MFront and OpenGeoSys

Connecting two open-source initiatives for simulations in environmental geosciences and energy geotechnics

Thomas Nagel, Francesco Parisio, Dmitri Naumov, Chrisoph Lehmann, Olaf Kolditz

Technische Universität Bergakademie Freiberg – TUBAF
Helmholtz Zentrum für Umweltforschung GmbH – UFZ
Technische Universität Dresden – TUD

Competence Centre for Environmental Geosciences – CC-EG

MFront User Meeting
17.10.–18.10.2019, Paris

Visit

`https://tu-freiberg.de/fakultaet3/gt/bodenmechanik`
`www.ufz.de/environmental-geotechnics`
`www.ufz.de/comp-energy-sys`

MFront and OpenGeoSys

Connecting two open-source initiatives for simulations in environmental geosciences and energy geotechnics

Thomas Nagel, Francesco Parisio, Dmitri Naumov, Chrisoph Lehmann, Olaf Kolditz

Technische Universität Bergakademie Freiberg – TUBAF
Helmholtz Zentrum für Umweltforschung GmbH – UFZ
Technische Universität Dresden – TUD

Competence Centre for Environmental Geosciences – CC-EG

MFront User Meeting
17.10.–18.10.2019, Paris

Visit

https://tu-freiberg.de/fakultaet3/gt/bodenmechanik
www.ufz.de/environmental-geotechnics
www.ufz.de/comp-energy-sys

InterPore in Qingdao

Content

Introduction

Prof. Dr. Thomas Nagel thomas.nagel@ifgt.tu-freiberg.de

Chair of Soil Mechanics and Foundation Engineering

Coupled Problems

T HERMAL
H YDRAULIC
M ECHANICAL
C HEMICAL
B IOLOGICAL

in Porous and Granular Media

Theory

Experiment

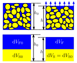
Application

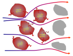
verification, parameterization, validation

Multiphysical problem formulation

T^3

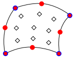
THERMODYNAMICS
THEORY OF POROUS MEDIA
THEORY OF MATERIALS

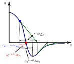




Numerical implementation

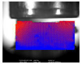
in scientific open-source software or
via user-interfaces in commerical software

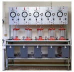




Geomechanical laboratory

application-oriented material and
process characterization based on
point, field and integral measurements



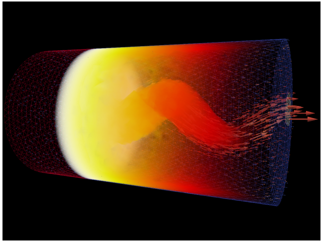


Geotechnical applications

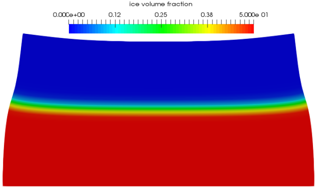
application-oriented assessments at the
site/field scale for design and optimization
in the presence of uncertainties

THMC simulations with finite elements (OpenGeoSys)

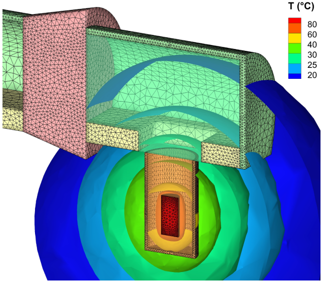
Deep and shallow geothermal, energy storage



Phase change in soil (s,l,g)

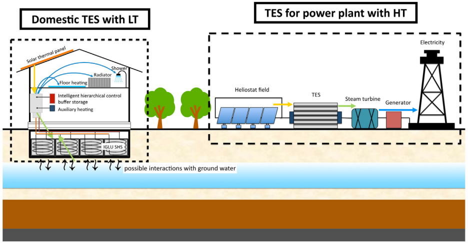


Radioactive and toxic waste disposal

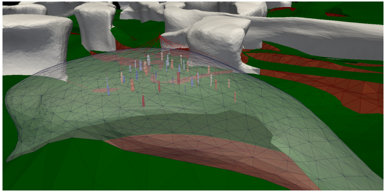


THMC simulations with finite elements (OpenGeoSys)

Thermal energy storage in building infrastructures

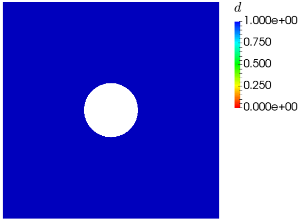


Hydrogen storage in salt caverns

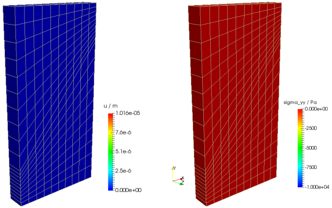


THMC simulations with finite elements (OpenGeoSys)

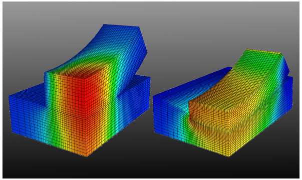
Thermally and hydraulically induced discontinuities in soils and rocks



Hydro-Mechanics of interfaces

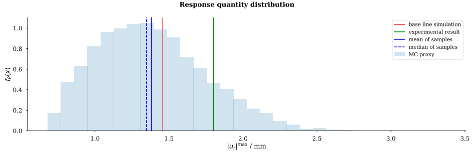


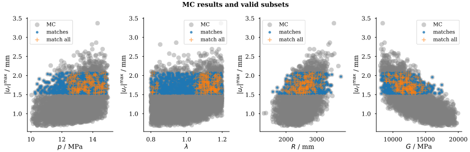
Constitutive models at finite deformations

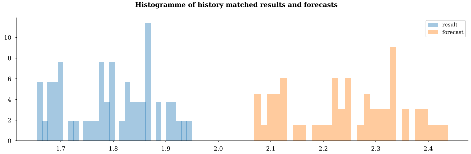


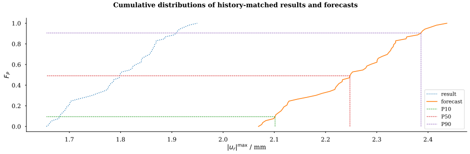
THMC simulations with finite elements (OpenGeoSys)

Quantification and assessment of uncertainties









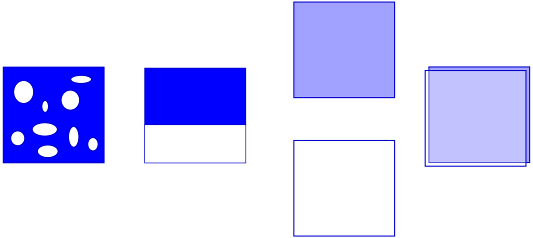
THMC problems in porous media

Theory of Porous Media

Ingredients: mixture theory & concept of volume fractions.

Truesdell's metaphysical principles (Truesdell and Noll, 1965):

1. All properties of the mixture must be mathematical consequences of the properties of the constituents.
2. So as to describe the motion of a constituent, we may in imagination isolate it from the rest of the mixture, provided we allow properly for the actions of the other constituents upon it.
3. The motion of the mixture is governed by the same equations as is a single body.



