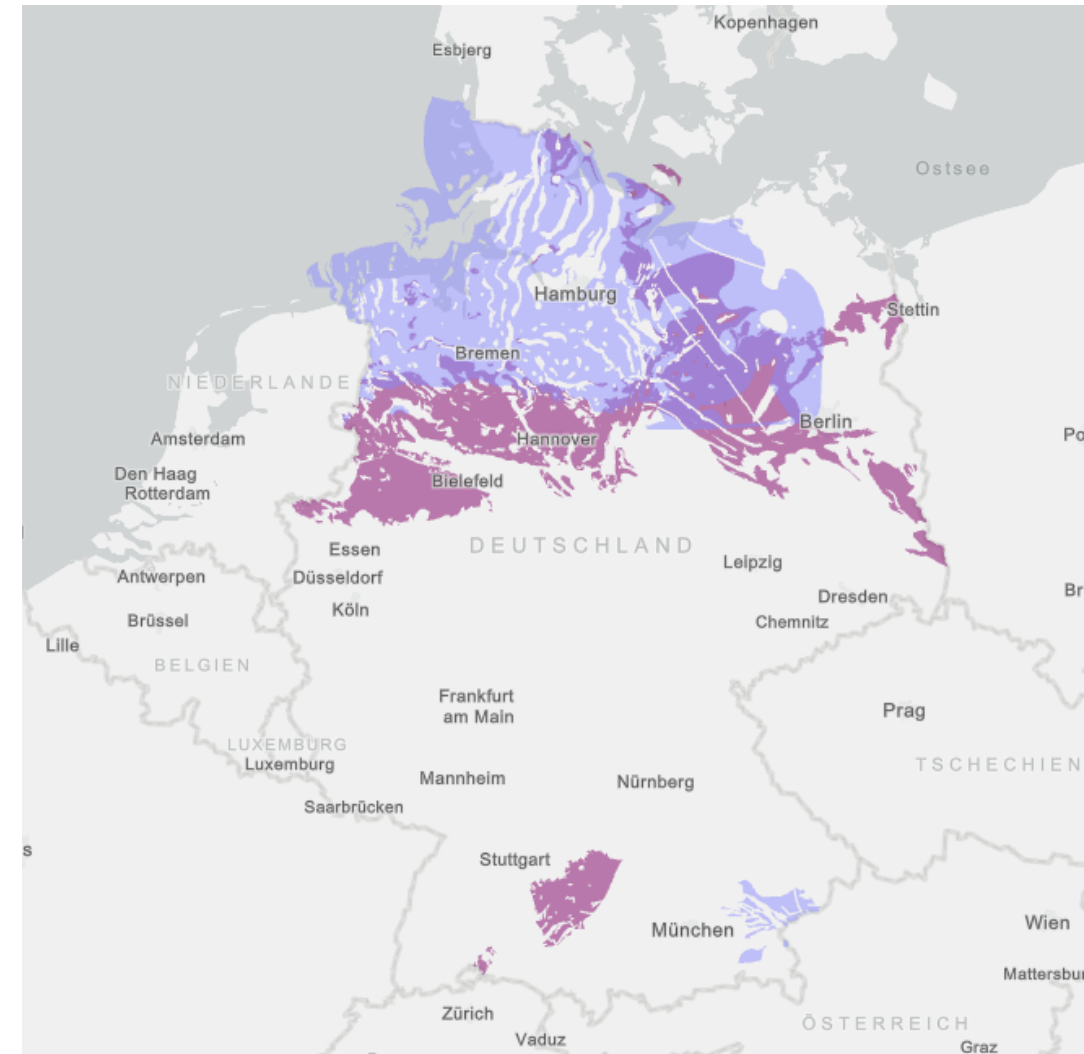


Implementation of clay rock and bentonite models using Mfront

Eric Simo, T. Helfer, P. Herold, M. Mánica, D. Masin, T. Nagel

Clay rock as potential host rock for high-level waste repositories

- Clay rock formations are considered to be a suitable host rock for the disposal of high-level waste (HLW)
- In Germany **nine formations** have been selected for further investigations
- The **safety** of a repository in a clay has to be proven for a period of **1 Million years**
- The understanding of the complex THM-behaviour of clay materials is therefore **necessary** for the safety assessment of repository



BGE (2020)

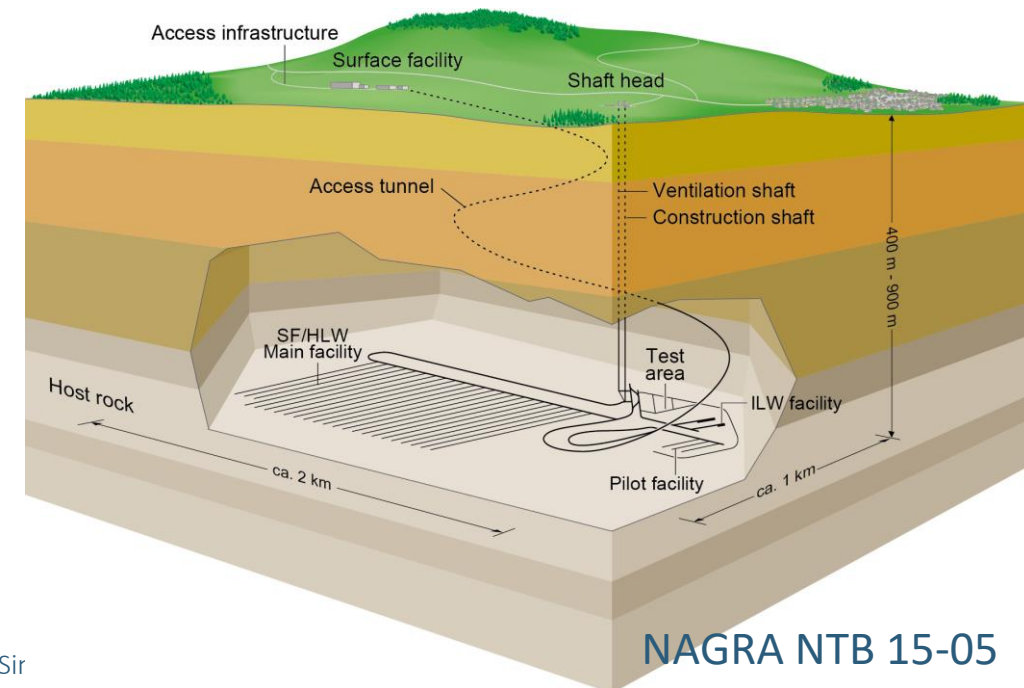
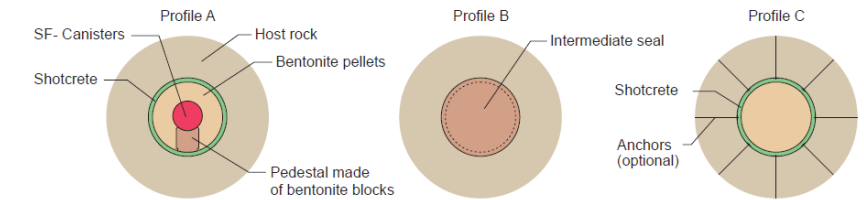
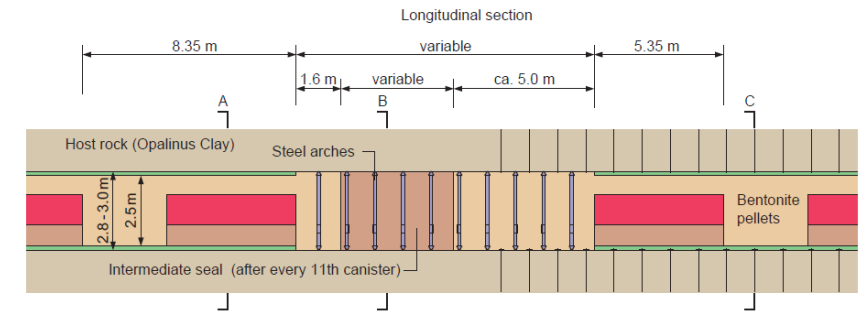
Bentonite as sealing material in radioactive waste repository

- Bentonite materials are considered as the main sealing element of the engineered barrier system for a HLW-repository in clay formations

- **Advantages of Bentonite:**

- Very low Permeability: 10^{-17} - 10^{-18} m²
- Swelling capacity
- Sorption capacity

- A suitable model for bentonite taking into account all relevant phenomena expected in the nearfield of the disposed cask is necessary for numerical based safety assessment



Hypoplastic THM-model for bentonite

Eric Simo

Material Behaviour of Bentonite

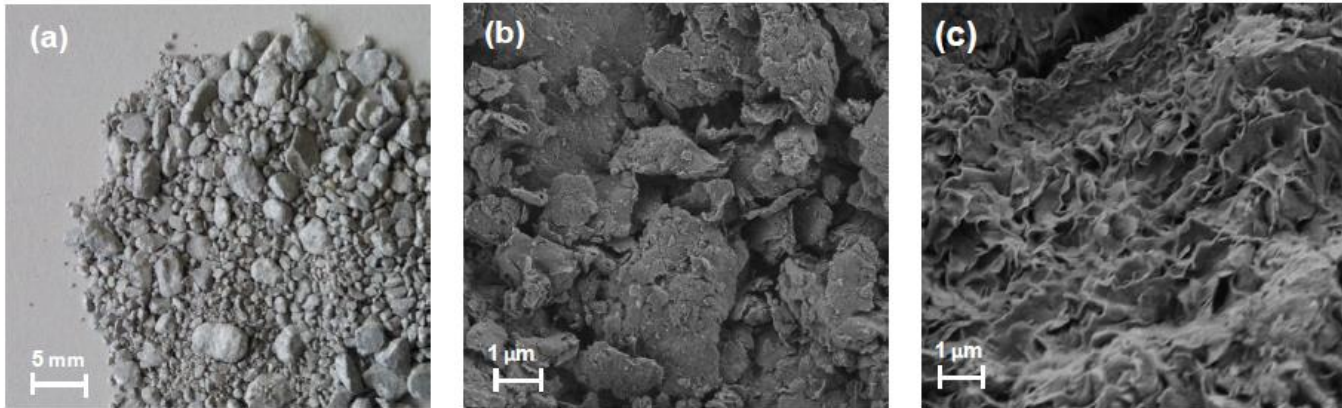
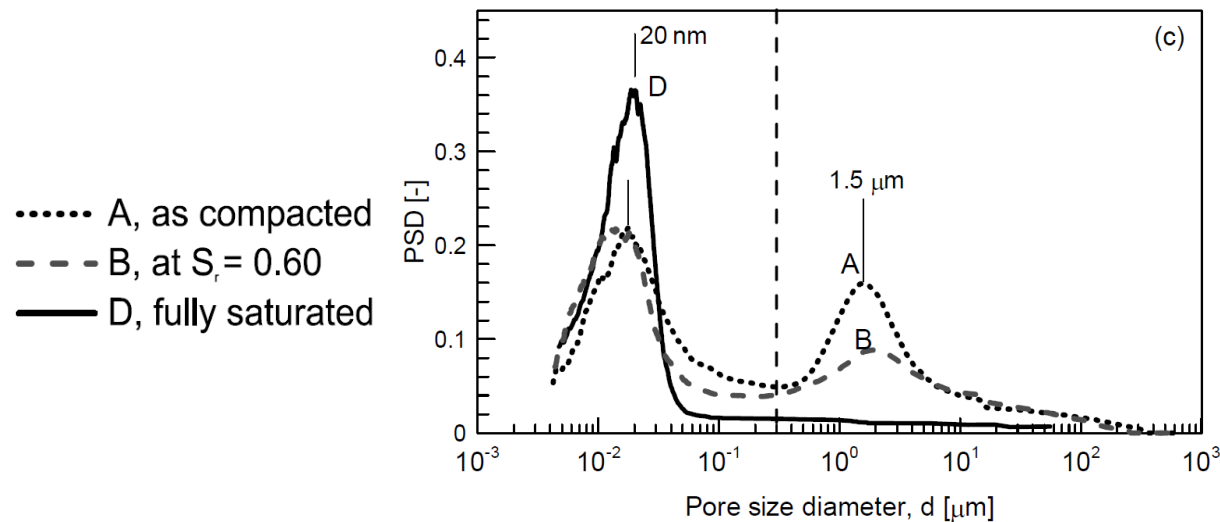
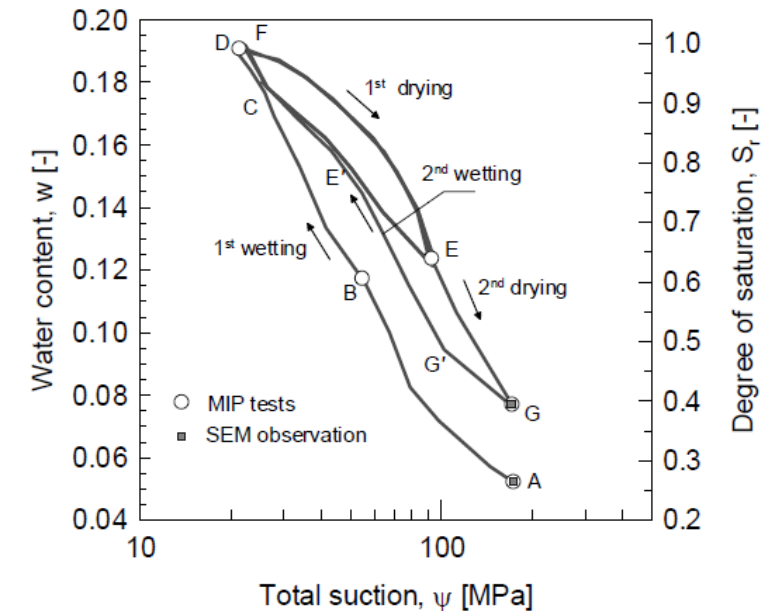


Fig. 1-4: Fabric of Wyoming granular bentonite: (a) appearance of granular bentonite at macroscopic scale; photomicrographs of the material at (b) the as compacted state, and (c) after wetting/drying cycles with significant modification of the fabric.



