GeomInt: Geomechanical integrity of host and barrier rocks—experiments, models and analysis of discontinuities

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Abstract

The present paper gives an overview of the GeomInt project “Geomechanical integrity of host and barrier rocks—experiment, modelling and analysis of discontinuities” which has been conducted from 2017–2020 within the framework of the “Geo:N Geosciences for Sustainability” program. The research concept of the collaborative project is briefly introduced followed by a summary of the most important outcomes. The research concept puts geological discontinuities into the centre of investigations—as these belong to the most interesting and critical elements for any subsurface utilisation. Thus, while research questions are specific, they bear relevance to a wide range of applications. The specific research is thus integrated into a generic concept in order to make the results more generally applicable and transferable. The generic part includes a variety of conceptual approaches and their numerical realisations for describing the evolution of discontinuities in the most important types of barrier rocks. An explicit validation concept for the generic framework was developed and realised by specific “model-experiment-exercises” (MEX) which combined experiments and models in a systematic way from the very beginning. 16 MEX have been developed which cover a wide range of fundamental fracturing mechanisms, i.e. swelling/shrinkage, fluid percolation, and stress redistribution processes. The progress in model development is also demonstrated by field-scale applications, e.g. in the analysis and design of experiments in underground research laboratories in Opalinus Clay (URL Mont Terri, Switzerland) and salt rock (research mine Springen, Germany).

Keywords GeomInt · Fracture flow · Fracture mechanics · Barrier integrity · Discontinuities · Open source · OpenGeoSys

Introduction

The use of the subsurface as a source of resources, a storage space and for installing underground municipal or traffic infrastructure has increased both in intensity and diversity in recent years Volchko et al. (2020). In addition to classical anthropogenic interventions such as mining, oil and gas production or tunnel construction, other forms of underground use have come into the focus of economic, political and scientific activities, particularly in connection with the transformation of energy systems and a global trend to urbanization McCartney et al. (2016). These include, for example, the extraction of energy (e.g. geothermal energy) and energy sources using new technologies (e.g. unconventional gas extraction) Field et al. (2018) as well as the geological short-term and long-term storage of energy carriers such as compressed air, hydrogen, and methane Kabuth et al. (2017); Bauer et al. (2012) and the safe storage of waste.
generated during energy production or in other industrial sectors, e.g. carbon dioxide, radioactive waste, or chemotoxic waste Hudson et al. (2001); Gens (2010); Birkholzer et al. (2019); Ringrose and Meckel (2019).

The rocks and rock mass themselves are characterised by complex material behaviour. Irreversible deformation, rate-dependence, swelling and shrinkage effects occur under real loading conditions. Damping aspects, for example in the range of low-frequency seismic waves, damage and physical-chemical ageing (e.g. solution and/or precipitation reactions) play an important role in many geotechnical applications and have their roots in the multiphase nature of geomaterials Buscarnera (2012); Steeb et al. (2014); Loret et al. (2002). One common theme in the deformation behaviour of geomaterials is localization leading to structural features such as shear bands, compaction bands, unloading fractures. The formation, presence and evolution of these features can quickly dominate the system evolution and is implicated in most geological processes such as tectonics, orogenesis, hydrothermal systems, etc. Hobbs et al. (1990); Jirásek (2007); Duretz et al. (2018); Döhmann et al. (2019); Parisio et al. (2019). Despite their importance, the topics of damage, crack formation and propagation as well as interface problems are aspects that require further clarification from a scientific perspective. Because of prevailing knowledge gaps in these areas, many such processes can currently not be adequately modelled with numerical simulation systems established in geotechnical practice and therefore represent topics in urgent need of research. The corresponding processes manifest themselves in diverse micro- and macro-mechanical phenomena in the considered materials and are here summarised under the umbrella term **discontinuities** (Fig. 1).