Kolumban Hutter and Jöhnk, 2004; Wolfgang Ehlers and Bluhm, 2002

Early history: Terzaghi and Fröhlich, 1936; Fillunger, 1936; Kögler and Scheidig, 1938; Biot, 1941; Skempton, 1960; Bowen, 1980; Mow et al., 1980; W. Ehlers, 1989

General balance equations (without interfaces or common lines/points)

The following local balance relations hold for the phases/constituents (assuming sufficient continuity):

$$(\rho_\alpha)'_\alpha + \rho_\alpha \operatorname{div} \mathbf{v}_\alpha = \hat{\rho}_\alpha \qquad \sum_\alpha \hat{\rho}_\alpha = 0$$

$$\operatorname{div} \boldsymbol{\sigma}_\alpha + \rho_\alpha \mathbf{b}_\alpha + \hat{\mathbf{s}}_\alpha - \hat{\rho}_\alpha \mathbf{v}_\alpha = \rho_\alpha \mathbf{a}_\alpha \qquad \sum_\alpha \hat{\mathbf{s}}_\alpha = \mathbf{0}$$

$$\boldsymbol{\sigma}_\alpha = \boldsymbol{\sigma}_\alpha^\mathsf{T}$$

$$\rho_\alpha (u_\alpha)'_\alpha = \boldsymbol{\sigma}_\alpha : \mathbf{d}_\alpha + \rho_\alpha r_\alpha - \operatorname{div} \mathbf{q}_\alpha + \hat{u}_\alpha - \hat{\mathbf{p}}_\alpha \cdot \mathbf{v}_\alpha - \hat{\rho}_\alpha \left(u_\alpha + \frac{1}{2} \mathbf{v}_\alpha \cdot \mathbf{v}_\alpha \right) \qquad \sum_\alpha \hat{u}_\alpha = 0$$

$$\rho_\alpha (\eta_\alpha)'_\alpha = \frac{\rho_\alpha r_\alpha}{T_\alpha} - \operatorname{div} \left(\frac{1}{T_\alpha} \mathbf{q}_\alpha \right) + \hat{\eta}_\alpha - \hat{\rho}_\alpha \eta_\alpha$$

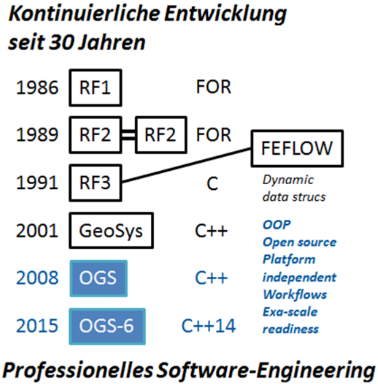
The first and second law can be combined to the Clausius-Duhem inequality (Coleman and W. Noll, 1963; Clifford Truesdell, 2012; other possibilities: Hutter, 1977; Woods, 1982; Müller, 1968; Müller and Ruggeri, 2013; Liu and Müller, 1984):

$$0 \leq \sum_\alpha \frac{1}{T_\alpha} \left[\boldsymbol{\sigma}_\alpha : \mathbf{d}_\alpha - \rho_\alpha [(\psi_\alpha)'_\alpha + \eta_\alpha (T_\alpha)'_\alpha] - \frac{1}{T_\alpha} \mathbf{q}_\alpha \cdot \operatorname{grad} T_\alpha + \hat{u}_\alpha - \hat{\mathbf{p}}_\alpha \cdot \mathbf{v}_\alpha - \right.$$

$$\left. - \hat{\rho}_\alpha \left(\psi_\alpha + \frac{1}{2} \mathbf{v}_\alpha \cdot \mathbf{v}_\alpha \right) \right]$$

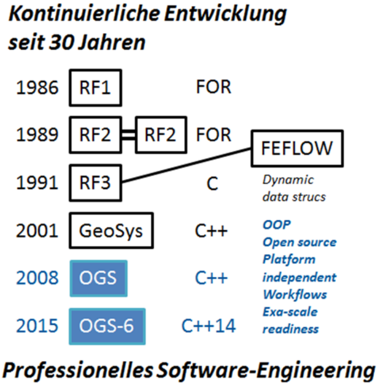
OpenGeoSys—open-source multiphysics for environmental and energy geotechnics

OpenGeoSys—an open-source finite element framework



→ Strongly coupled multi-physical processes in fractured porous media: **T**hermal-**H**ydraulic-**M**echanical-**C**hemical/**B**iological (THMC/B)

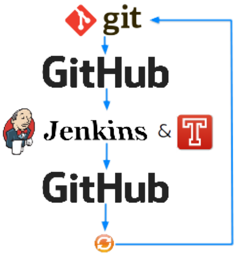
OpenGeoSys—an open-source finite element framework



→ Strongly coupled multi-physical processes in fractured porous media:
Thermal-**H**ydraulic-**M**echanical-**C**hemical/**B**iological (THMC/B)

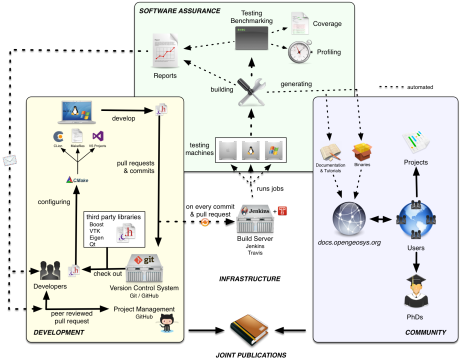
Elements of code QA

- Code is open-source
- Development discussion is public



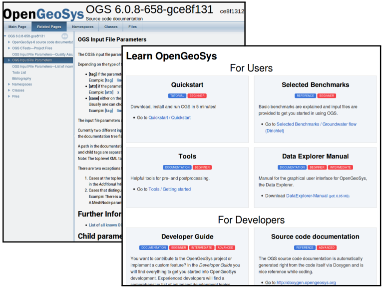
Elements of code QA

- Code is open-source
- Development discussion is public
- Automated compilation & testing on different platforms
- Complex testing in intervals (e.g. memory leaks, runtime checks)
- Automated deployment of binaries



Elements of code QA

- Code is open-source
- Development discussion is public
- Automated compilation & testing on different platforms
- Complex testing in intervals (e.g. memory leaks, runtime checks)
- Automated deployment of binaries
- Automated & manual documentation



Elements of code QA

- Code is open-source
- Development discussion is public
- Automated compilation & testing on different platforms
- Complex testing in intervals (e.g. memory leaks, runtime checks)
- Automated deployment of binaries
- Automated & manual documentation
- Participation in international benchmarking initiatives
- Results of benchmarks published

Elements of code QA

- Code is open-source
- Development discussion is public
- Automated compilation & testing on different platforms
- Complex testing in intervals (e.g. memory leaks, runtime checks)
- Automated deployment of binaries
- Automated & manual documentation
- Participation in international benchmarking initiatives
- Results of benchmarks published
- Tutorials published → international training courses

Elements of code QA

- Code is open-source
- Development discussion is public
- Automated compilation & testing on different platforms
- Complex testing in intervals (e.g. memory leaks, runtime checks)
- Automated deployment of binaries
- Automated & manual documentation
- Participation in international benchmarking initiatives
- Results of benchmarks published
- Tutorials published → international training courses
- Community contributions

Elements of code QA

- Code is open-source
- Development discussion is public
- Automated compilation & testing on different platforms
- Complex testing in intervals (e.g. memory leaks, runtime checks)
- Automated deployment of binaries
- Automated & manual documentation
- Participation in international benchmarking initiatives
- Results of benchmarks published
- Tutorials published $\rightarrow$ international training courses
- Community contributions

Transport in Porous Media
https://doi.org/10.1007/s11242-019-01310-1

Check for updates

Development of Open-Source Porous Media Simulators: Principles and Experiences

Lars Bilke[1] · Bernd Flemisch[2] · Thomas Kalbacher[1] · Olaf Kolditz[1,3] · Rainer Helmig[2] · Thomas Nagel[1,4]