Seiphoori (2015)



Description of the Bentonite Model

- Expression of the model proposed by (Mašín, 2013 & 2017)

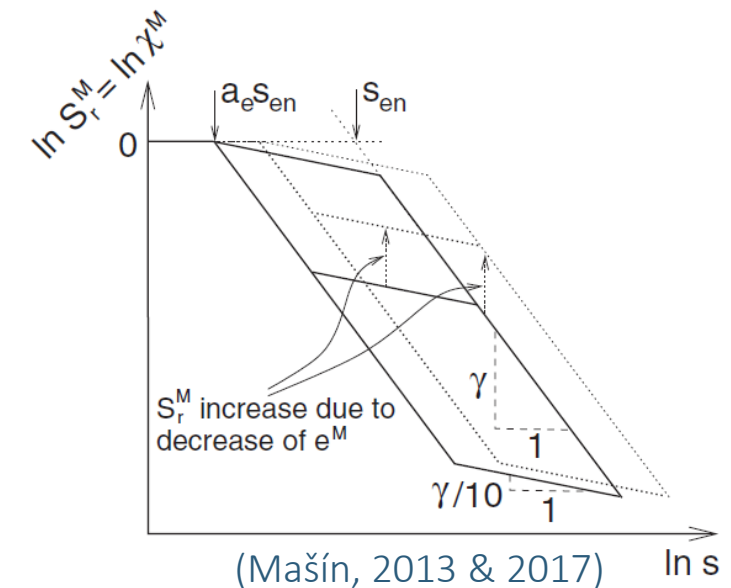
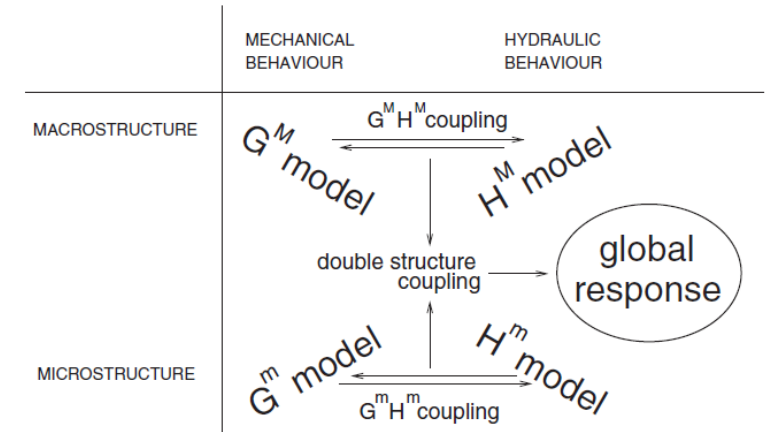
$$\dot{\boldsymbol{\sigma}}^M = f_s [\mathcal{L} : (\dot{\boldsymbol{\epsilon}} - f_m \dot{\boldsymbol{\epsilon}}^m) + f_d \mathbf{N} \|\dot{\boldsymbol{\epsilon}} - f_m \dot{\boldsymbol{\epsilon}}^m\|] + f_u (\mathbf{H}_S + \mathbf{H}_T)$$

- Behaviour of the macrostructure based on hypoplasticity and Bishop equation: $\boldsymbol{\sigma}^M = \boldsymbol{\sigma}^{net} - \mathbf{1} S_r^M S$

- Behaviour of microstructure using elastic volumetric model and Terzaghi stress hypothesis:

$$\dot{\boldsymbol{\epsilon}}^m = \frac{1}{3} \left(\alpha_s \dot{T} - \frac{\kappa_m}{p^m} \dot{p}^m \right) \quad \boldsymbol{\sigma}^m = \boldsymbol{\sigma}^{net} - \mathbf{1} S$$

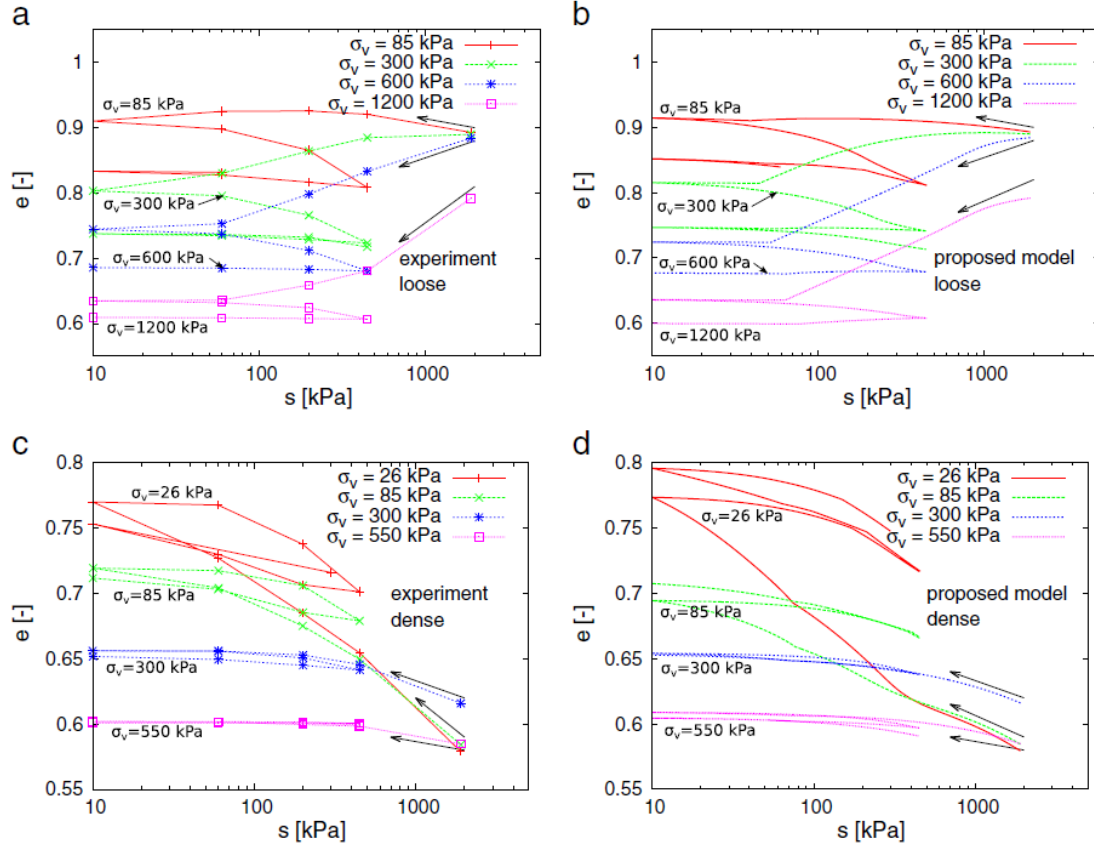
- Double structure coupling through the factor f_m
- Hydraulic and thermal effect considered through $(\mathbf{H}_S + \mathbf{H}_T)$
- f_u controls the overconsolidation ratio, f_s and f_d control the effect of stress and void ratio on macrostructural soil stiffness



Description of the Bentonite Model

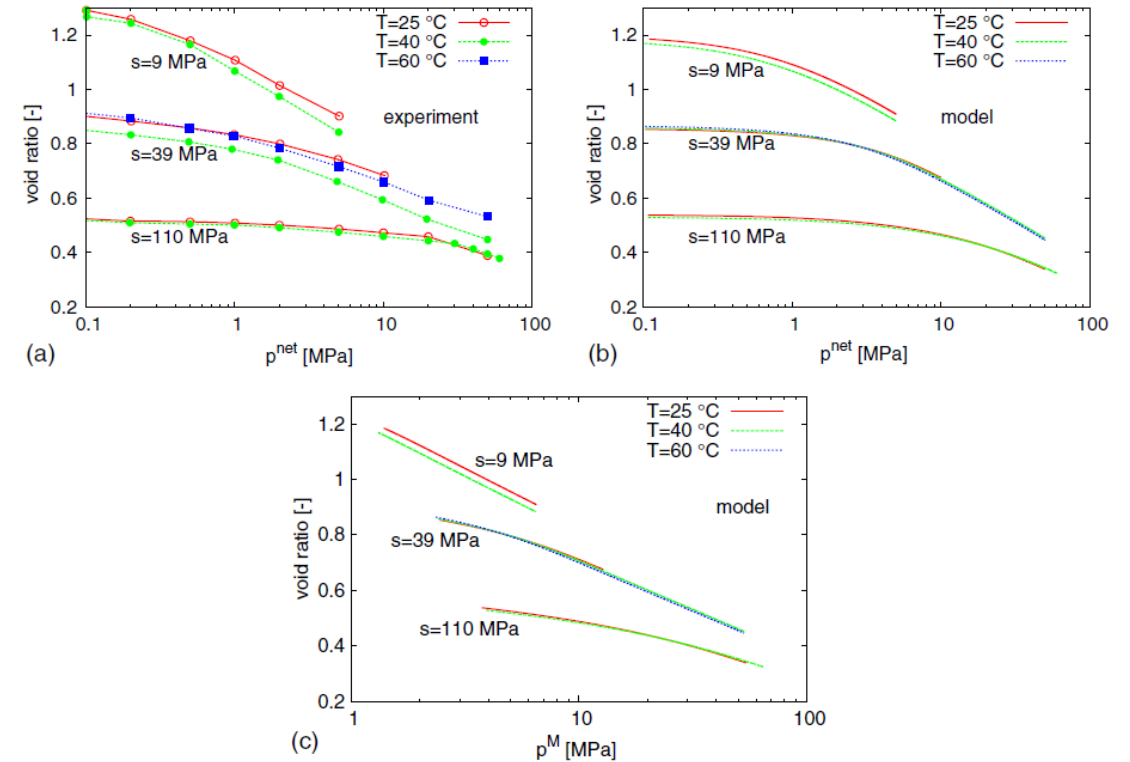
- Some applications of the model

wetting–drying oedometric experiments on Boom clay



Mašín(2013)

Isotropic compression tests at various suctions and temperatures

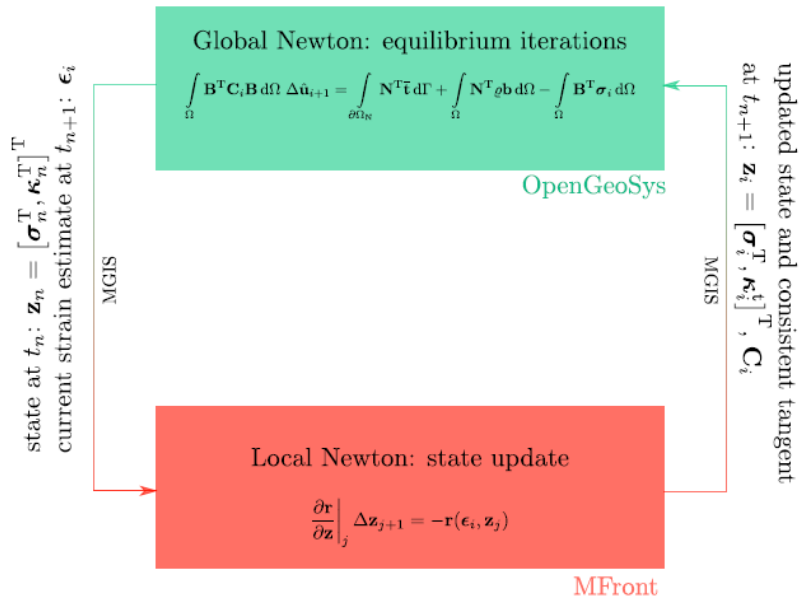


Mašín(2017)