Geological systems in their natural state feature a range of discontinuities which, from a modelling perspective, can be loosely categorised into weak discontinuities, such as material interfaces, and strong discontinuities, such as fractures Armero and Garikipati (1996); Hansbo and Hansbo (2004). These existing discontinuities determine the in-situ stress-state as well as hydrothermal flow fields encountered when attempting to establish a particular geotechnology at a given site. Such anthropogenic intervention locally disturbs the quasi-steady state of the system and shifts it further away from equilibrium, thus triggering a range of multi-physical processes. These thermo-hydro-mechanical-chemical-microbiological (THMCB) processes can in turn trigger the formation of new discontinuities in the form of stress fractures, hydraulic fractures, quenching fractures or chemical wormholes Regenauer-Lieb et al. (2013); Liu et al. (2019). From the perspectives of operational and environmental safety, several consequences are of interest, such as induced seismicity due to the formation of new fractures or

**Fig. 1** Graphical abstract of the GeomInt project: geological reservoir-barrier systems and geomechanical integrity. The formation of new discontinuities and their connectivity to existing fracture networks can dominate system evolution and needs to be thoroughly understood.
the reactivation of existing faults Guglielmi et al. (2015); Ucar et al. (2017); Chang and Segall (2016); Parisio et al. (2019). Very often the creation of new fluid pathways and of connectivity to existing fractures or fracture networks is of primary importance: it is desired in fossil or geothermal resource extraction and to be avoided in hazardous waste disposal applications Quintal et al. (2014); Armand et al. (2014); Lei et al. (2017). However, in all applications the formation of new discontinuities has to occur in a controlled manner within a data-poor environment. Therefore, a sound theoretical understanding of the evolution of discontinuities is required for virtually all geotechnologies (Fig. 1). The aim of the GeomInt project is to contribute to this knowledge base and its transfer to practical engineering.

GeomInt is dealing with specific research questions concerning the evolution of discontinuities:

- Swelling and shrinkage processes in clay rocks are related to the key question of barrier integrity under changing moisture conditions. To what degree can the low permeability of clay rock be maintained under desaturation-induced shrinkage during the heating process and can it be fully re-established by swelling processes upon subsequent resaturation? (see work package WP1)
- Fluid percolation processes have been studied in both clay and salt rocks. How does fluid percolation depend on the surrounding stress regimes? How can the related threshold be defined for both rock types? How can the evolution of the discontinuities be described effectively in the presence of initial stress effects? (see work package WP2)
- Stress redistribution is a fundamental mechanism of fracture initiation in brittle rocks. How will cyclic loading of rock fractures influence the evolution of fracture permeability? (see work package WP3)

but also more general questions concerning the transferability of experimental and numerical methods for various rock types:

- How to determine anisotropic and lamination effects in different clay rocks, i.e. from sandy and clayey facies (see “Experimental platform”)?
- How to compare and combine different conceptual (continuum and discontinuum) and numerical approaches (lattice, finite and distinct elements) for accurate description of discontinuity evolution in various brittle and ductile rock types (see “Numerical platform”)?
- How to combine experimental and modelling approaches in an optimal way to build cross-scale approaches for the analyses of discontinuity propagation (see Model-Experiment (MEX) concept)?
WP3 is investigating discontinuities formed by and subjected to stress redistribution in brittle materials. Stress redistribution constitutes a fundamental fracturing mechanism that is also closely linked to the processes studied in WPs 1 and 2, where the multiphysical couplings are stronger McDermott et al. (2018); Parisio et al. (2019).

Granite rock samples are obtained from locations in the Ore Mountains, i.e. from Kirchberg and Freiberg (URL Reiche Zeche). Experimental investigations are conducted in the Freiberg (TU Freiberg) and Stuttgart labs (University of Stuttgart). Constant Normal Load (CNL) and Constant Normal Stiffness (CNS) experiments are conducted to study fluid flow in rough fractures under confining stresses. Rock samples from Freiberg will be also used within the “Crystalline Task” of the new DECOVALEX-2023 phase.