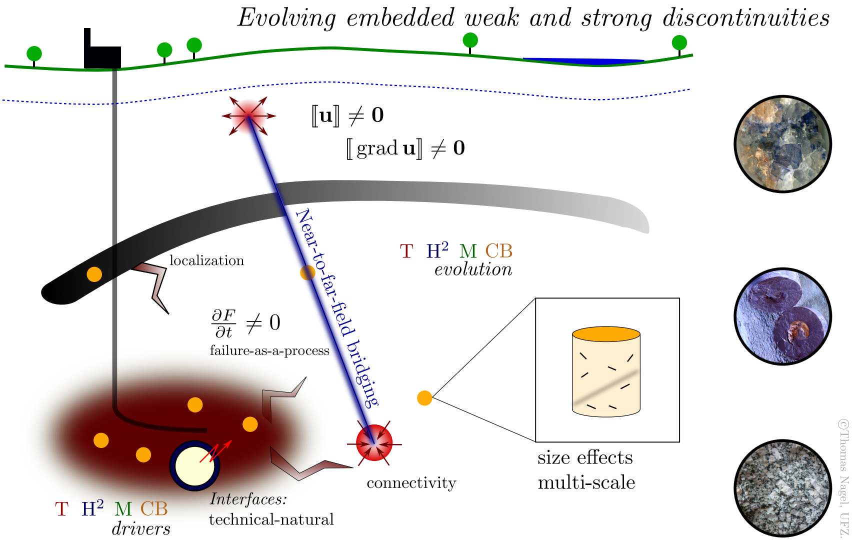
Received: 21 December 2018 / Accepted: 17 June 2019

Abstract
By its very nature, research into multi-physical processes occurring in porous and fractured media requires a collaborative approach. An interdisciplinary approach has led to the adoption of collaborative software development paradigms in this field relying on software for scientific computing as research infrastructures. The development of open-source software has become a cornerstone of computational approaches in academia and has even spawned successful business models in the commercial world. This article is geared toward readers who want to learn more about potential benefits of open-source software in porous media research and who want to familiarize themselves with typical workflows required to become an active contributor to or user of open-source solutions for porous media simulation. The article puts general principles, motivations and concepts into the specific context of experiences and lessons learned from the authors developing the open-source software projects OpenGeoSys and DuMu^x.

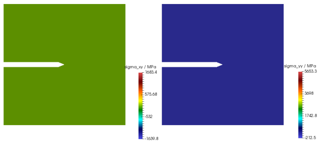
Keywords Open-source · Multi-physics · THMC · Software development · Porous media

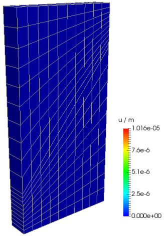
Fractures and damage in geomaterials

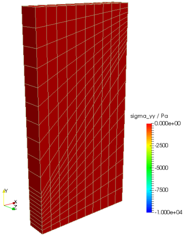
Evolving embedded discontinuities for barrier integrity assessment

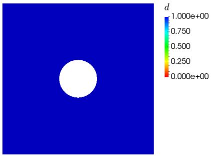


Numerical methods & goals









- **Efficient**, **quality-assured** and **error-controlled** numerical simulation frameworks for evolving **fluid pathways** in **multi-phase systems** with embedded **discontinuities**.
- **Thermodynamically consistent constitutive models**
- **Incorporation of size effects** for physically meaningful scale transitions from laboratory to field scale

$$\bar{u}(\mathbf{x}) = \int\limits_{\Omega_l} u(\mathbf{x} + \boldsymbol{\xi})\omega(\boldsymbol{\xi})\,\mathrm{d}\Omega$$

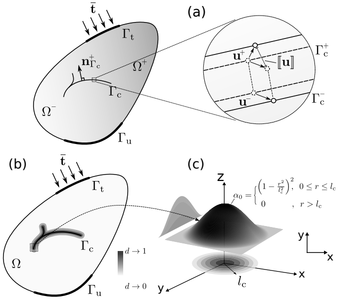
$$u(\mathbf{x}) = \sum_{i=1}^{m} N^i(\mathbf{x})\hat{u}^i + \sum_{j=1}^{n} N^j(\mathbf{x}) \sum_{k=1}^{o} \bar{N}^k(\mathbf{x})\hat{a}^{jk}$$

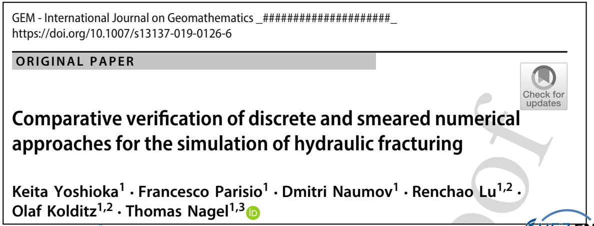
$$\mathbf{0} = \operatorname{Div} \boldsymbol{\Sigma} + \mathbf{g}$$

$$(\mathbf{u}^*, \Gamma^*) = \underset{\mathbf{u},\Gamma}{\arg\min} \left[\Pi^{\text{mech}}(\mathbf{u}, \Gamma) + G_\mathrm{c}\mathcal{H}^{N-1}(\Gamma)\right]$$

$$\mathcal{H}^{N-1}(\Gamma) \to \int\limits_{\Omega} \gamma(d)\,\mathrm{d}\Omega$$

Numerical approaches for hydraulic fracturing: development and cross-verification





GEM - International Journal on Geomathematics _####################_
https://doi.org/10.1007/s13137-019-0126-6

ORIGINAL PAPER

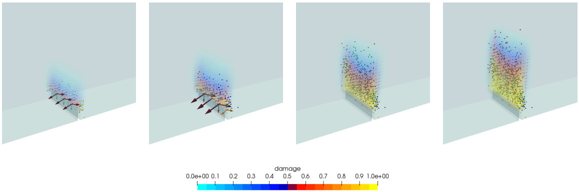
Check for updates

Comparative verification of discrete and smeared numerical approaches for the simulation of hydraulic fracturing

Keita Yoshioka[1] · Francesco Parisio[1] · Dmitri Naumov[1] · Renchao Lu[1,2] · Olaf Kolditz[1,2] · Thomas Nagel[1,3]

- Hydraulic fracturing in toughness-dominated regime
- Variational phase-field approach vs. non-local plastic-damage vs. locally enriched cohesive-zone elements
- extensive cross-verification
- physical richness vs. parameterization
- consistent quantification of crack-length and energy release rate for phase-field (smeared approach)

Elasto-plastic model with non-local damage: beyond linear elastic fracture mechanics



Contents lists available at ScienceDirect

International Journal of Solids and Structures

journal homepage: www.elsevier.com/locate/ijsolstr

ELSEVIER

Experimental characterization and numerical modelling of fracture processes in granite

Francesco Parisio[a,*], Ali Tarokh[b], Roman Makhnenko[b], Dmitri Naumov[a], Xing-Yuan Miao[a,c], Olaf Kolditz[a,c], Thomas Nagel[a,d,1]

[a] Department of Environmental Informatics, Helmholtz Centre for Environmental Research – UFZ, Leipzig, Germany
[b] Department of Civil and Environmental Engineering, University of Illinois at Urbana-Champaign, USA
[c] Applied Environmental Systems Analysis, Technische Universität Dresden, Dresden, Germany
[d] Department of Mechanical and Manufacturing Engineering, School of Engineering, Trinity College Dublin, College Green, Dublin, Ireland

- Transition between strength-dominated and toughness-dominated failure
- Parameterization using standard tests (UCS, US, ITS)
- Validation with global (force-displacement) and local quantities (AE)
- Configurational forces used to assess energy release rates
- Dissipation in the fracture process zone accounted for

Recent studies in energy geotechnics and environmental geotechnics

HIGHER: enhanced supercritical geothermal systems

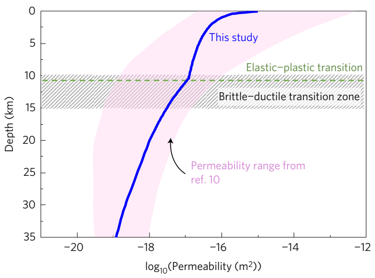


Figure 3 | Comparison between the experimental results summarized in equations (1)–(3) and a permeability–depth relation from the literature[10]. The permeability–depth relation in this study is consistent with those suggested in the literature, which indicates no abrupt decrease in permeability at the brittle–ductile transition. The elastic–plastic transition occurs at a depth of approximately 11 km (temperature, 285 °C; effective confining stress, 177 MPa).