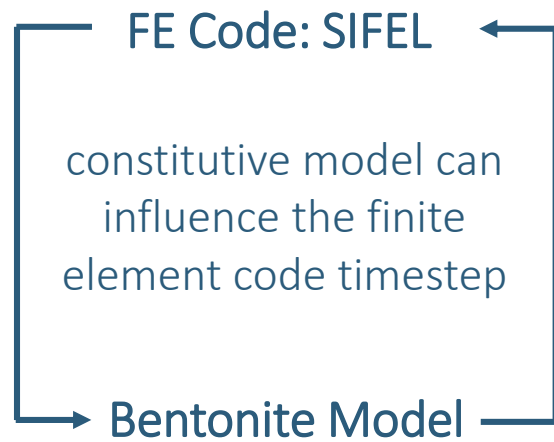
Implementation in Mfront

- Conceptual approach

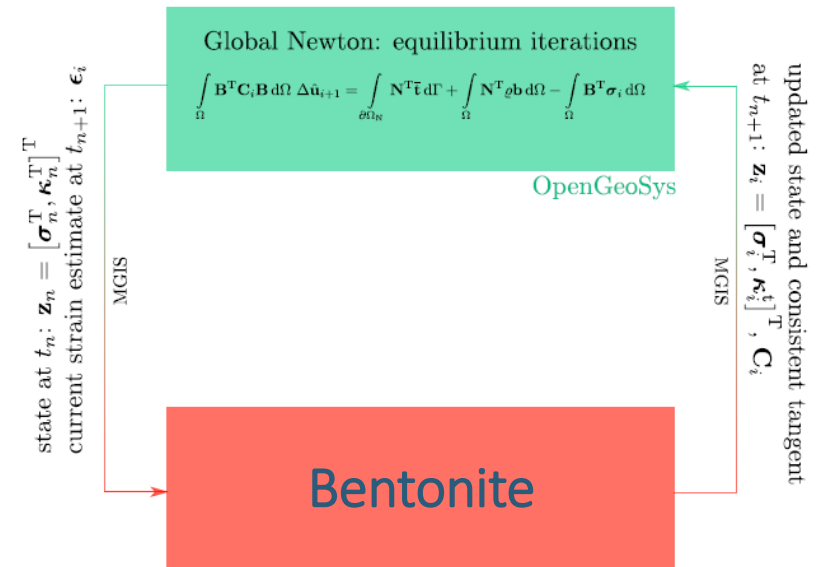
Model implementation in OGS



Actual implementation of the model in FE-Code SIFEL

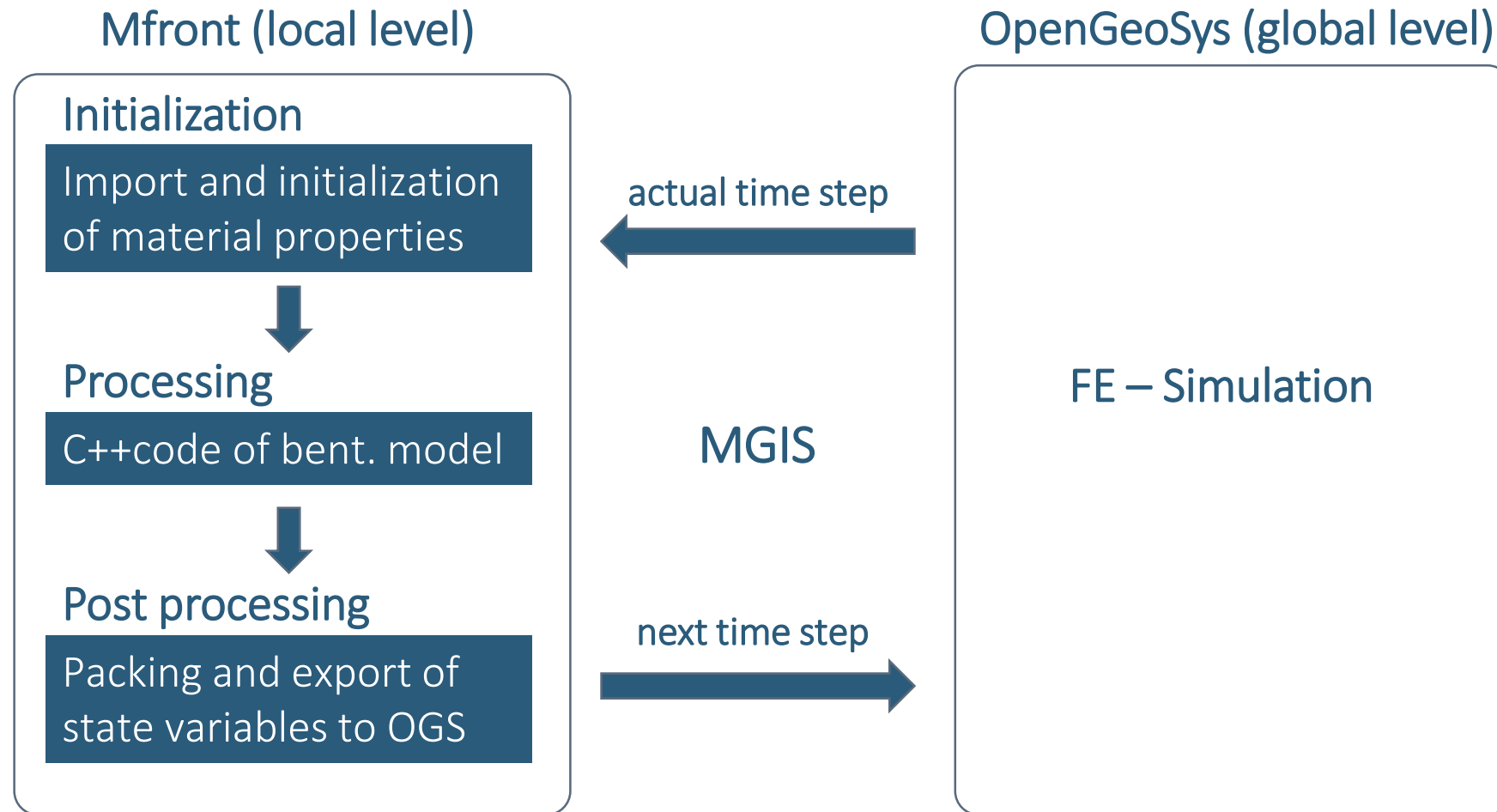


Integration of the bentonite model in Mfront



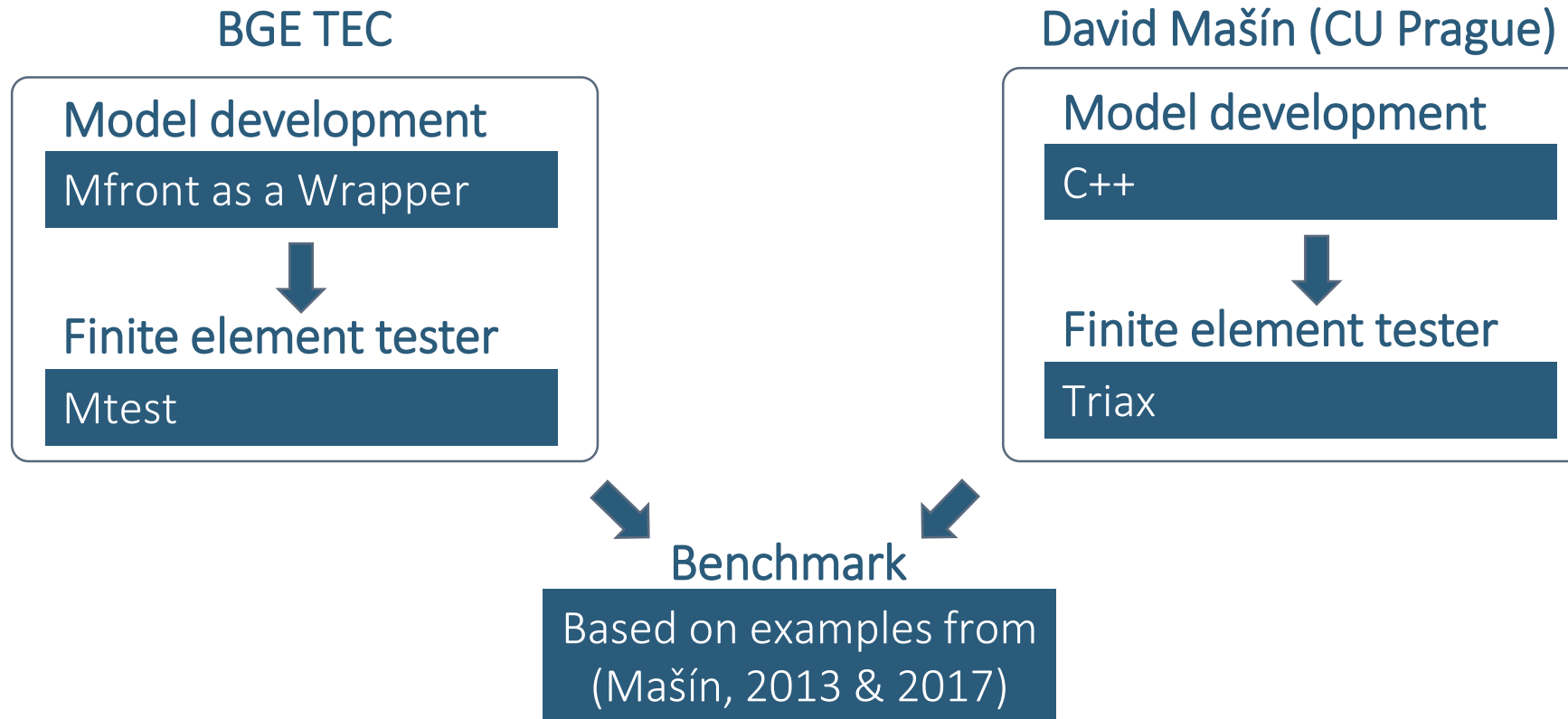
Implementation in Mfront

- The available code of the bentonite model was included in Mfront as a C++Library



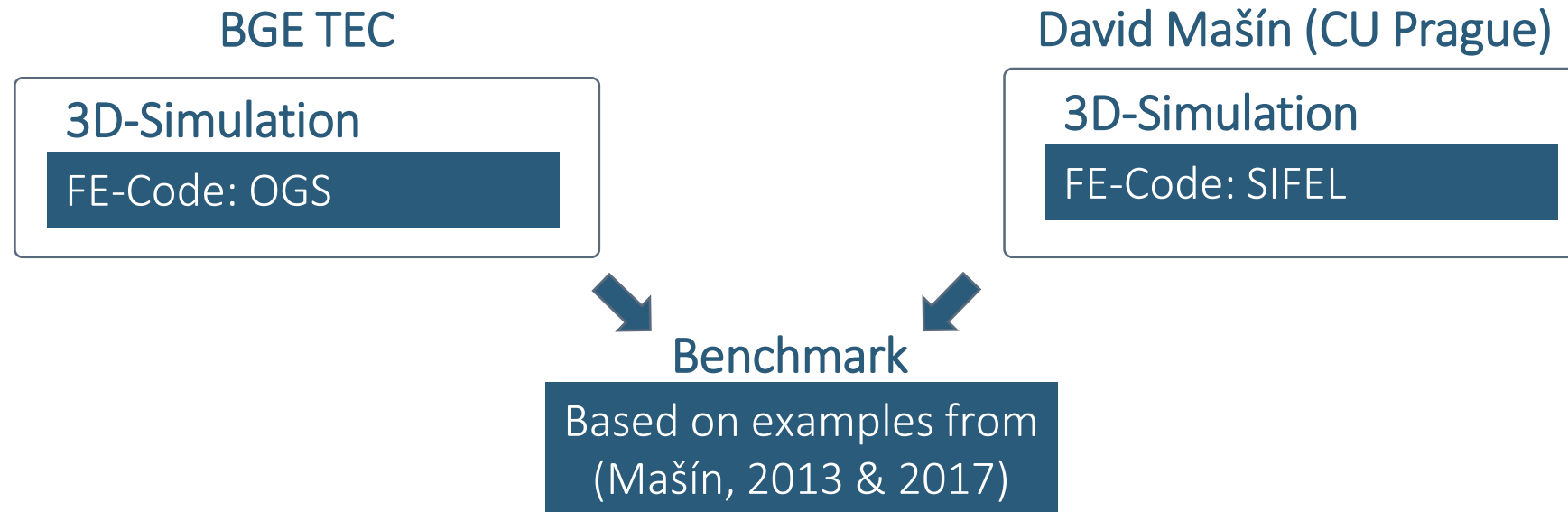
Implementation in Mfront

- Testing of the implementation: at local level



Implementation in Mfront

- Testing of the implementation: at global level



First results

- Suction and axial stress were applied then saturation was calculated:

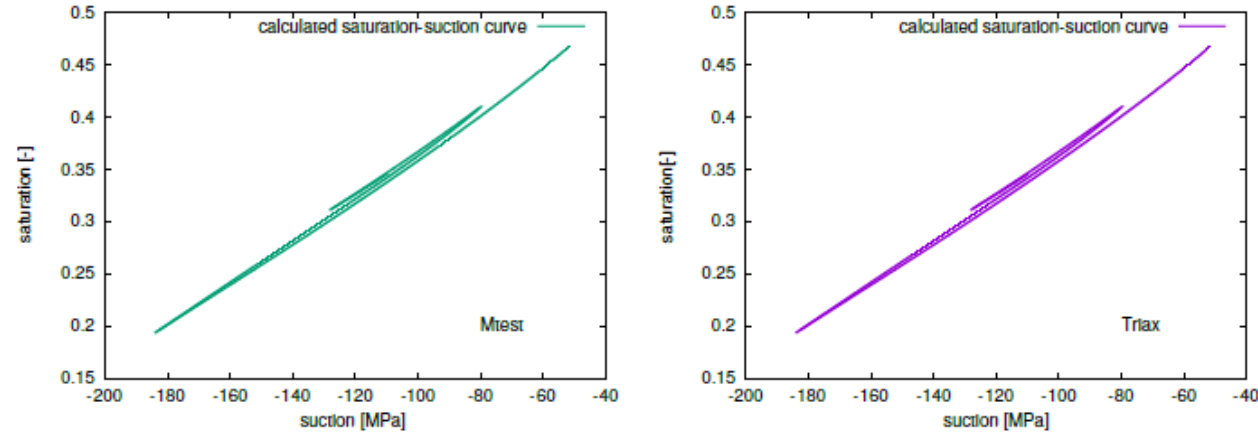


Figure 1: Comparison of the saturation computed with MTest and the saturation computed with TRIAX for the first test

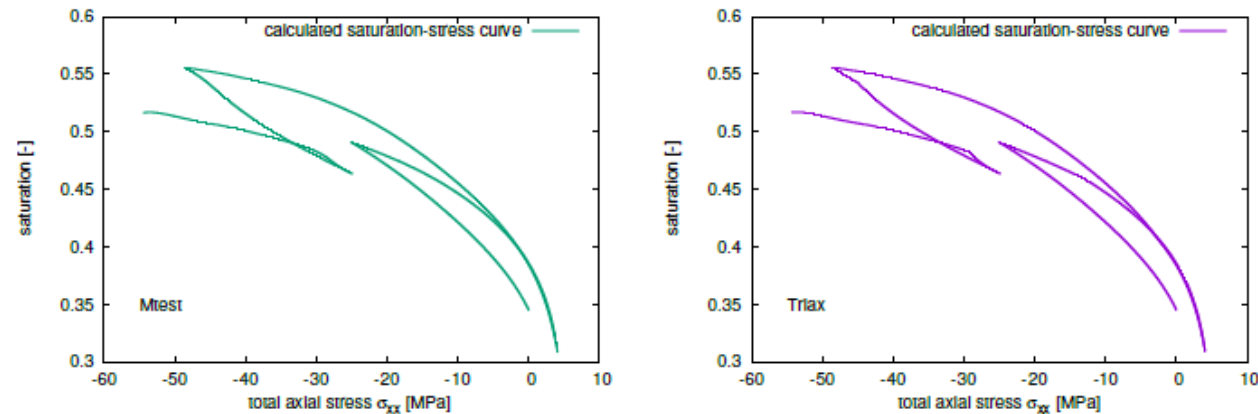


Figure 2: Comparison of the saturation computed with MTest and the saturation computed with TRIAX for the second test

A nonlocal HM-model for clay rocks

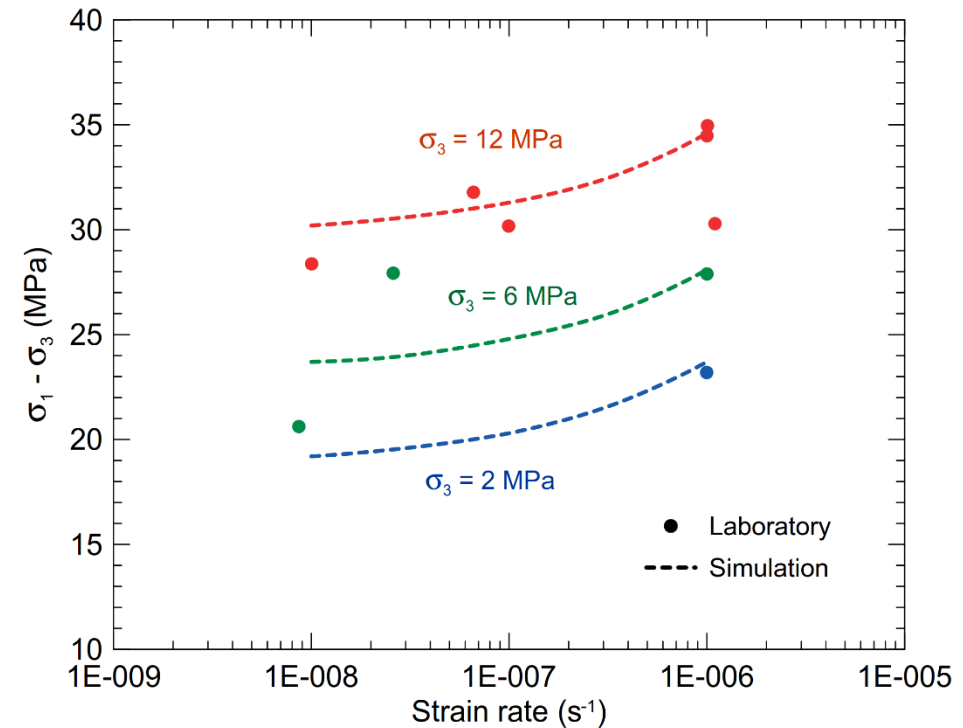
Miguel Mánica

Material behaviour of claystone

- Observed behaviour:

Material behaviour of claystone

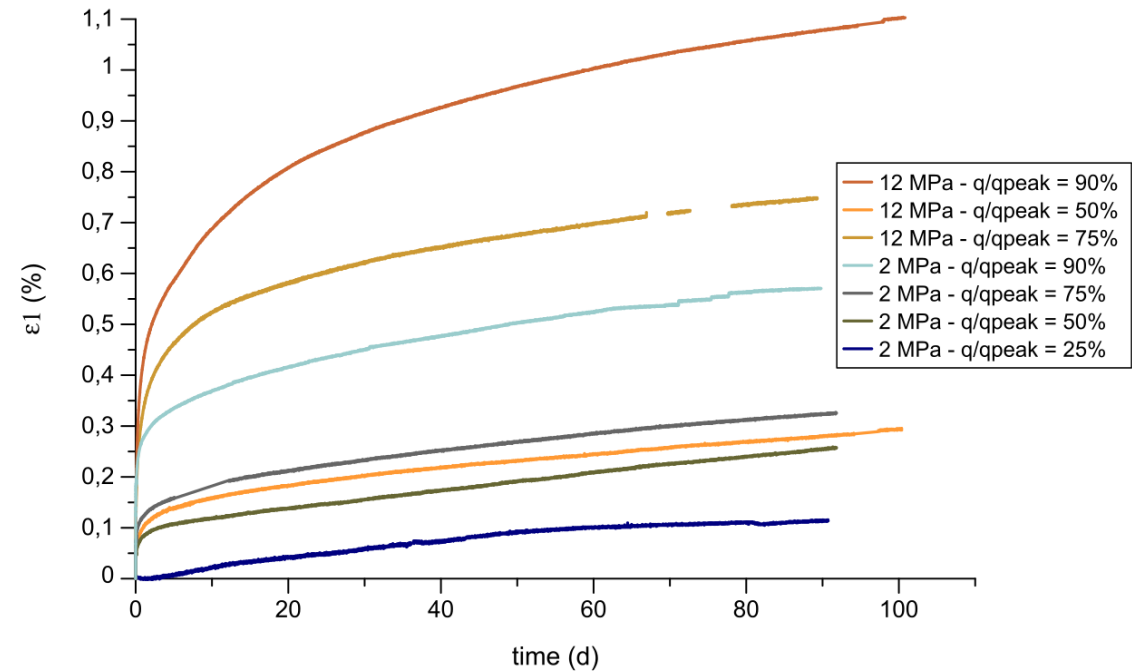
- Observed behaviour:
 - Rate dependency



Callovo-Oxfordian argillite
(Armand et al., 2017)

Material behaviour of claystone

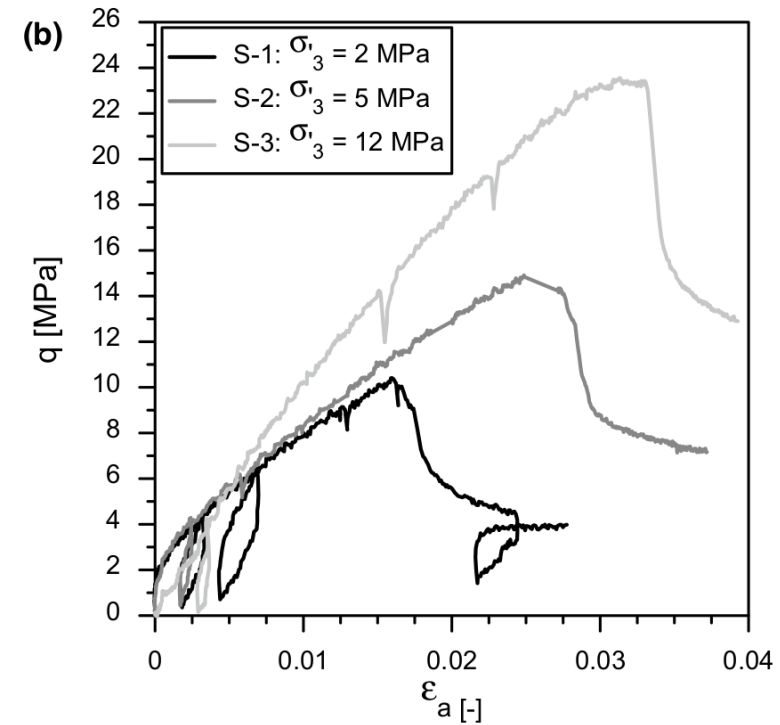
- Observed behaviour:
 - Rate dependency
 - Creep



Callovo-Oxfordian argillite
(Armand et al., 2017)

Material behaviour of claystone

- Observed behaviour:
 - Rate dependency
 - Creep
 - **Significant softening**



Opalinus clay
(Favero et al., 2018)

Material behaviour of claystone

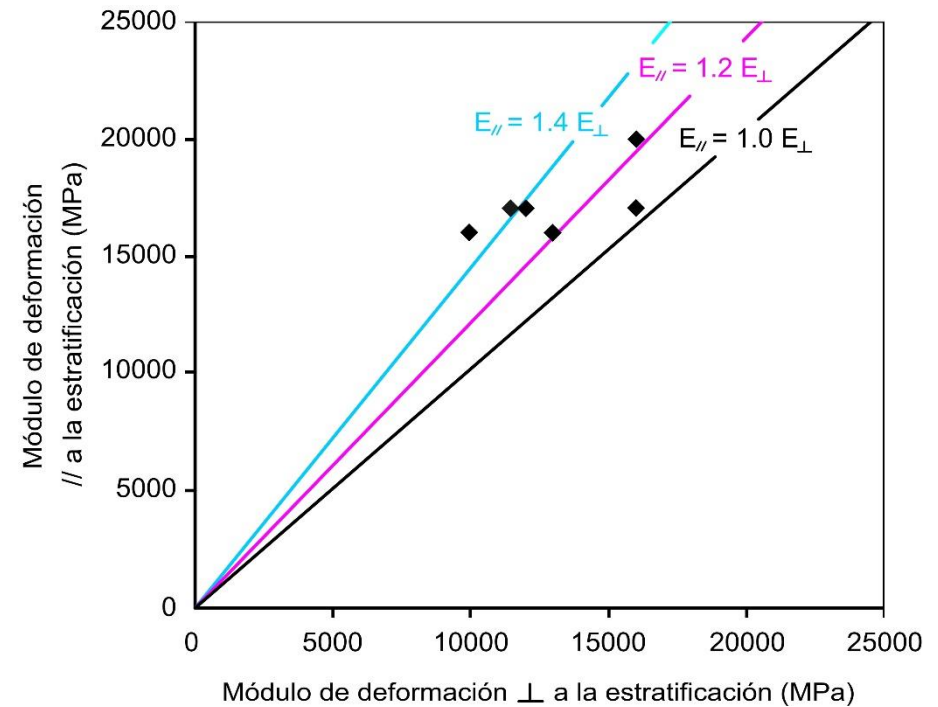
- Observed behaviour:
 - Rate dependency
 - Creep
 - Significant softening
 - Localised deformations