For building strong links between the above described work packages, laboratory work (LAB), modelling (MOD) and in-situ experiments (URL for Underground Research Laboratories) are clustered (Fig. 2 upper right). Experimental and modelling platforms have been established during project in order to foster collaboration between the rock type oriented groups (see sections “Experimental platform” and “Numerical platform”, respectively). The clear structure of the GeomInt project is part of its specific research methodology. The process-oriented work packages are interlinked at methodological levels (lower left) and GeomInt is using Virtual Reality (VR) methods for data and model integration (lower right)

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GeomInt relies on a very close link between experimental and modelling works. To this purpose 16 Model-Experiment-Exercises (MEX) have been defined at the beginning of the project (see section “Model-Experiment-Exercises (MEX)”). Within these exercises various numerical methods have been applied to same experimental data sets in order to determine advantages / disadvantages of particular numerical methods (see section “In-situ experiments (URL)”) and e.g. for experimental design of the CD-A experiment in Mont Terri (see section “Synthesis–Numerical methods capabilities”).

To link the laboratory experiments to the in-situ experiments and related applications of current interest, samples for the lab work are taken from the URLs. Figure 3 illustrates the geographical WP workflows from in-situ sampling to geomechanical laboratories and modelling. The main sources for rock samples are (i) Mont Terri for clay (ii) Springen for salt and (iii) Freiberg/Kirchberg for crystalline rock specimens. Moreover, there is collaboration with other URLs (Bure, Grimsel) concerning experimental and modelling work—mainly for testing transferability of the methodology to other rock types (e.g. Callovo-Oxfordian Clay—COx).
Experimental platform

For the coordinated experimental analysis of the THM properties and behaviour of clay, salt and crystalline rocks an experimental platform has been established within GeomInt, which comprises both laboratory (LAB) and in-situ test in Underground Research Laboratories (URL) (Fig. 2). After a brief introduction of the experimental platform of GeomInt (section “Laboratory experiments (LAB)” one laboratory research result is highlighted (section “LAB highlight: Anisotropy of clay rocks”).

Laboratory experiments (LAB)

The laboratory facilities of the project partners were used for the characterisation of rock samples from clay, salt, and crystalline for the description of discontinuities under various loads (THM conditions) and at various spatial scales. Specimens have been gathered from various URLs such as Mt. Terri, Springen and from the Ore Mountains (see Fig. 3) to cover the required barrier rock types. Newly accessible samples have been tested, e.g. from core drilling campaigns in the sandy facies of the Opalinus Clay in the Mont Terri URL.

The experimental work on the various rock types by the project partners has been distributed in principle as follows:

- CAU\(^1\): investigated Opalinus Clay from the URL Mont Terri (sandy and shaley facies). The rock specimens were sampled and provided by BGR\(^2\)
- IFG\(^3\): contributed their long-term experience salt mechanics and investigated salt rock from the Springen salt mine.
- TUBAF\(^4\): studied fracture behaviour of crystalline rock samples from the Kirchberg mine.
- UoS\(^5\): used their µXRCT facility for the structural characterisation of crystalline rocks.

The following types of laboratory experiments have been conducted with the aim of obtaining basic material parameters on the one hand and of increasing the understanding of more complex multiphysical phenomena on the other:

- three-point bending tests
- Brazilian tests
- conventional triaxial deformation tests
- shrinkage and swelling behaviour of Opalinus Clay under free and in-situ stress conditions
- fluid-driven percolation in clay and salt using either gas or brine
- cyclic (mechanical, hydraulic) percolation tests to study healing and sealing effects
- direct shear tests, mechanical and hydraulic fracture properties under normal and shear load conditions
- cyclic tests to study the evolution of fracture properties

Figure 4 illustrates an overview of the experimental facilities of the LAB platform. The results of the experimental investigations are published in a series of papers Rizvi et al. (2019); Vowinckel et al. (2020); Frühwirt et al. (2021); Sattari et al. (2020) and a book publication Kolditz et al. (2021). Here, a general selection is presented:

- characterisation of rock properties, e.g. fracture toughness, splitting strength, mechanical and thermal properties under various loading conditions (THM),
- influence of embedded layering on material strength, deformation behaviour and fracture propagation
- influence of anisotropy on shrinkage and swelling effects,
- fluid-driven (gas and brine) percolation in clay and salt and its impact on permeability changes.