From (Watanabe, Numakura, et al., 2017).

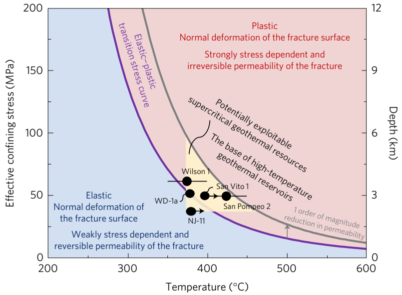
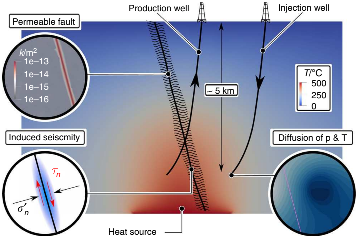
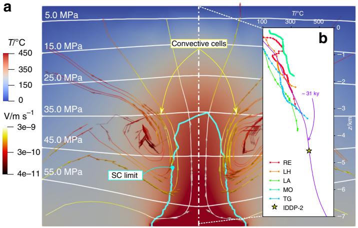


Figure 4 | Temperature and effective confining stress (depth) conditions for the base of high-temperature geothermal reservoirs, and potentially exploitable supercritical geothermal resources. Given that the elastic–plastic transition causes a gradual change from a higher-permeability regime to a lower-permeability regime in the crust, productive supercritical geothermal resources from 375 °C to approximately 460 °C may form at effective confining stresses of approximately 30–100 MPa or corresponding depths of approximately 2–6 km, depending on temperature, even if the rocks are nominally ductile.

From (Watanabe, Numakura, et al., 2017).

HIGHER: enhanced supercritical geothermal systems





nature COMMUNICATIONS

ARTICLE

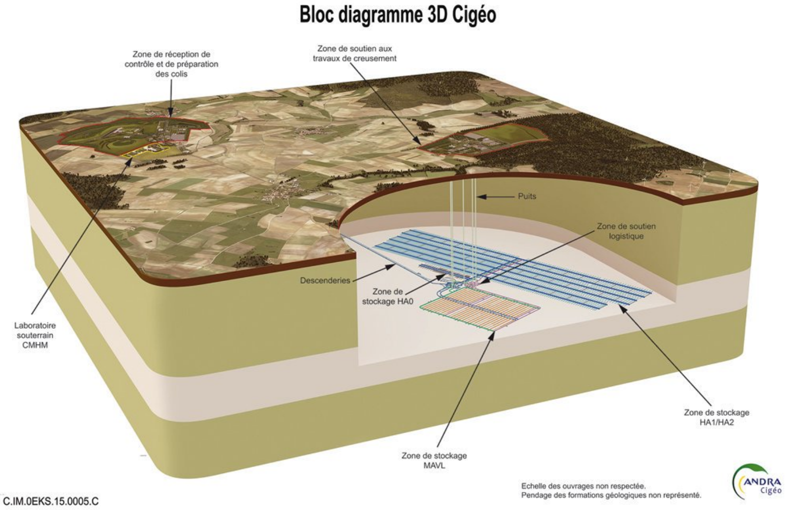
https://doi.org/10.1038/s41467-019-12146-0 OPEN

The risks of long-term re-injection in supercritical geothermal systems

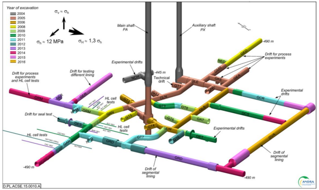
Francesco Parisio [1,2*], Victor Vilarrasa [3,4], Wenqing Wang[1], Olaf Kolditz[2,5] & Thomas Nagel [1,2]

- Induced seismicity due to THM effects (cooling, pressurization, stress redistribution)
- Cooling can trigger fault reactivation
- Around the injection well a combination of tensile and shear failure modes exists
- Pressure distributions change transiently due to phase change and viscosity change

Upscaling heater experiments in URL

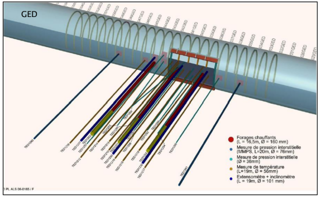


Upscaling heater experiments in URL

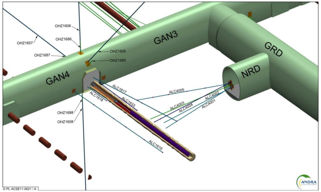


1 Meuse/Haute-Marne URL plan and principal stress directions.

Meuse/Haute Marne URL



Small-scale heater experiment (TED)



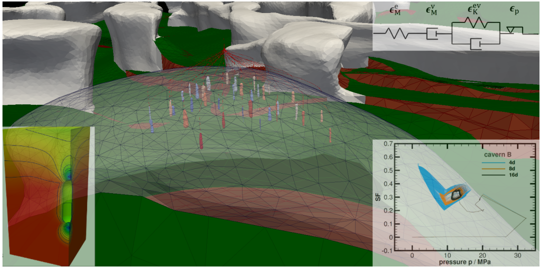
Real-scale heater experiment (ALC)

- THM-behaviour of Callovo-Oxfordian clay stone
- Interpretive and predictive modelling of URL experiments from small scale to repository scale
- Decovalex teams: ANDRA, Quintessa, LBNL, UFZ/BGR

DECOVALEX 2019

www.decovalex.org

Cyclic storage of hydrogen in rock salt caverns



Environ Earth Sci (2017)76:98
DOI 10.1007/s12665-017-6414-2

CrossMark

THEMATIC ISSUE

Thermo-mechanical investigation of salt caverns for short-term hydrogen storage

Norbert Böttcher[1,2] · Uwe-Jens Görke[2] · Olaf Kolditz[2,3] · Thomas Nagel[2,4]

Bundesministerium für Bildung und Forschung

ENERGIESPEICHER
Forschungsinitiative der Bundesregierung

- Salt caverns as utility-scale storage in renewable energy systems
- Gas thermodynamics
- Thermo-elasto-visco-plastic models (Minkley)
- extension to percolation: work in progress → H2UGS HYPOS

MFront, MGIS and OGS

Nested Newton iterations for constitutive updates in OGS (prior to MFront)

Global System—ith Netwon iteration

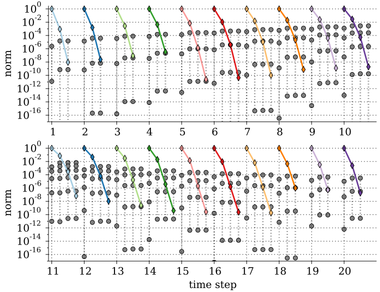
$$\int_\Omega \mathbf{B}^\mathrm{T} \boldsymbol{D}^i \mathbf{B} \,\mathrm{d}\Omega \, \Delta\hat{\boldsymbol{u}}^{i+1} = \int_{\partial\Omega} \mathbf{N}^\mathrm{T} \bar{\boldsymbol{t}}^{t+\Delta t} \mathrm{d}\Gamma - \int_\Omega \mathbf{B}^\mathrm{T} \boldsymbol{\sigma}^i \mathrm{d}\Omega$$

Local System—jth Netwon iteration

$\boldsymbol{\epsilon}^i$

$$\left.\frac{\partial \boldsymbol{r}}{\partial \boldsymbol{z}}\right|_j \Delta \boldsymbol{z}^{j+1} = -\boldsymbol{r}^j$$

$\boldsymbol{D}^i$, $\boldsymbol{\sigma}^i$



Ingredients:

- Eigen library
- Kelvin mapping for tensor quantities (Nagel et al., 2016)

Nested Newton iterations for constitutive updates in OGS (using MFront)

state at t_n: $\mathbf{z}_n = \left[\boldsymbol{\sigma}_n^{\mathrm{T}}, \boldsymbol{\kappa}_n^{\mathrm{T}}\right]^{\mathrm{T}}$
current strain estimate at t_{n+1}: $\boldsymbol{\epsilon}_i$