Opalinus clay
(Naumann et al., 2007)

Material behaviour of claystone

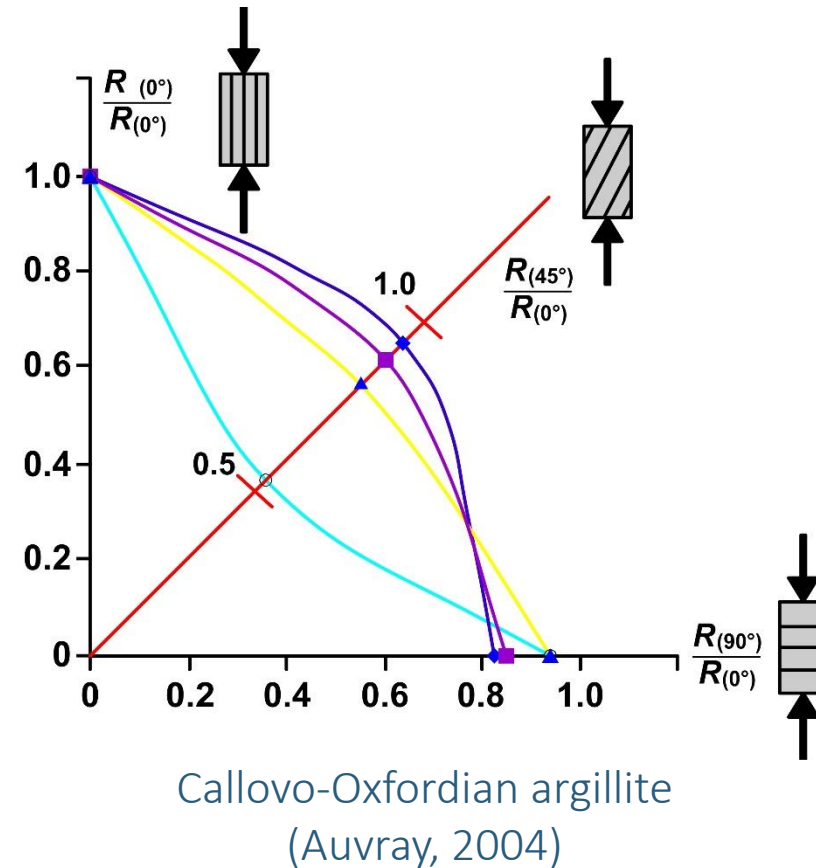
- Observed behaviour:
 - Rate dependency
 - Creep
 - Significant softening
 - Localised deformations
 - Anisotropic properties:
 - **Stiffness**



Callovo-Oxfordian argillite
(Auvray, 2004)

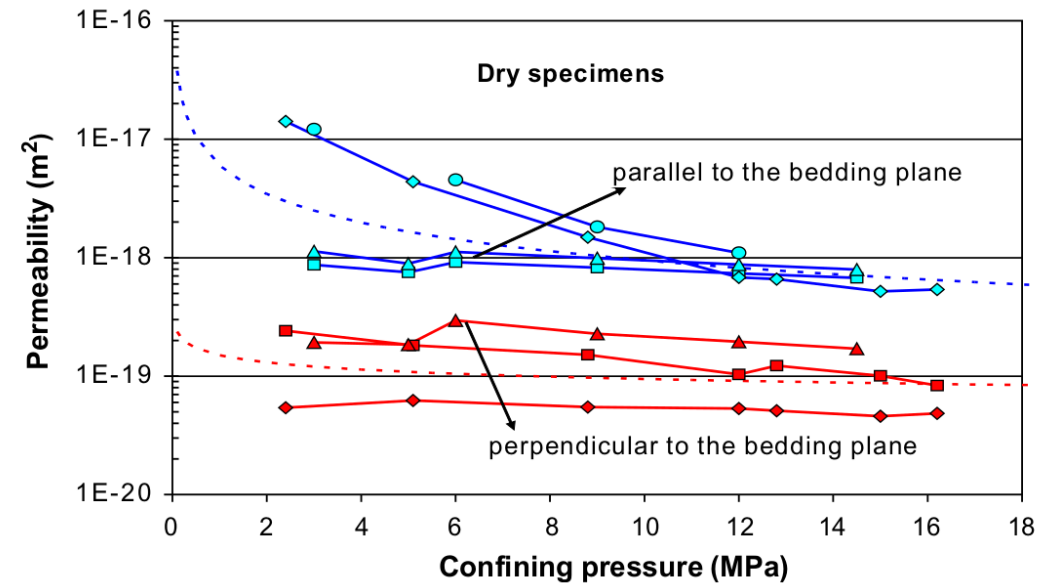
Material behaviour of claystone

- Observed behaviour:
 - Rate dependency
 - Creep
 - Significant softening
 - Localised deformations
 - Anisotropic properties:
 - Stiffness
 - Strength



Material behaviour of claystone

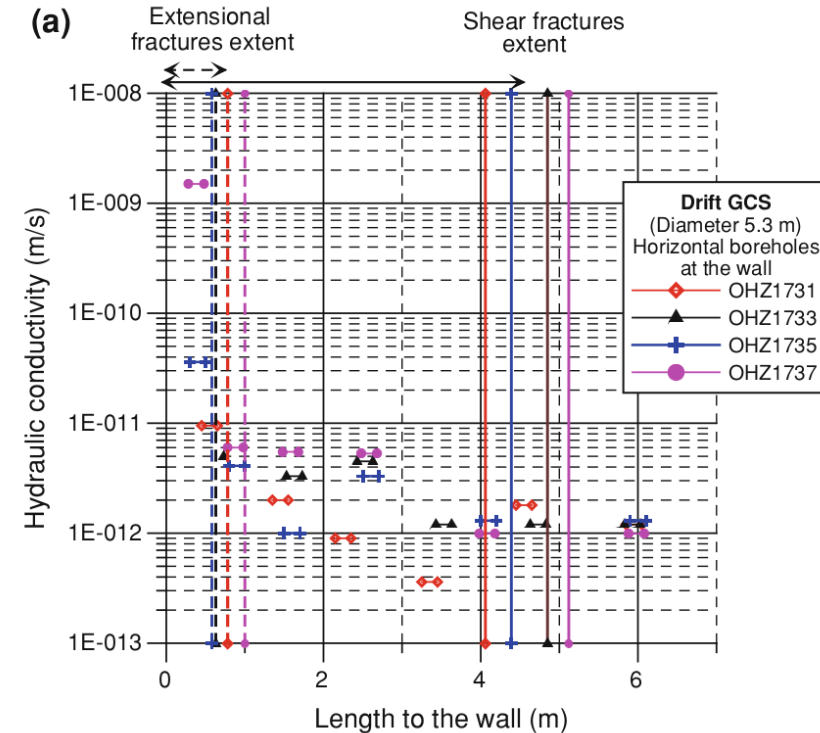
- Observed behaviour:
 - Rate dependency
 - Creep
 - Significant softening
 - Localised deformations
 - Anisotropic properties:
 - Stiffness
 - Strength
 - Permeability



Callovo-Oxfordian argillite
(Zhang & Rothfuchs, 2004)

Material behaviour of claystone

- Observed behaviour:
 - Rate dependency
 - Creep
 - Significant softening
 - Localised deformations
 - Anisotropic properties:
 - Stiffness
 - Strength
 - Permeability
 - Increase of permeability with damage



Callovo-Oxfordian argillite
(Armand et al., 2014)

Material behaviour of claystone

- Nonlocal elasto-viscoplastic constitutive model (Manica, 2018).
- Incorporates the mentioned behavioural features for indurated clayey materials.
- Implemented in the FEM code Plaxis.

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Scientific open-source initiative for the numerical simulation of thermo-hydro-mechanical/chemical (THMC) processes in porous and fractures media (Kolditz, 1990; Wollrath, 1990; Kroehn, 1991; Helmig, 1993; Kolditz et al., 2012; Bilke et al., 2019)

<https://www.opengeosys.org/>

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Scientific open-source initiative for the numerical simulation of thermo-hydro-mechanical/chemical (THMC) processes in porous and fractures media (Kolditz, 1990; Wollrath, 1990; Kroehn, 1991; Helmig, 1993; Kolditz et al., 2012; Bilke et al., 2019)

<https://www.opengeosys.org/>



No introduction required here ;)
(Helfer et al., 2015)

<http://tfel.sourceforge.net/>

Brief description of the formulation

Description	Equation	Parameters
Strain decomposition	$d\epsilon = d\epsilon^e + d\epsilon^{vp} + d\epsilon^c$	-

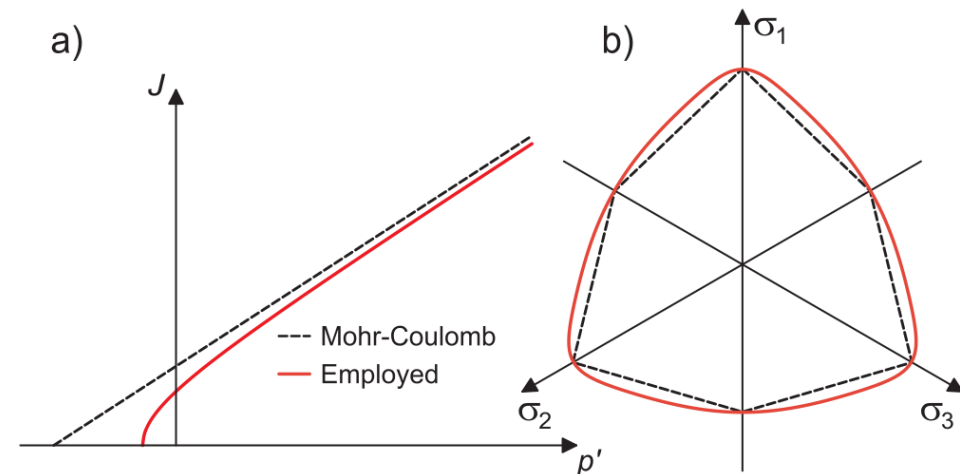
Brief description of the formulation

Description	Equation	Parameters
Strain decomposition	$d\boldsymbol{\epsilon} = d\boldsymbol{\epsilon}^e + d\boldsymbol{\epsilon}^{vp} + d\boldsymbol{\epsilon}^c$	-
Elastic behaviour	$d\boldsymbol{\sigma} = \hat{\mathbf{D}}^e d\boldsymbol{\epsilon}^e$ $\hat{\mathbf{D}}^e = \mathbf{T}^T \mathbf{D}^e \mathbf{T}$	$E_1, E_2, G_2, \nu_1, \nu_2, \alpha^{\text{rot}},$ β^{rot}

$$\mathbf{D}^e = \begin{bmatrix} E_1 \frac{1 - \bar{n}\nu_2^2}{(1 + \nu_1)\bar{m}} & E_1 \frac{\nu_1 + \bar{n}\nu_2^2}{(1 + \nu_1)\bar{m}} & E_1 \frac{\nu_2}{\bar{m}} & 0 & 0 & 0 \\ E_1 \frac{\nu_1 + \bar{n}\nu_2^2}{(1 + \nu_1)\bar{m}} & E_1 \frac{1 - \bar{n}\nu_2^2}{(1 + \nu_1)\bar{m}} & E_1 \frac{\nu_2}{\bar{m}} & 0 & 0 & 0 \\ E_1 \frac{\nu_2}{\bar{m}} & E_1 \frac{\nu_2}{\bar{m}} & E_2 \frac{1 - \nu_1}{\bar{m}} & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{E_1}{2(1 + \nu_1)} & 0 & 0 \\ 0 & 0 & 0 & 0 & G_2 & 0 \\ 0 & 0 & 0 & 0 & 0 & G_2 \end{bmatrix}$$