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\(^4\) Technische Universität Bergakademie Freiberg.
\(^5\) University of Stuttgart.
Fig. 4 Experimental facilities of the LAB platform for the mechanical characterisation barrier rocks (clay, crystalline, and salt rocks): (second row) THM Laboratory Tests - e.g. mechanical properties of all rock types; (third row) Shrinkage and Swelling Tests for clay rocks; Percolation Tests for salt rocks; (lower row) Stress Redistribution Tests: Dynamic big shear box device at TU Freiberg (left: Overview of apparatus; mid: Preparation of sample for shear test, right: Shear box with displacement transducers ready for testing)
LAB highlight: Anisotropy of clay rocks

The published data for Opalinus Clay rock indicate a strong dependence of its thermo-hydro-mechanical properties on sample heterogeneity and inherent anisotropy Sarout et al. (2014); Favero et al. (2018); Minardi et al. (2016). The embedded layering orientation in these sedimentary rocks results in a high anisotropy factor along the material’s principal axes. Therefore, based on fluid percolation tests conducted on cubic clay samples, the dependency of fracture openings on the imposed stress state as well as sample orientation were investigated (Fig. 5a). A similar approach has been followed for salt rock samples by Kamlot (2009). A true triaxial device is used to apply and control the principal stresses along the axes. Pressurised oil using a syringe pump is used to perform the hydraulic fracturing. The experiments are conducted under two main boundary conditions: the direction of the applied borehole pressure perpendicular or parallel to the embedded layering orientations. In both cases the layering orientation controls the fracking paths and flow surfaces.

The inherent anisotropy in Opalinus Clay rocks also affects the material response during the wetting and drying processes Minardi et al. (2016). Thin-section samples were prepared and placed inside a desiccator under different total suction values (Fig. 5b). The suction applied by means of saturated salt solutions ranged from 3.2 up to 367.5 MPa, which results in shrinkage and swelling of the samples. One sample was used to determine the surface linear strains along two different orientations, one parallel to the embedded layering orientation and the other one perpendicular to it. A second sample was used to determine the weight change during the entire process. The room temperature was kept constant around 20 °C during the test period. Equilibrium inside the desiccator is defined once the weight change of the sample during three consecutive readings equalled zero, where tolerance is set to be 1%. Along a drying path, the results indicate higher strains perpendicular to the embedded layers. When the suction exceeded 150 MPa, the strains in the perpendicular direction were almost 4.5 times larger than those parallel to the bedding. Similar behaviour was also observed by Minardi et al. (2016), however, the conducted experiment here was extended to cover a wider range of suction values. Previous results from Minardi et al. (2016) were limited to a suction range of 9.8 up to 139 MPa and did not provide results for air-entry pressure values. Interestingly, along the wetting path, the differences between the strain gauges were much less pronounced. According to the water content data, the air-entry pressure for a sandy Opalinus Clay was found to be around 25 MPa.

In-situ experiments (URL)

The in-situ part of the experimental work is formed by the collaborating underground research labs (URLs) from which the sample material was obtained and distributed according to the defined workflow (Fig. 3) for use in the laboratory experiments described above. As an example, Opalinus Clay samples have been provided from the AD experiment in Mt. Terri for fluid percolation experiments and simulations Bossart et al. (2017). In addition, several in-situ experiments have been analysed within the GeomInt project such as the CD experiment in Mont Terri Ziefle et al. (2019) or the large wellbore test in Springen Nest and Naumann (2020).

These analyses were possible due to links to related projects in which the partners of the present consortium were involved, such as the Mt. Terri and DECOVALEX projects as well as the Geo:N project StimTec Schmidt et al. (2020).

URL highlight: In-situ experiments in Mont Terri

The Mont Terri rock laboratory provides unique direct access to the Middle Jurassic Opalinus Clay formation in the Swiss Jura Mountain Belt. It branches off from the security gallery of the motorway tunnel near the town of St. Ursanne (NW Switzerland). Depending on the topography, it lies at 230 m to 320 m depth below ground Heitzmann and Bossart (2001). The Opalinus Clay in the rock laboratory offers a thickness of about 130 m Hostettler et al. (2018), the sedimentary bedding plane is dipping with about 40° towards SE. Within the Mont Terri project, 21 institutions from nine
countries are currently investigating the Opalinus Clay as a potential host rock for the storage of nuclear waste. Since 1996, a total of 1400 m of galleries and niches have been excavated in the Mont Terri rock laboratory (Fig. 17a) and more than 140 experiments have been carried out. Almost 50 of them are still running Bossart and Milnes (2018). Some of them are noteworthy within the context of the GeomInt-Project.

