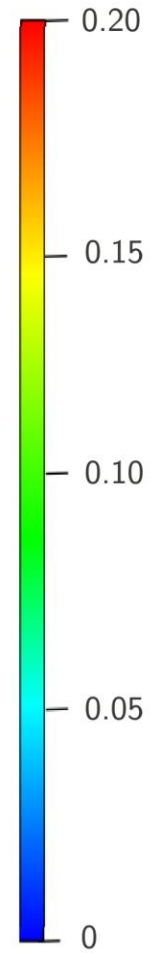
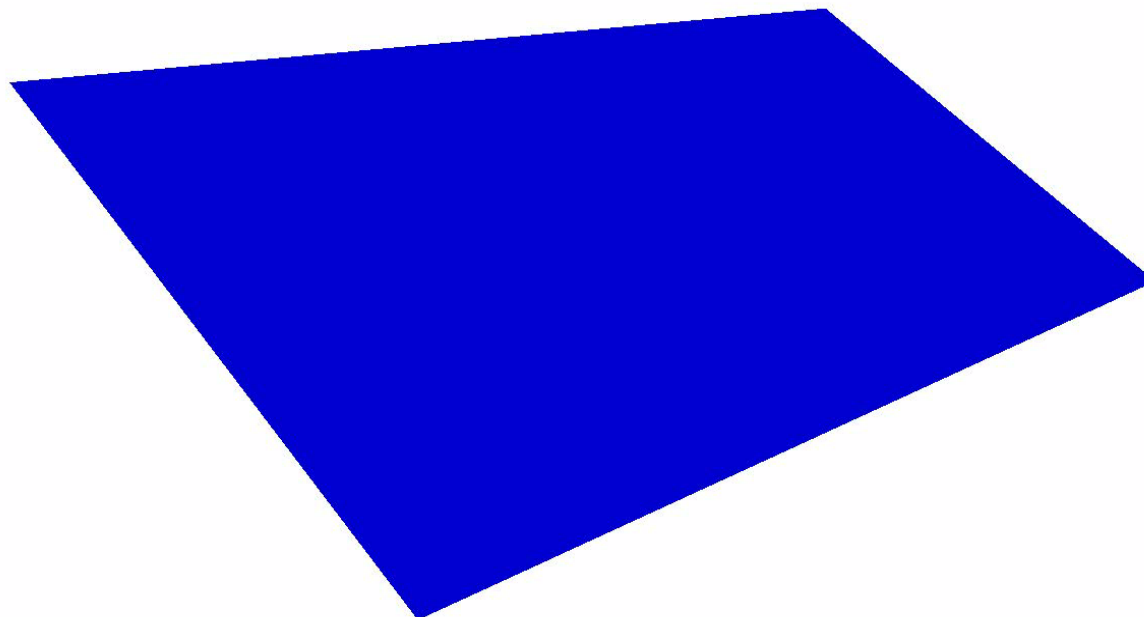
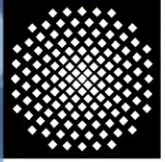
Parameter	Abb.	Value	Unit
1st Lamé constant	μ^S	$5.583 \cdot 10^6$	N/m ²
2nd Lamé constant	λ^S	$8.375 \cdot 10^6$	N/m ²
solid effective density	ρ^{SR}	2720	kg/m ³
fluid effective density	ρ^{FR}	1000	kg/m ³
initial volume fraction	n_{0S}^S	0.67	
Darcy permeability	k^F	10^{-2}	m/s

• Load:





➤ Result



$|\mathbf{u}_S|$ [mm]

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➤ Summary

- Theory of porous media
- Numerical treatment (discretisation in space and time)
- DUNE-PANDAS Interface (procedure overview)
- Numerical example (wave propagation)

➤ Outlook

- Complete data transfer between DUNE and PANDAS (history variables, etc.)
- Parallel execution

Thank you for your attention!