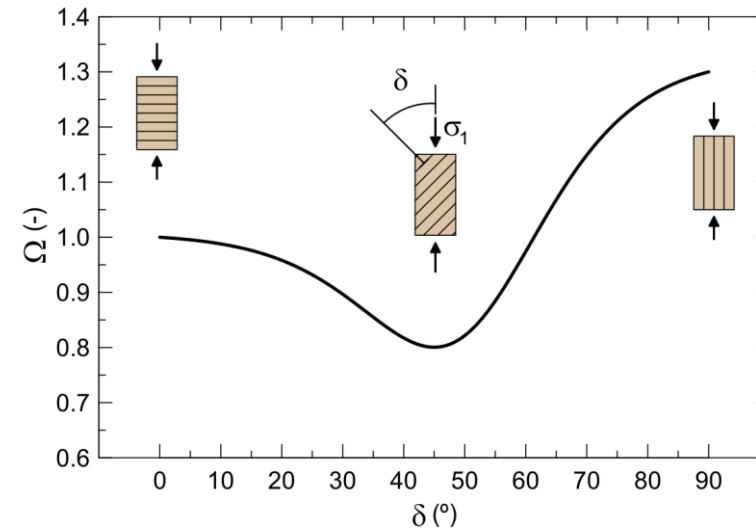
Brief description of the formulation

Description	Equation	Parameters
Strain decomposition	$d\boldsymbol{\epsilon} = d\boldsymbol{\epsilon}^e + d\boldsymbol{\epsilon}^{vp} + d\boldsymbol{\epsilon}^c$	-
Elastic behaviour	$d\boldsymbol{\sigma} = \hat{\mathbf{D}}^e d\boldsymbol{\epsilon}^e$ $\hat{\mathbf{D}}^e = \mathbf{T}^T \mathbf{D}^e \mathbf{T}$	$E_1, E_2, G_2, \nu_1, \nu_2, \alpha^{\text{rot}}, \beta^{\text{rot}}$
Yield criterion	$F = \sqrt{\frac{J_2}{f_d(\theta)} + (c^* + p_t \tan \phi^*)^2} - (c^* + p' \tan \phi^*)$ $f_d(\theta) = \alpha_d (1 + B_d \sin 3\theta)^{n_d}$	α_d



Brief description of the formulation

Description	Equation	Parameters
Strength anisotropy	$c^* = \Omega(\delta)c_0^*$ $p_t = \Omega(\delta)p_{t0}$ $\Omega = \frac{Ae^{(\delta_m - \delta)n}}{[1 + e^{(\delta_m - \delta)n}]^2} + \frac{B}{1 + e^{(\delta_m - \delta)n}} + C$ $A = \frac{2(e_1 + 1)(e_2 + 1)(e_1 - e_2 + \Omega_{90} + e_1 e_2 + e_1 \Omega_{90} - e_2 \Omega_{90} - 2e_1 \Omega_m + 2e_2 \Omega_m - e_1 e_2 \Omega_{90} - 1)}{(e_1 - e_2)(e_1 - 1)(e_2 - 1)}$ $B = \frac{\Omega_{90} - \frac{Ae_1}{(e_1 + 1)^2} + \frac{Ae_2}{(e_2 + 1)^2} - 1}{\frac{1}{e_1 + 1} - \frac{1}{e_2 + 1}}$ $C = 1 - \frac{Ae_2}{(e_2 + 1)^2} - \frac{B}{e_2 + 1}$ $e_1 = e^{n(\delta_m - 90)}$ $e_2 = e^{n\delta_m}$	$\Omega_{90}, \Omega_m, \delta_m, n$



Brief description of the formulation

Description	Equation	Parameters
-------------	----------	------------

Softening laws

$$\tan \phi^* = \tan \phi_{\text{peak}}^* - \left(\tan \phi_{\text{peak}}^* - \tan \phi_{\text{res}}^* \right) \left[1 - e^{-b_{\text{res}}(\epsilon_{\text{eq}}^{\text{P}})} \right]$$

ϕ_{peak}^* , ϕ_{res}^* , $c_{0 \text{ peak}}^*$, $p_{t \text{ peak}}$,

$$c_0^* = \left(c_{0 \text{ peak}}^* - c_{0 \text{ post}}^* \right) e^{-b_{\text{post}}(\epsilon_{\text{eq}}^{\text{P}})} + c_{0 \text{ post}}^* e^{-b_{\text{res}}(\epsilon_{\text{eq}}^{\text{P}})}$$

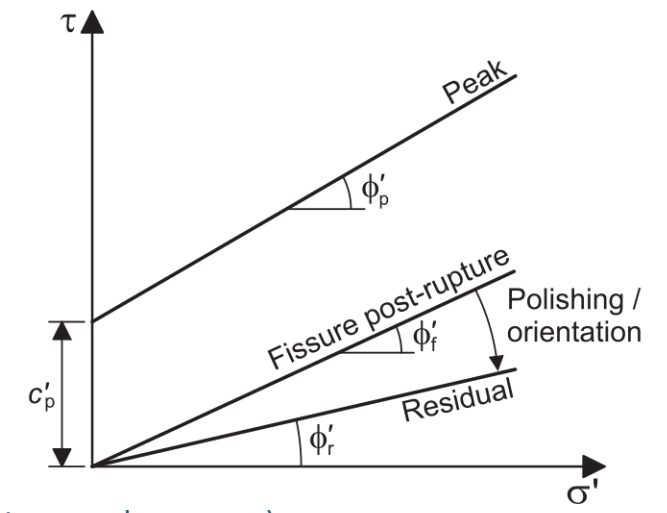
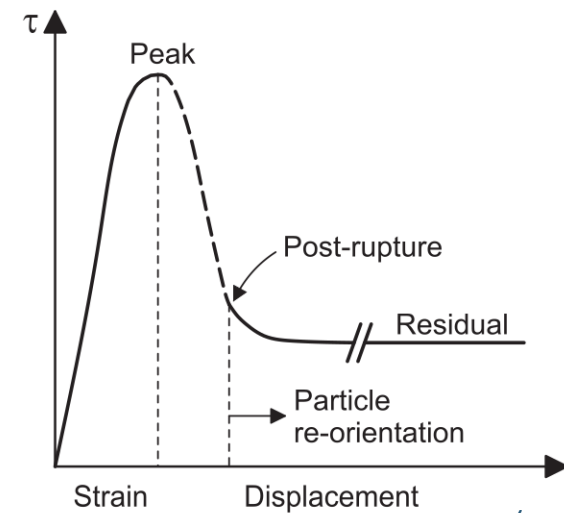
r_{post} , b_{post} , b_{res}

$$p_{t0} = \left(p_{t0 \text{ peak}} - p_{t0 \text{ post}} \right) e^{-b_{\text{post}}(\epsilon_{\text{eq}}^{\text{P}})} + p_{t0 \text{ post}} e^{-b_{\text{res}}(\epsilon_{\text{eq}}^{\text{P}})}$$

$$\epsilon_{\text{eq}}^{\text{P}} = (\epsilon^{\text{P}} : \epsilon^{\text{P}})^{1/2}$$

$$\epsilon^{\text{P}} = \epsilon^{\text{vp}} + \epsilon^{\text{c}}$$

$$r_{\text{post}} = \frac{c_{0 \text{ post}}^*}{c_{0 \text{ peak}}^*} = \frac{p_{t0 \text{ post}}}{p_{t0 \text{ peak}}}$$



(Jardin et al., 2004)

Brief description of the formulation

Description	Equation	Parameters
Softening laws	$\tan \phi^* = \tan \phi_{\text{peak}}^* - \left(\tan \phi_{\text{peak}}^* - \tan \phi_{\text{res}}^* \right) \left[1 - e^{-b_{\text{res}}(\epsilon_{\text{eq}}^{\text{P}})} \right]$ $c_0^* = \left(c_{0 \text{ peak}}^* - c_{0 \text{ post}}^* \right) e^{-b_{\text{post}}(\epsilon_{\text{eq}}^{\text{P}})} + c_{0 \text{ post}}^* e^{-b_{\text{res}}(\epsilon_{\text{eq}}^{\text{P}})}$ $p_{t0} = \left(p_{t0 \text{ peak}} - p_{t0 \text{ post}} \right) e^{-b_{\text{post}}(\epsilon_{\text{eq}}^{\text{P}})} + p_{t0 \text{ post}} e^{-b_{\text{res}}(\epsilon_{\text{eq}}^{\text{P}})}$ $\epsilon_{\text{eq}}^{\text{P}} = (\epsilon^{\text{P}} : \epsilon^{\text{P}})^{1/2}$ $\epsilon^{\text{P}} = \epsilon^{\text{VP}} + \epsilon^{\text{C}}$ $r_{\text{post}} = \frac{c_{0 \text{ post}}^*}{c_{0 \text{ peak}}^*} = \frac{p_{t0 \text{ post}}}{p_{t0 \text{ peak}}}$	$\phi_{\text{peak}}^*, \phi_{\text{res}}^*, c_{0 \text{ peak}}^*, p_{t \text{ peak}},$ $r_{\text{post}}, b_{\text{post}}, b_{\text{res}}$
Plastic potential	$\frac{\partial G}{\partial \sigma'} = \omega \frac{\partial F}{\partial p} \frac{\partial p}{\partial \sigma'} + \frac{\partial F}{\partial J_2} \frac{\partial J_2}{\partial \sigma'} + \frac{\partial F}{\partial \theta} \frac{\partial \theta}{\partial \sigma'}$	ω

Brief description of the formulation

Description	Equation	Parameters
Softening laws	$\tan \phi^* = \tan \phi_{\text{peak}}^* - \left(\tan \phi_{\text{peak}}^* - \tan \phi_{\text{res}}^* \right) \left[1 - e^{-b_{\text{res}}(\epsilon_{\text{eq}}^{\text{P}})} \right]$ $c_0^* = \left(c_{0 \text{ peak}}^* - c_{0 \text{ post}}^* \right) e^{-b_{\text{post}}(\epsilon_{\text{eq}}^{\text{P}})} + c_{0 \text{ post}}^* e^{-b_{\text{res}}(\epsilon_{\text{eq}}^{\text{P}})}$ $p_{t0} = \left(p_{t0 \text{ peak}} - p_{t0 \text{ post}} \right) e^{-b_{\text{post}}(\epsilon_{\text{eq}}^{\text{P}})} + p_{t0 \text{ post}} e^{-b_{\text{res}}(\epsilon_{\text{eq}}^{\text{P}})}$ $\epsilon_{\text{eq}}^{\text{P}} = (\epsilon^{\text{P}} : \epsilon^{\text{P}})^{1/2}$ $\epsilon^{\text{P}} = \epsilon^{\text{VP}} + \epsilon^{\text{C}}$ $r_{\text{post}} = \frac{c_{0 \text{ post}}^*}{c_{0 \text{ peak}}^*} = \frac{p_{t0 \text{ post}}}{p_{t0 \text{ peak}}}$	$\phi_{\text{peak}}^*, \phi_{\text{res}}^*, c_{0 \text{ peak}}^*, p_{t \text{ peak}},$ $r_{\text{post}}, b_{\text{post}}, b_{\text{res}}$
Plastic potential	$\frac{\partial G}{\partial \sigma'} = \omega \frac{\partial F}{\partial p} \frac{\partial p}{\partial \sigma'} + \frac{\partial F}{\partial J_2} \frac{\partial J_2}{\partial \sigma'} + \frac{\partial F}{\partial \theta} \frac{\partial \theta}{\partial \sigma'}$	ω
Visco-plasticity	$d\epsilon^{\text{VP}} = \frac{\langle \Phi(F) \rangle}{\eta} \frac{\partial G}{\partial \sigma'} dt$ $\Phi(F) = \left(\frac{F}{p_{\text{atm}}} \right)^N$	N, η

Brief description of the formulation

Description	Equation	Parameters
Creep deformations	$d\epsilon^c = \dot{\epsilon}^c dt$ $\dot{\epsilon}^c = \begin{cases} \mathbf{0} & \text{if } \epsilon_{\text{eq}}^p \leq \epsilon_{\text{thr}} \\ \gamma e^{(-m\epsilon_{\text{eq}}^c)} (\mathbf{s} + \mu p' \mathbf{I}) & \text{if } \epsilon_{\text{eq}}^p > \epsilon_{\text{thr}} \end{cases}$ $\epsilon_{\text{eq}}^c = (\epsilon^c : \epsilon^c)^{1/2}$	$\gamma, \mu, m, \epsilon_{\text{thr}}$