Serving the need for core samples for the GeomInt laboratory investigation program, the AD-experiment has been initiated. Therein, two fully cored boreholes with a diameter of 131 mm were drilled parallel and perpendicular to the sedimentary bedding, respectively. The 15.35 m long horizontal borehole is located entirely in the lower sandy facies. The second borehole is oriented perpendicular to the bedding (with a dip of 43°), thus crossing the upper shaly, lower sandy, carbonate-rich sandy-facies and lower shaly facies of the Opalinus Clay. The cores have been geologically characterised Galletti and Jaeggi (2019) and analysed by thin section-microscopy and mineralogical-geochemical techniques Kneuker and Furche (2021). Furthermore, geophysical in-situ-borehole-measurements have been conducted Furche (2020). These analysis bring out that the Opalinus Clay is characterised by a high intrafacies variability perpendicular to bedding, especially for the sandy and carbonate-rich parts, but a low variability parallel to bedding, except for the carbonate-rich sandy facies Kneuker et al. (2020); Kneuker and Furche (2021).

The Model-Experiment-Exercise MEX 1-4 is based on the CD/LP experiment, which investigates the long-term cyclic deformation (CD) in a niche of the rock laboratory, as depicted in Fig. 6. The related long-term coupled hydro-mechanically effects are characterised by the interaction of various effects like the redistribution of stresses due to the excavation, swelling and shrinkage of the host rock, related changes of material parameters, as well as plastic and viscous effects. Within the GeomInt project these effects have been modelled with a fully coupled hydro-mechanically approach showing consistent results. Nevertheless, the complex interaction of these effects is not yet fully understood and is subject of the follow-up experiment CD-A and the GeomInt II project. The Fault Slip (FS) experiment addresses the fault reactivation due to pressure-induced percolation in a low-permeability, large-scale discontinuity in the Mont Terri rock laboratory. Within the GeomInt project it was shown that the implemented hydro-mechanically coupled model approach, using the Lower-Interface-Element (LIE)-method, is principally capable to reproduce the measured evolution of the deformation at the fault and the injected water volume.

URL highlight: In-situ experiments in the salt mine Kalibergwerk Springen/Merkers

The large-scale test site Merkers benefits from the unique mining situation in the bedded salt mass of the Werra salt formation (z1, Zechstein sequence) where two potash seams were mined in a room-and-pillar system at 275 m (1st floor, potash seam “Hessen”, z1KH) and 360 m (2nd floor, potash seam “Thüringen”, z1KTh) depth, respectively. The evaporite rocks of the Zechstein formation were laid down during the Permian period around 250 million years ago. The intact mineral deposit was locally disturbed between 14 and 25 million years ago by tertiary volcanism, leading to the mutation of some potash salts to sylvinate, and the creation of pockets of CO₂ under high pressure.

The in-situ tests for pressure-driven percolation are conducted between the two potash seams in the very homogeneous Middle Werra rocksalt (z1Na). It consists mostly of very pure halite layers intersected by thin anhydrite lines or bands of rock salt with finely distributed anhydrite accessories indicating the sedimentary bedding.

Because the test results depend mainly on the acting stress field, i.e. the minimum principal stress distribution in the rock mass around the test area, it has been measured and characterised by hydro-frac measurements, and is thus well-known. The minimal stresses in the contour increase with progressive distance from the underground openings until reaching a constant value at a depth of around 15 m. The measured value of an undisturbed stress state of around 8 MPa corresponds fairly well to calculated lithostatic stresses of 7.8 to 8.8 MPa.

The in-situ tests for pressure-driven percolation in the salt mine Kalibergwerk Springen/Merkers
For monitoring of micro-seismic events, e.g. due to creation of an excavated damage zone around underground openings or fluid flow-driven damage, a highly sensitive acoustic emission (AE) network was installed in observation boreholes, which were drilled parallel to the main borehole. This network has constantly been updated and extended over the past years. Signals of magnitude $M < -4$ can be detected in a frequency range from 1 kHz to 200 kHz corresponding to intergranular microcracking along grain boundaries on a millimeter- to centimeter-scale.