MGIS

Global Newton: equilibrium iterations

$$\int_\Omega \mathbf{B}^{\mathrm{T}} \mathbf{C}_i \mathbf{B}\, \mathrm{d}\Omega\, \Delta\hat{\mathbf{u}}_{i+1} = \int_{\partial\Omega_{\mathrm{N}}} \mathbf{N}^{\mathrm{T}} \bar{\mathbf{t}}\, \mathrm{d}\Gamma + \int_\Omega \mathbf{N}^{\mathrm{T}} \varrho \mathbf{b}\, \mathrm{d}\Omega - \int_\Omega \mathbf{B}^{\mathrm{T}} \boldsymbol{\sigma}_i\, \mathrm{d}\Omega$$

OpenGeoSys

Local Newton: state update

$$\left.\frac{\partial \mathbf{r}}{\partial \mathbf{z}}\right|_j \Delta\mathbf{z}_{j+1} = -\mathbf{r}(\boldsymbol{\epsilon}_i, \mathbf{z}_j)$$

MFront

MGIS

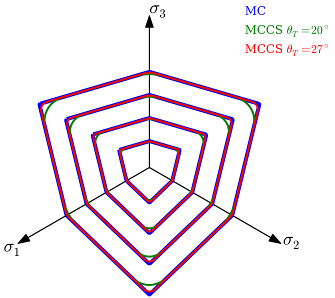
updated state and consistent tangent
at t_{n+1}: $\mathbf{z}_i = \left[\boldsymbol{\sigma}_i^{\mathrm{T}}, \boldsymbol{\kappa}_i^{\mathrm{T}}\right]^{\mathrm{T}}$, $\mathbf{C}_i$

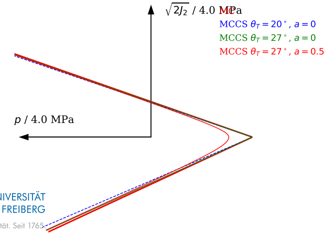
Advantages of using MFront

- syntax very close to equations
- little coding overhead
- easier to learn for engineers
- fewer coding errors
- testing outside of the FE environment with MTest and Python interface
- Availability of models
- Common interfaces, common language across platforms

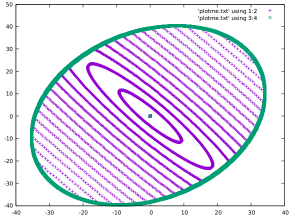
Implementations so far...

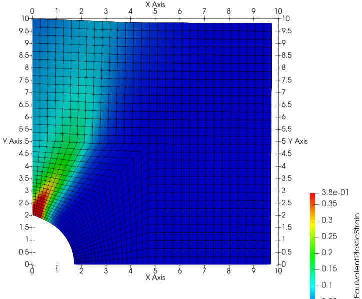
Mohr-Coulomb:



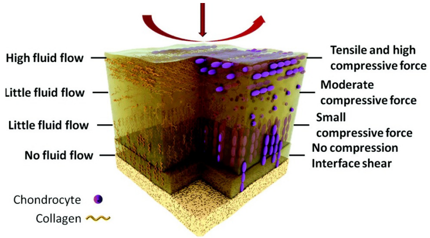


Anisotropic Drucker-Prager:



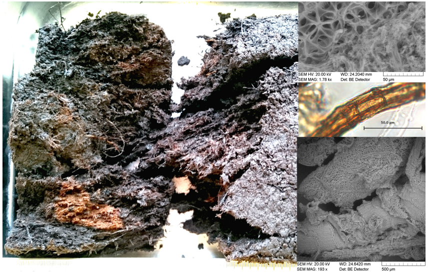


Two organic porous media: peat and articular cartilage



https://tinyurl.com/yczeanao (http://pubs.rsc.org)

- High water content
- Anisotropic (fibrous)
- Nonlinear rate-dependence
- Large deformation
- Multiple fluid compartments
- Swelling



- High water content
- Anisotropic (fibrous)
- Nonlinear rate-dependence
- Large deformation
- Multiple fluid compartments
- Equilibrium hysteresis (plasticity)

$\rightarrow$ Striking similarities motivate use of common model foundations and constitutive approaches. But ...

Typical features of granular geomaterials and constitutive formulations

- Elastic range can be very small
- Bulk moduli highly dependent on compaction
- High non-linearity already under very small strains (viz. small-strain stiffness)
- Initial stress state (not known very well) typically not associated with an initial (elastic) strain
- Dilatant and contractant flow
- Often negligible tensile strength
- Fluidization possible
- Typically multi-phase systems
- Constitutive response may depend on state variables of other processes[1] (T, χp_{cap}, c_{eq}, ...)

$\rightarrow$ Typical material categories: hyper(visco)plasticity, hypo(visco)plasticity

[1] Additional linearization components needed in case of monolithic coupling schemes.

Example: Hypoplasticity

General formulation:

$$\overset{\circ}{\boldsymbol{\sigma}} = f_\mathrm{s} \left(\boldsymbol{\mathcal{L}} : \mathbf{d} + f_\mathrm{d} \mathbf{N} \, \|\mathbf{d}\| \right)$$

with the constitutive tensors $\boldsymbol{\mathcal{L}}$ and $\mathbf{N}$ and the the barotropy and pyknotropy factors f_s and f_d.

A hypoplastic Cam-Clay model:[2]

$$\overset{\circ}{\boldsymbol{\sigma}} = f_\mathrm{s} \boldsymbol{\mathcal{L}} : \mathbf{d} - \left(\frac{p}{p_e^*} \right) \frac{M^2 + \eta^2}{M^2} \left(f_\mathrm{s} \boldsymbol{\mathcal{L}} + \frac{1}{\lambda^*} \boldsymbol{\sigma} \otimes \mathbf{1} \right) : \mathbf{n}_\mathrm{as} \, \|\mathbf{d}\|$$

with

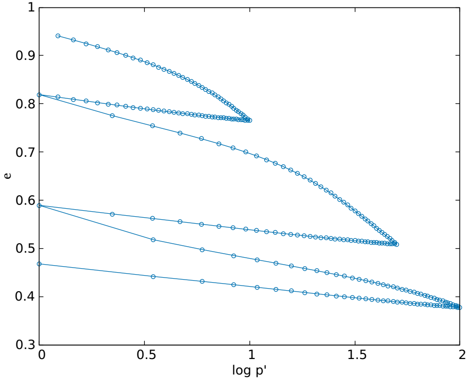
$$p_e^* = p_\mathrm{r} \exp \left[\frac{N - \ln(1+e)}{\lambda^*} \right] , \quad f_\mathrm{s} = \frac{3p}{2} \left(\frac{1}{\lambda^*} + \frac{1}{\kappa^*} \right) \frac{1 - 2\nu}{1 + \nu} , \quad \eta = \frac{q}{p}$$

$$\boldsymbol{\mathcal{L}} = \boldsymbol{\mathcal{I}} + \frac{\nu}{1 - 2\nu} \mathbf{1} \otimes \mathbf{1} , \quad \mathbf{n}_\mathrm{as} = \frac{3\boldsymbol{\sigma}^\mathrm{D} - {}^1\!/_3\, p(M^2 - \eta^2)}{\left\| 3\boldsymbol{\sigma}^\mathrm{D} - {}^1\!/_3\, p(M^2 - \eta^2) \right\|}$$

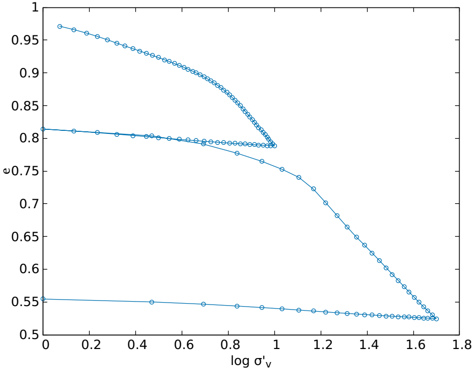
[2] Mašín, 2012

A hypoplastic Cam-Clay model (Mašín, 2012)