Brief description of the formulation

Description	Equation	Parameters
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Creep deformations

$$d\epsilon^c = \dot{\epsilon}^c dt$$

$\gamma, \mu, m, \epsilon_{thr}$

$$\dot{\epsilon}^c = \begin{cases} \mathbf{0} & \text{if } \epsilon_{eq}^p \leq \epsilon_{thr} \\ \gamma e^{(-m\epsilon_{eq}^c)} (\mathbf{s} + \mu p' \mathbf{I}) & \text{if } \epsilon_{eq}^p > \epsilon_{thr} \end{cases}$$

$$\epsilon_{eq}^c = (\epsilon^c : \epsilon^c)^{1/2}$$

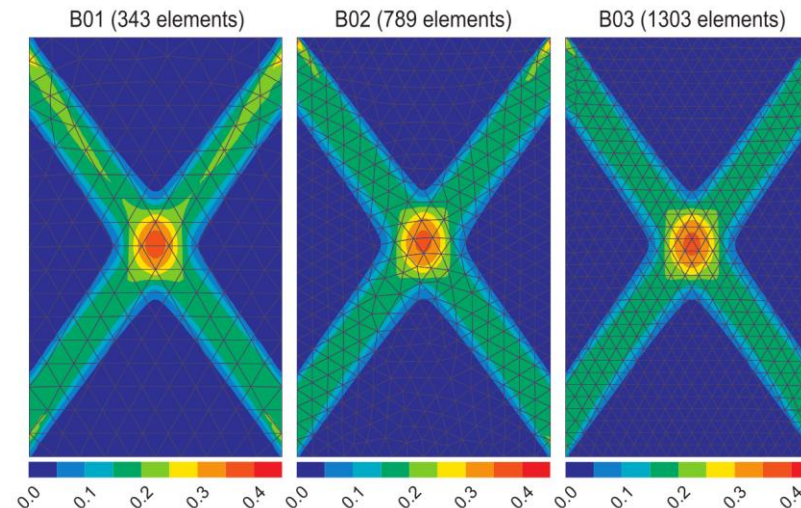
Nonlocal regularisation

$$\bar{\epsilon}_{eq}^p(\mathbf{x}) = \int_V w(\mathbf{x}, \boldsymbol{\xi}) \epsilon_{eq}^p(\boldsymbol{\xi}) d\boldsymbol{\xi}$$

l_s

$$w(\mathbf{x}, \boldsymbol{\xi}) = \frac{w_0(\|\mathbf{x} - \boldsymbol{\xi}\|)}{\int_V w_0(\|\mathbf{x} - \boldsymbol{\zeta}\|) d\boldsymbol{\zeta}}$$

$$w_0 = \frac{\|\mathbf{x} - \boldsymbol{\xi}\|}{l_s} e^{-\left(\frac{\|\mathbf{x} - \boldsymbol{\xi}\|}{l_s}\right)^2}$$

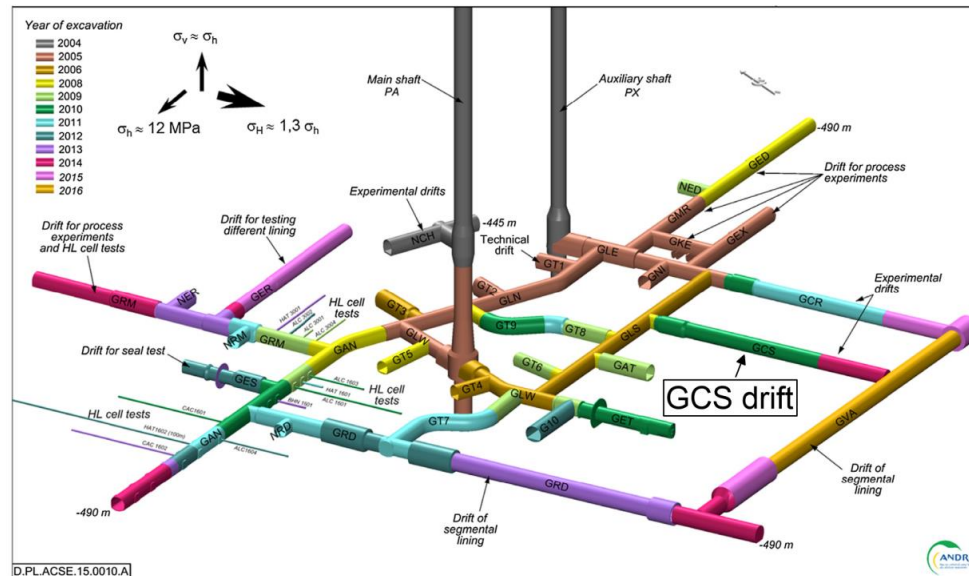


Brief description of the formulation

Description	Equation	Parameters
Hydro-mechanical coupling	$\boldsymbol{\sigma}' = \boldsymbol{\sigma} + S_e s B \mathbf{I}$ $S_e = \frac{S_l - S_{lr}}{S_{ls} - S_{lr}} = \left[1 + \left(\frac{s}{P} \right)^{\frac{1}{1-\lambda}} \right]^{-\lambda}$ $\mathbf{q} = -\frac{\mathbf{k}k_r}{\mu_w} (\nabla p_l - \rho_w \mathbf{g})$ $k_r = S_e^{\frac{1}{2}} \left[1 - \left(1 - S_e^{\frac{1}{\lambda}} \right)^\lambda \right]^2$ $\mathbf{k} = \mathbf{k}_0 \left[1 + \beta (\epsilon_{eq}^p)^3 \right]$	$B, \lambda, P, \beta, k_h, k_v$

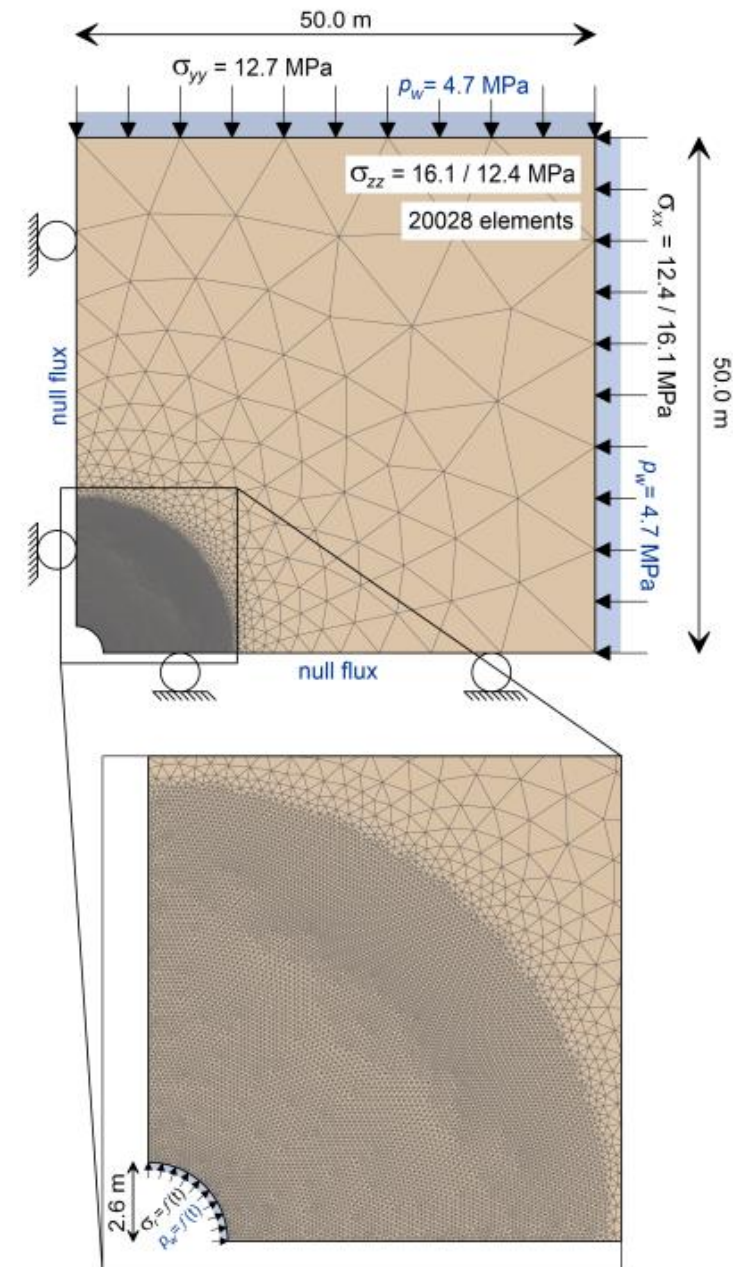
Application example

- Simulation of drifts at the Meuse/Haute Marne Underground Research Laboratory.



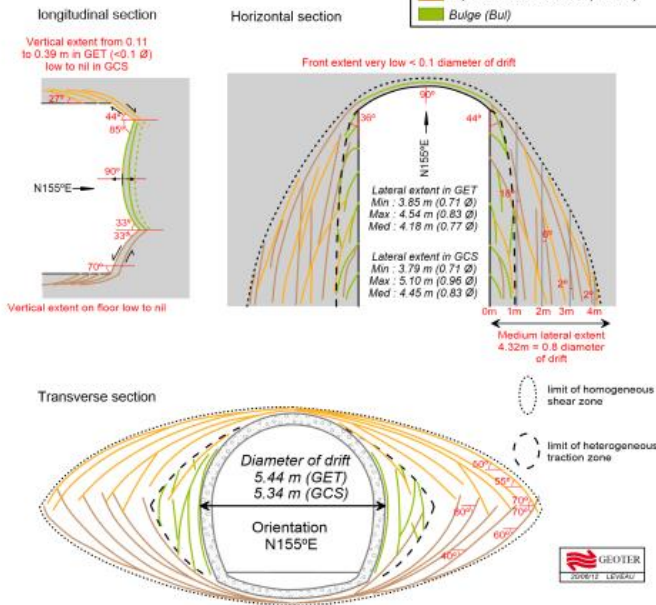
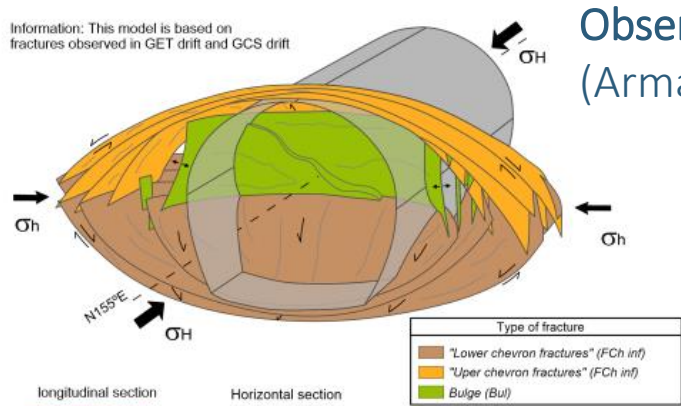
(Seyedi et al., 2017)

Details in: Mánica M (2018) Analysis of underground excavations in argillaceous hard soils–weak rocks. Technical University of Catalonia, PhD.



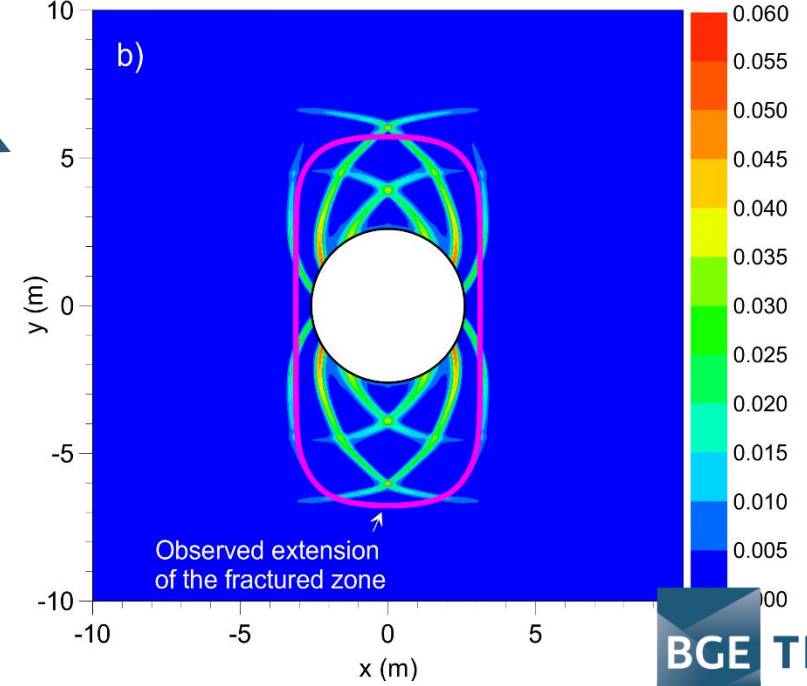
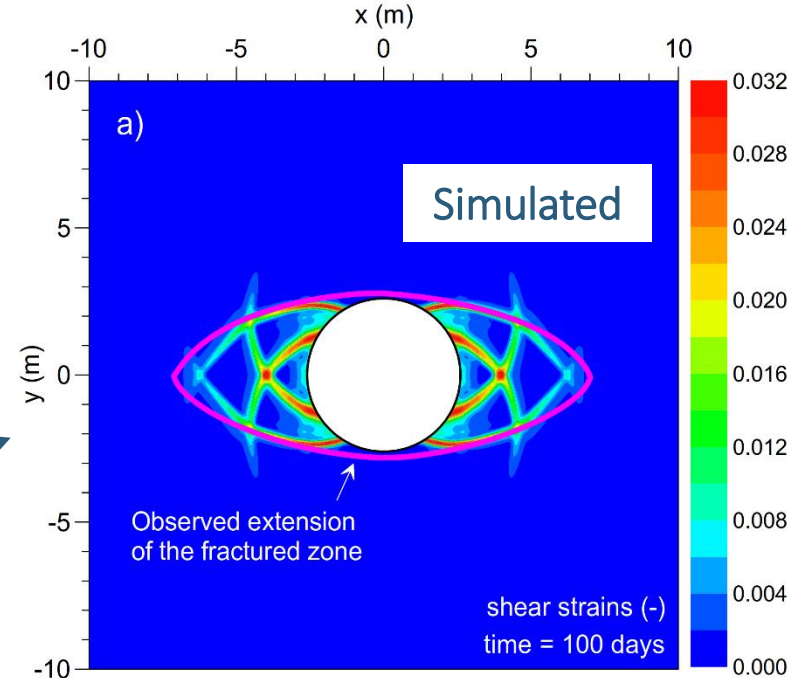
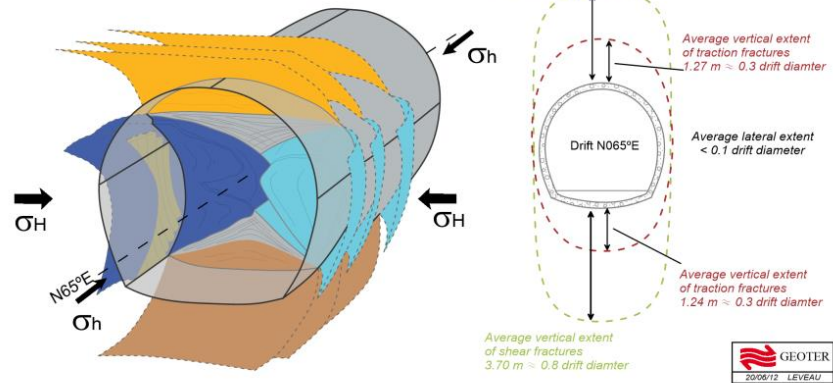
Application example