As an example, we present an experiment performed in 2018, where the borehole was loaded with brine. Figure 8 shows the last three pressure spikes over a span of 50 days. They were created by pumping brine with rates of 2 l/h, 3.3 l/h and 5.5 l/h, respectively. Each time, a rapid drop in pressure was observed consistent with the high bulk modulus of brine. This behaviour is very different from gases (think natural gas/nitrogen blanket), where the pressure decreases very slowly. The central part of the figure shows, that the decay of the pressure still continues 6 weeks after the pressure spike, showing the slow expansion of the brine into the surrounding area. The final spike was an attempt to determine the highest pressure obtainable with available equipment.

**Numerical platform**

In order to render the gathered experimental data useful for the analysis of current and future geosystems and geotechnologies, it needs to be integrated into software used for the design and assessment of such applications. An essential scientific goal of the GeomInt project was, therefore, the analysis of potentials and limitations of different numerical approaches for the modelling of discontinuities in the rocks under consideration of multi-physical processes. An important prerequisite is the improved understanding of the diverse set of methods available to the analyst and their synergies with regard to theoretical and numerical fundamentals. The following numerical methods were included in the comparison and development efforts:

- discontinuous “Lattice Element Method” (LEM),
- discontinuous “Discrete Element Method” (DEM),
- Lagrangian “Smoothed Particle Hydrodynamics” (SPH),
- imaging-based “Forces on Fracture Surfaces” (FFS),
- continuum-based “Phase-Field Method” (PFM),
- continuum-based “Non-Local Damage” (NLD) formulation,
- co-dimensional continua-based method using “Lower-Interface-Elements” (LIE) and the “Hybrid-Dimensional Finite-Element-METHOD” (HDF).

The methods were systematically investigated and appropriately extended based on experimental results. The specific arrangement of the numerical methods along scales represents typical applications within the GeomInt project. In general, numerical methods can be applied at different scales depending on the specific purpose of investigation.

For example, smeared (phase field, non-local damage) and discrete (co-dimensional LIE) representations of fractures were compared for the case of hydraulic fracture propagation in Yoshioka et al. (2019). While all methods were able to simulate fracture propagation in a toughness-dominated regime, they strongly differ in several aspects:

- The type and number of material parameters used: The PFM model for brittle fracture requires a discretisation-related length-scale parameter and otherwise well defined material parameters such as Young’s modulus, Poisson’s ratio and fracture toughness. Other choices are implic-
ity made, e.g., by the choice of degradation function and phase-field driving forces. The LIE approach with a cohesive-zone model requires stiffness and damage parameters of the lower-dimensional fracture zone, which in turn can be linked to quantities such as fracture toughness (critical energy release rate).

– The impact of discretisation and how it can be compensated for: For example, an effective critical energy release rate can be determined for the PFM approach that maintains energetic equivalence to the sharp interface approach for a given choice of regularisation length and discretisation.

– The accessibility of important physical measures of the fractured system: While methods such as LIE or HDF readily allow a quantification of the fracture aperture, smeared approaches such as PFM and NLD have to determine these values based on additional criteria and post-processing effort. This becomes particularly relevant for coupled processes, where the fracture aperture determines flow and transport through the fractured porous medium.

**NUM highlight: Phase-field method for fracturing processes**

In order to facilitate comparisons such as this one and to advance the development of the individual methods in light of the experimental work packages, so-called model-experiment exercises were introduced, cf. Section “Model-Experiment-Exercises (MEX)”. One of the exercises is concerned with pressure-driven fluid percolation and hydraulic fracturing in salt rock samples under anisotropic confining stresses. Cubic samples with a side length of 100 mm were prepared with a borehole drilled in the centre to a depth of 50 mm. The wellbore is cased with a steel tubing with a diameter of 4 mm, leaving the bottom 20 mm open for fluid entrance (Fig. 9).

Pressurised oil is injected through the wellbore in the sample until eventual failure. Two different configurations of the confining stresses were considered as shown in Fig. 10. As the vertical stress applied is the minimum principal stress (compression positive) in the first configuration, a crack on the horizontal plane was induced (Fig. 10a). Similarly for the second configuration, a vertical crack is developed according to the confining stress configuration (Fig. 10b).