Isotropic consolidation

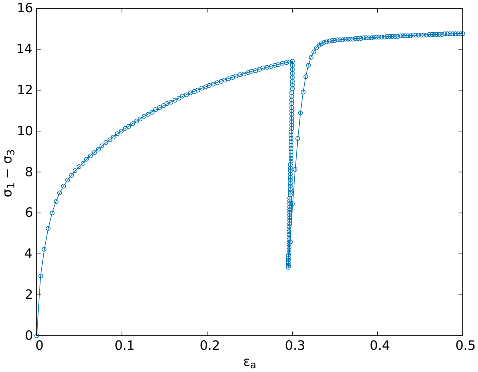


Oedometric compression

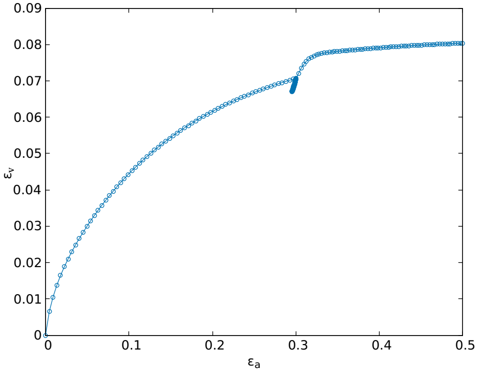


A hypoplastic Cam-Clay model (Mašín, 2012)

Triaxial compression, high e_0, low σ_3



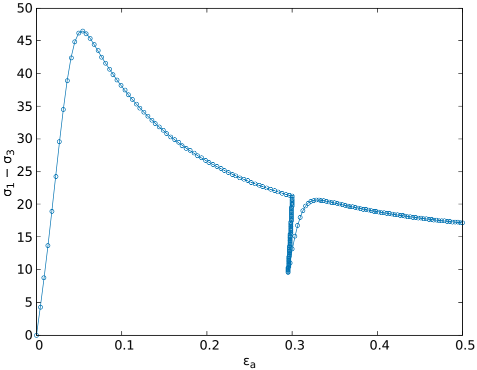
Triaxial compression, high e_0, low σ_3



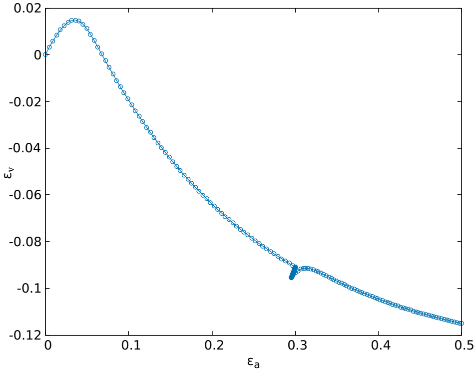
Next slide: effect of increase in initial density → pyknotropy

A hypoplastic Cam-Clay model (Mašín, 2012)

Triaxial compression, low e_0, low σ_3



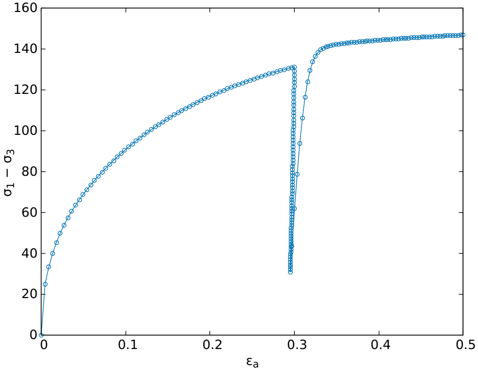
Triaxial compression, low e_0, low σ_3



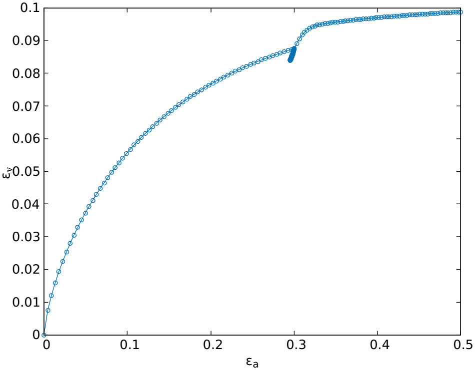
Next slide: effect of increase in confinement $\rightarrow$ barotropy

A hypoplastic Cam-Clay model (Mašín, 2012)

Triaxial compression, low e_0, high σ_3



Triaxial compression, low e_0, high σ_3



A promising alternative: Continuous Hyperplasticity

- smooth/continuous stress-strain behaviour
- internal functions instead of internal variables
- models based on two scalar potential functionals (thermodynamic consistency guaranteed) $\rightarrow$ model can in principle be built with automatic differentiation or using a symbolic differentiation tool (numerical differentiation used in (Puzrin, 2001))
- closer to standard elasto-plasticity with all the benefits in terms of physical interpretation
- Means of model classification according to potential dependencies and structure
- Transformation of existing hardening plasticity models possible (e.g. Modified Cam-Clay in Einav et al., 2003)
- Extension to multiphysics and rate-dependence likely to follow common routes (Likitlersuang and Houlsby, 2006)

Outlook

- Comparison to some native implementations
- MFront as standard implementation for solid models
- Functionalities use of external state variables in case of monolithic coupling would be required
- Integration of MFront into our lower-dimensional interface elements using `@DSL DefaultCZM` $\rightarrow$ constitutive models for faults
- Automatic differentiation following the provision of two scalar potentials?
- Simplified interface for hypoplasticity as another material class, maybe in collaboration with `soilmodels.info`

Thank you for your attention!

Special thanks to Thomas Helfer for idea, initiative and involvement!

References I

- Bilke, Lars, Bernd Flemisch, Thomas Kalbacher, Olaf Kolditz, Rainer Helmig, and Thomas Nagel (06/2019). "Development of Open-Source Porous Media Simulators: Principles and Experiences". In: *Transport in Porous Media* in press.
- Biot, Maurice A (1941). "General theory of three-dimensional consolidation". In: *Journal of applied physics* 12.2, pp. 155–164.
- Bowen, R.M. (1980). "Incompressible porous media models by use of the theory of mixtures". In: *International Journal of Engineering Science* 18, pp. 1129–1148.
- Coleman, B.D. and W. Noll (1963). "The thermodynamics of elastic materials with heat conduction and viscosity". In: *Archive for Rational Mechanics and Analysis* 13.1, pp. 167–178.
- Ehlers, W. (1989). "Poröse Medien: ein kontinuumsmechanisches Modell auf der Basis der Mischungstheorie". PhD thesis. Der Dekan des Fachbereichs 10 – Bauwesen der Universität-Gesamthochschule-Essen.
- Ehlers, Wolfgang and Joachim Bluhm (2002). *Porous media: theory, experiments and numerical applications*. Springer Science & Business Media.
- Einav, I, A.M. Puzrin, and G.T. Houlsby (03/2003). "Continuous hyperplastic models for overconsolidated clays". In: *Mathematical and Computer Modelling* 37.5-6, pp. 515–523.
- Fillunger, Paul (1936). *Erdbaumechanik?* Selbstverl. d. Verf.