- Obtained results – damaged zone



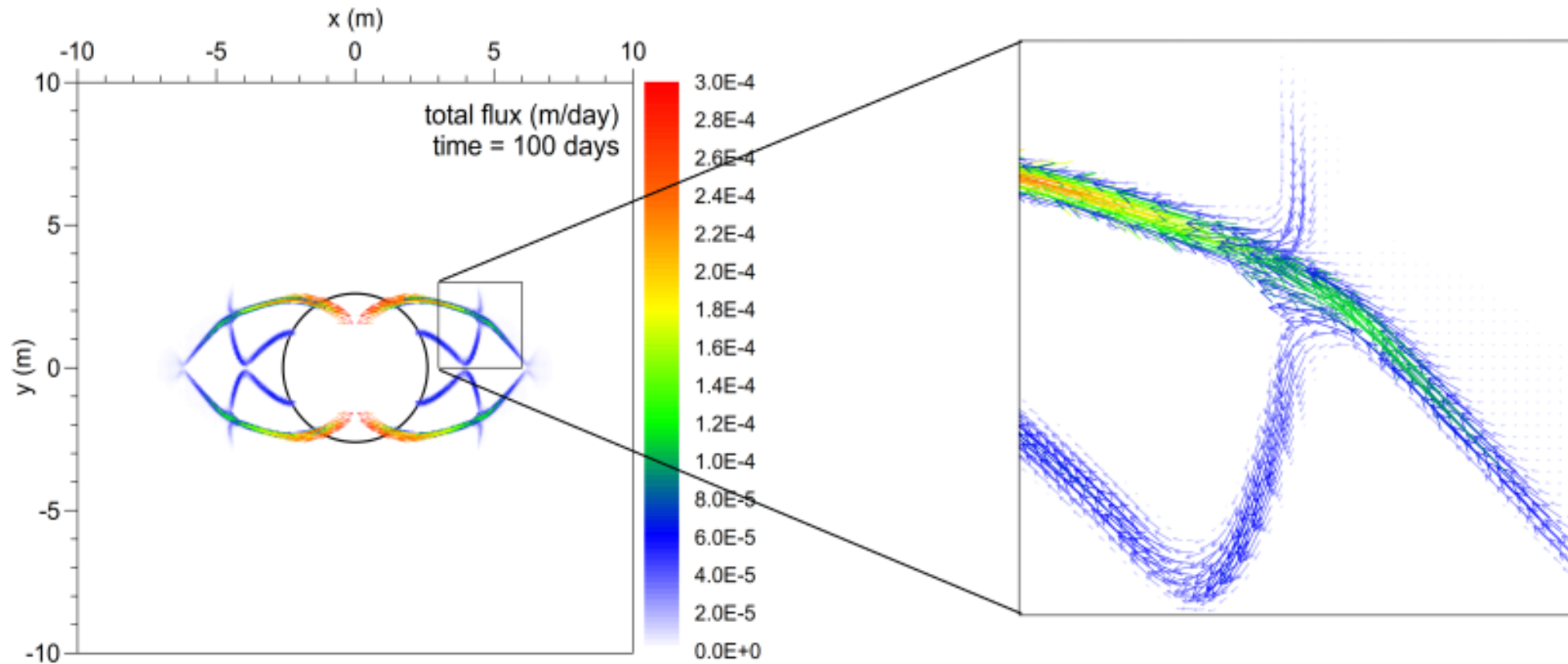
parallel to the major horizontal stress

parallel to the minor horizontal stress



Application example

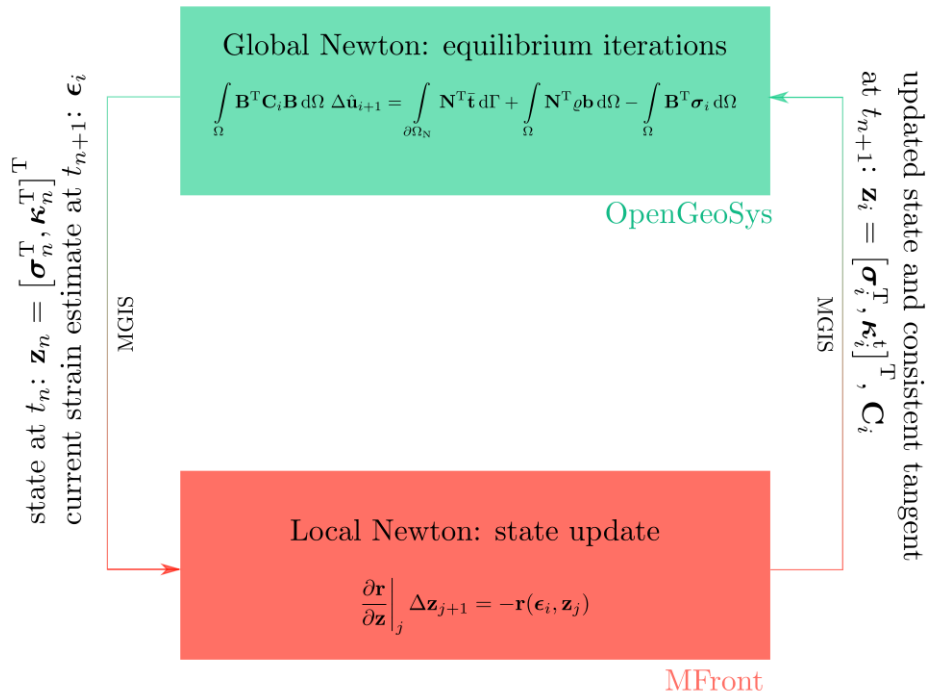
- Obtained results – localized water flow



Implementation - MFront

- Implementation of the described model in **OpenGeoSys**: recently started project.

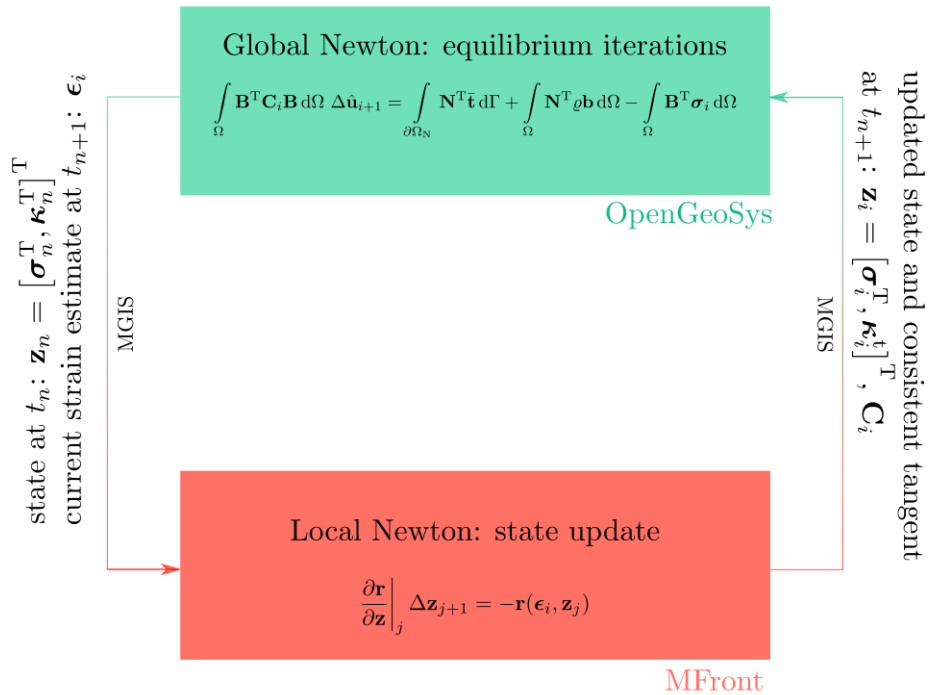
Implementation - MFront



(Nagel et al., 2019)

- Implementation of the described model in **OpenGeoSys**: recently started project.
- Support for **MFront** already provided in **OpenGeoSys** (Nagel et al., 2019) through the **MFrontGenericInterfaceSupport (MGIS)** library (Helfer et al., 2020).

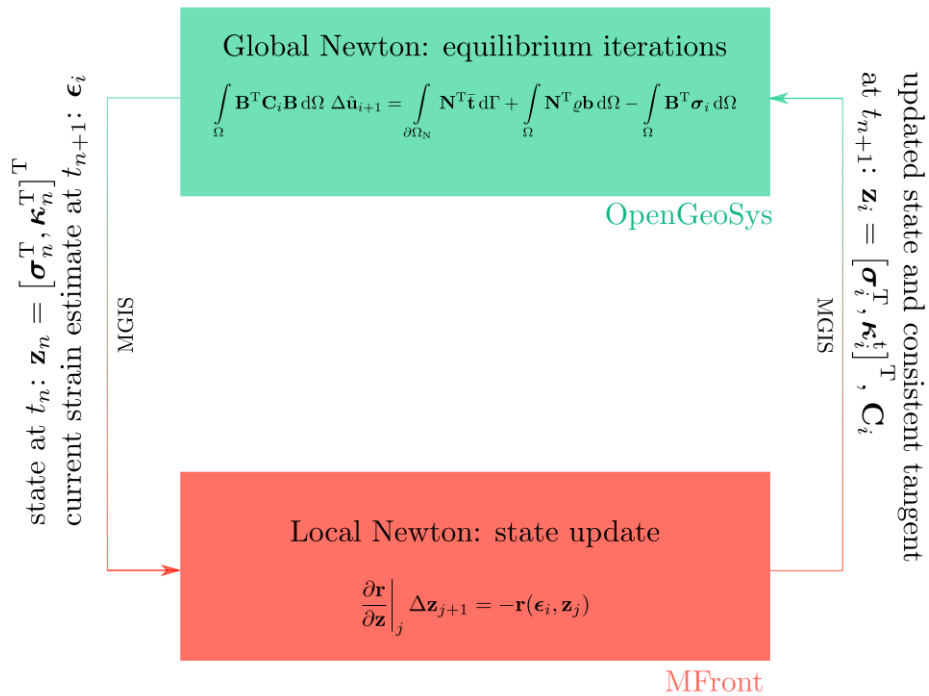
Implementation - MFront



(Nagel et al., 2019)

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Implementation - MFront



(Nagel et al., 2019)

- Implementation of the described model in **OpenGeoSys**: recently started project.
- Support for **MFront** already provided in **OpenGeoSys** (Nagel et al., 2019) through the **MFrontGenericInterfaceSupport (MGIS)** library (Helfer et al., 2020).
- Local version of the model straightforward.
- Nonlocal version – more challenging:
 - Already exists a native implementation in **OGS** (Parisio et al., 2019).
 - Main requirement – access to state variables from neighboring Gauss points.
 - It could be directly addressed in **MFront**.

Next steps

- **Bentonite model:**
 - Development work in OpenGeoSys to consider the generalized state variable vector for THM-simulation
 - Numerical tests and Benchmarks in OpenGeoSys and SIFEL
- **Clay stone model**
 - Implementation of the local model in Mfront
 - Theoretical work to deal with nonlocal plasticity in Mfront



Thank you for your attention!