References II

- Hutter, K (1977). "The foundations of thermodynamics, its basic postulates and implications. A review of modern thermodynamics". In: *Acta Mechanica* 27.1-4, pp. 1–54.
- Hutter, Kolumban and Klaus Jöhnk (2004). *Continuum methods of physical modeling: continuum mechanics, dimensional analysis, turbulence*. Springer.
- Kögler, Franz and Alfred Scheidig (1938). *Baugrund und Bauwerk*. Ernst & Sohn.
- Likitlersuang, S. and G. T. Houlsby (03/2006). "Development of hyperplasticity models for soil mechanics". In: *International Journal for Numerical and Analytical Methods in Geomechanics* 30.3, pp. 229–254.
- Liu, I-Shih and Ingo Müller (1984). "Thermodynamics of mixtures of fluids". In: *Rational thermodynamics*. Springer, pp. 264–285.
- Mašín, D. (06/2012). "Hypoplastic Cam-clay model". In: *Géotechnique* 62.6, pp. 549–553.
- Mow, V. C., S. C. Kuei, W. M. Lai, and C. G. Armstrong (02/1980). "Biphasic creep and stress relaxation of articular cartilage in compression? Theory and experiments.". In: *J Biomech Eng* 102.1, pp. 73–84.
- Müller, Ingo (1968). "A thermodynamic theory of mixtures of fluids". In: *Archive for Rational Mechanics and Analysis* 28.1, pp. 1–39.
- Müller, Ingo and Tommaso Ruggeri (2013). *Rational extended thermodynamics*. Vol. 37. Springer Science & Business Media.

References III

- Nagel, Thomas, Uwe-Jens Görke, Kevin M. Moerman, and Olaf Kolditz (2016). "On advantages of the Kelvin mapping in finite element implementations of deformation processes". In: *Environmental Earth Sciences* 75.11, pp. 1–11.
- Puzrin, A (08/2001). "A thermomechanical framework for rate-independent dissipative materials with internal functions". In: *International Journal of Plasticity* 17.8, pp. 1147–1165.
- Skempton, AW (1960). "Terzaghi's discovery of effective stress". In: *From Theory to Practice in Soil Mechanics: Selections from the Writings of Karl Terzaghi*, pp. 42–53.
- Terzaghi, Karl and Otto Karl Fröhlich (1936). *Theorie der Setzung von Tonschichten: eine Einführung in die analytische Tonmechanik*. Franz Deuticke.
- Truesdell, C and W Noll (1965). *Handbuch der Physik, Band III/3. Die Nicht-Linearen Feldtheorien der Mechanik*. Springer-Verlag. Chap. Die Nicht-Linearen Feldtheorien der Mechanik.
- Truesdell, Clifford (2012). *Rational thermodynamics*. Springer Science & Business Media.
- Watanabe, Noriaki, Motoki Egawa, Kiyotoshi Sakaguchi, Takuya Ishibashi, and Noriyoshi Tsuchiya (06/2017). "Hydraulic fracturing and permeability enhancement in granite from subcritical/brittle to supercritical/ductile conditions". In: *Geophysical Research Letters* 44.11, pp. 5468–5475.
- Watanabe, Noriaki, Tatsuya Numakura, Kiyotoshi Sakaguchi, Hanae Saishu, Atsushi Okamoto, Steven E. Ingebritsen, and Noriyoshi Tsuchiya (2017). "Potentially exploitable supercritical geothermal resources in the ductile crust". In: *Nature Geoscience* January, pp. 1–6.

References IV

Woods, L. C. (1982). “Thermodynamic Inequalities in Continuum Mechanics”. In: *IMA Journal of Applied Mathematics* 29.3, pp. 221–246. eprint: http://imamat.oxfordjournals.org/content/29/3/221.full.pdf+html.

THM-coupled model

- Thermal process (T): advective and conductive heat transfer

$$(\varrho c_p)^{\text{eff}} \frac{\mathrm{d}_\mathrm{S} T}{\mathrm{d}t} + \phi_\mathrm{F} \varrho_\mathrm{FR} c_{p\mathrm{F}} \,\mathrm{grad}\, T \cdot \mathbf{w}_\mathrm{FS} - \mathrm{div}\left[\boldsymbol{\lambda}^{\text{eff}} \,\mathrm{grad}\, T\right] = Q_T$$

- Hydraulic process (H): pore pressure change due to thermal expansion and volume strain change in fully saturated conditions for compressible constituents

$$\left(\phi_\mathrm{F}\beta_{p\mathrm{F}} + \frac{\alpha_\mathrm{B} - \phi_\mathrm{F}}{K_\mathrm{SR}}\right)\frac{\mathrm{d}_\mathrm{S} p}{\mathrm{d}t} - \left[\phi_\mathrm{F}\beta_{T\mathrm{F}} + 3(1-\phi_\mathrm{F})\alpha_{T\mathrm{S}}\right]\frac{\mathrm{d}_\mathrm{S} T}{\mathrm{d}t} + \alpha_\mathrm{B}\,\mathrm{div}\,\mathbf{u}'_\mathrm{S} + \mathrm{div}\,\phi_\mathrm{F}\mathbf{w}_\mathrm{FS} = Q_H$$

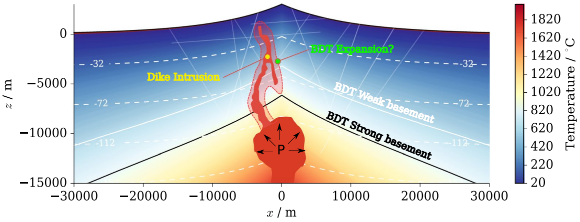
- Mechanical process (M): stress redistribution due to thermal expansion and pore pressure redistribution

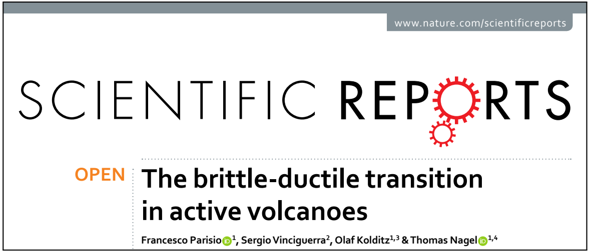
$$\mathrm{div}\left[\boldsymbol{\sigma}_\mathrm{S}^\mathrm{E} - \alpha_\mathrm{B} p\mathbf{I}\right] + \varrho^{\text{eff}}\mathbf{g} = \mathbf{0} \quad \text{with} \quad \boldsymbol{\sigma}_\mathrm{S}^\mathrm{E} = \boldsymbol{\mathcal{C}} : (\boldsymbol{\epsilon} - \boldsymbol{\alpha}_{T\mathrm{S}}\Delta T\mathbf{I})$$

with $\phi_\mathrm{F}\mathbf{w}_\mathrm{FS}$ the seepage velocity defined by Darcy's law

$$\phi_\mathrm{F}\mathbf{w}_\mathrm{FS} = -\frac{\mathbf{k}_\mathrm{F}}{\mu_\mathrm{FR}}\left[\mathrm{grad}\, p - \varrho_\mathrm{FR}\mathbf{g}\right]$$

GEMex: enhanced supercritical geothermal reservoirs





www.nature.com/scientificreports

SCIENTIFIC REPORTS

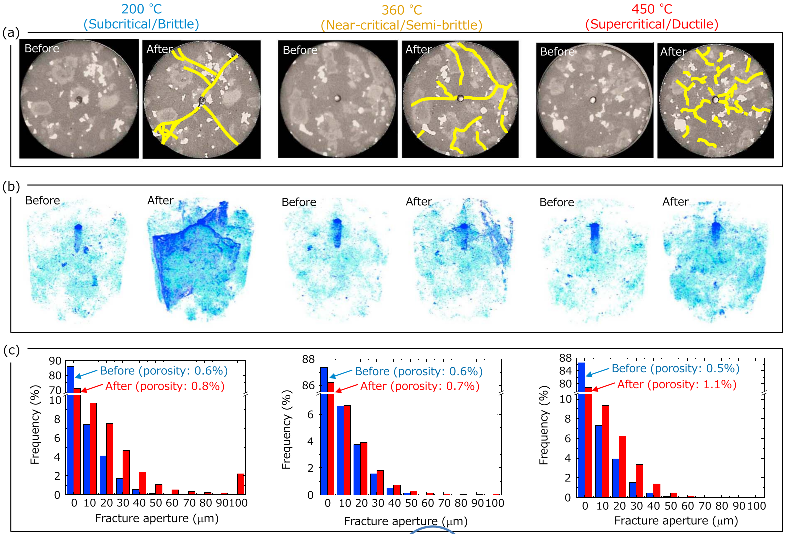
OPEN

The brittle-ductile transition in active volcanoes

Francesco Parisio[1], Sergio Vinciguerra[2], Olaf Kolditz[1,3] & Thomas Nagel[1,4]

- BDT in volcanic regions with dilatancy as indicator
- Context: Super-hot geothermal systems with high enthalpy
- Supercritical fluids (water: $T_{cr} = 374\,^\circ\mathrm{C}$, $p_{cr} = 22.1\,\mathrm{MPa}$, brittle-to-ductile failure modes
- Are these systems exploitable? Can they be enhanced? What role do solid and fluid rheology play?
- $\rightarrow$ continuation in DFG-JSPS project

HIGHER: enhanced supercritical geothermal systems



From Watanabe, Egawa et al., 2017.

HIGHER: enhanced supercritical geothermal systems

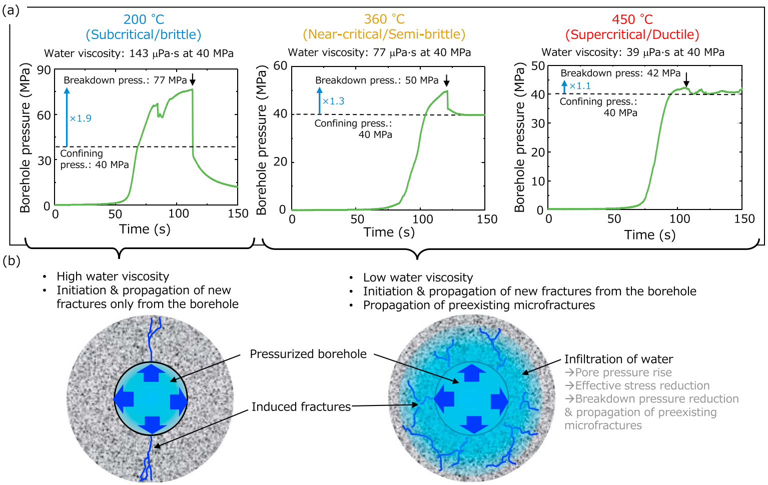


Figure 4. (a) Changes in borehole pressure with time during the experiments, suggesting (b) two types of fracturing mechanisms.

From Watanabe, Egawa, et al., 20 $p_{frac} = 2p_{conf} + \sigma_t - p$.

About InterPore

INTERPORE

International Society for Porous Media

non-profit independent scientific organization for all porous media researchers from academia and industry
www.interpore.org

Since **2008**

Who we are

InterPore is a **non-profit, independent** scientific organization established in 2008.

InterPore aims to **advance** and **disseminate knowledge** for the understanding, description and modeling of natural and industrial porous media systems.

Our topics

Porous media

- **Manufactured**
- **Geological**
- **Biological**

INTERPORE

Disciplines

Applied Mathematics
Biological and Medical Sciences
Engineering
Petroleum Science
Materials Sciences
Physics
Geosciences
Chemistry

What we aim

- facilitate collaboration between industry and academia
- bring together porous media theoreticians, modellers, and experimentalists
- provide a forum for exchanging ideas and expertise for the improvement of porous media models
- identify research questions that will lead to major improvements in the theories and models of complex porous media and to define modelling challenges
- play a role in setting up strategic research priorities of major funding agencies on national and European levels
- identify sources of funding for collaborative research among partners and facilitate the establishment of collaborative research projects
- facilitate training and education

Scope of Activities

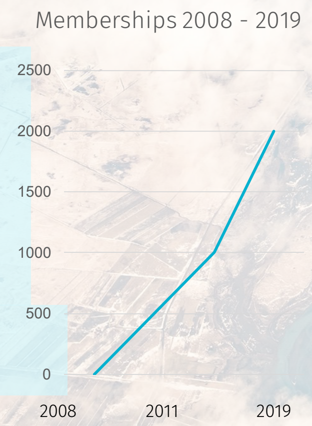
Setting up and maintaining a **website** where news, lists, and documents can be shared among members of the Society and the general porous media community

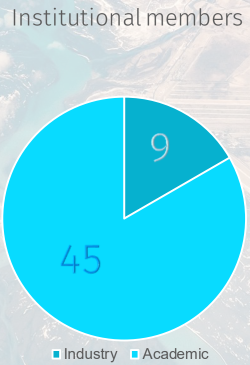
Organizing an **Annual Conference** on porous media as well as annual business meeting

Support national chapters all over the world

Offer various awards to porous media researchers

Facts and Figures





All over the world
in 16 countries

INTERPORE Foundation

InterPore Foundation for Porous Media Science and Technology

Since 2016

Mission

- Supporting educational and outreach activities of InterPore
- Honouring distinguished researchers and lecturers
- Sponsoring InterPore conference grants

www.interpore.org/foundation

Contact us

President

Laura Pyrak-Nolte
ljpn@purdue.edu

Managing Director

S. Majid Hassanizadeh
S.M.Hassanizadeh@uu.nl

Executive Officer

Karolin Weber
karolin.weber@interpore.org

Join us

At the next annual conference

Or become part of it!

INTERPORE

International Society for Porous Media

www.interpore.org

InterPore2020 in Qingdao

INTERPORE

International Society for Porous Media

12th International Conference on Porous Media & Annual Meeting

25-28 May 2020 – Qingdao, China

Join us in Qindao!

The scientific program is covering porous media subjects from **pore-scale modeling**, **pore-scale imaging**, to **experimental** and **numerical methods**, to **sensitivity and uncertainty analysis**.

Presentations of all kind of porous media processes in very diverse applications such as **geological reservoirs**, **soil**, **food**, **wood**, **biological tissues**, **filters**, **membranes**, **paper and textiles** and many more, will be given.

High-quality and lively poster presentation, sessions and exhibitions.

Qingdao, chosen as one of the **most livable** cities in China, is a very international **port city at the yellow sea**. Best known for Tsingtao Beer and international festivals which promote **friendship**, **economic & cultural exchanges** between China and others all over the world.

More than 90% of last years participants have recommended attending InterPore meetings

www.interpore.org/qingdao

conference2020@interpore.org

Plenary and invited lectures InterPore 2019

Plenary speakers:

Dominik Obrist, University of Bern, TBA

Qinjun Kang, Los Alamos National Lab; Pore-scale direct numerical simulation of flow and transport in energy and environment

Thomas Ramstadt, Principal Researcher Reservoir Technology, Trondheim; Developing a digital workflow for analysis of flow in porous media: Research on transport phenomena from pore to field scale for reservoir engineering applications

Invited speakers:

Bernd Flemisch, University of Stuttgart; Modelling flow and transport processes in complex porous media

Sylvie Lorthols, IMF Toulouse; Modeling of blood flow in complex tissue systems

James McClure, Virginia Polytechnic Institute and State University; Topology and its effects on fluid flow

Fred Vermolen, TU Delft; Research on modelling the brain as a porous medium and using effects of vibrations from heart beat on the brain for an early diagnosis of brain diseases

Olga Vizika, IFPEN; Experimental investigation and modeling of the effect of microstructure and heterogeneities at different scales on the displacement mechanisms and macroscopic flow properties of sandstones and carbonates

Martin Vohralík, Inria Paris; A posteriori error estimates and adaptive solvers for porous media flows

Moran Wang, Tsinghua University; Electrokinetic and ion transport in micro / nanoporous media

Guang Yang, Shanghai Jiao Tong University; Coupling free flow and porous-media flow, applications to aerospace and mechanical engineering