The variational phase-field model bases its origin on the generalised Griffith’s theory Francfort and Marigo (1998) and one of its main advantages is to account for arbitrary numbers of cracks without imposing geometrical restrictions on their topology. It represents a crack set \( \Gamma \) by a scalar phase-field variable, \( v : \Omega \mapsto [0, 1] \) which transitions from an intact \( (v = 1.0) \) to a fully broken state \( (v = 0.0) \) continuously. The transition length is controlled by a regularisation parameter with the dimension of a length, \( \ell_s > 0 \) Bourdin et al. (2000). In the computation, we seek a pair of displacement \( u \) and phase-field \( v \) that minimise the following energy functional given loading in a quasi-static manner Bourdin et al. (2012); Yoshioka et al. (2019)

\[
\mathcal{F}_\epsilon = \int_\Omega \nu^2 W dV - \int_{\partial \Omega_0} \mathbf{\tau} \cdot \mathbf{u} dS + \int_\Omega p \mathbf{u} \cdot \nabla v dV + \frac{1}{4c_n} \int_\Omega G_c \left( \frac{(1-v)^n}{\epsilon^2} + \epsilon |\nabla v|^2 \right) dV, \tag{1}
\]

where \( W \) is the strain energy density, \( G_c \) is the fracture toughness, and \( c_n \) is a normalisation parameter defined as \( c_n : = \int_0^1 (1 - \eta)^{n/2} d\eta \).

The two confining pressure cases above were simulated by the variational phase-field model (Fig. 10). Though the crack propagation direction is not prescribed, the stress concentration is correctly identified through the energy minimisation process and the cracks propagated in the expected direction with the expected orientation.

**NUM highlight: Hybrid-dimensional finite-element-method (HDF) for high resolution investigations on the influence of transient fracture volume changes**

Another modelling exercise is concerned with the identification of hydro-mechanical effects throughout characterisation of a single, fluid-filled fracture embedded in crystalline rock. Transient perturbations of the fracture’s equilibrium state by
Fig. 10  Two different confining stress states considered in the fluid percolation experiments in rock salt Kamlot (2009) and simulation results (simulated stresses are displayed in MPa)
systematic alterations of the fluid pressure induce fluid flow and changes of the fracture volume. The strong interaction of flow, transient geometrical properties such as the fracture’s permeability and changes in fracture volume are studied on a cylindrical sample with a radius of \(r = 15\) mm and height \(h = 75\) mm, separated by a single fracture (Fig. 11). The fluid pressure within the fracture is varied by pressure controlled experiments in a triaxial cell through a borehole located at the samples centre.

The water-filled fracture is stimulated by harmonic oscillations of the fluid pressure to study hydro-mechanical effects on the pressure \(p\)-flow \(q\) transients. Variation of the pressure amplitude lead to varying mechanically induced volumetric changes and flow characteristics of the fracture resulting in a non-linear \(p - q\) relationship. These effects are sensitive regarding the fracture’s volume, since small absolute variations in the \(\mu\)m range might induce large relative changes and is continuously influencing the flow characteristics within a single stimulation period.

These phenomena are governed by a hybrid-dimensional element formulation, which is motivated by pressure driven, Poiseuille-type creeping flow conditions and low Reynolds numbers. The lower dimensional flow domain is not explicitly accounting for the fracture’s geometry, but considers initial fracture apertures in terms of a material parameter and transient changes by means of the deformation state of the surrounding rock matrix. Consistent evaluation of the balance equations results in

\[
\frac{\partial p}{\partial t} = \frac{\delta^2}{12 \eta_R^R} \nabla \cdot \nabla p - \frac{\delta}{12 \eta_R^R \beta_l} \nabla \delta \cdot \nabla p - \frac{\delta}{12 \eta_R^R \beta_l} \nabla \cdot (\delta^2 \nabla p) + \frac{1}{\delta \beta_l} \frac{\partial \delta}{\partial t} = \frac{q_{lk}}{q}
\]

(2)

where \(p\) is the fluid pressure and \(\delta\) the fracture aperture. Eq. 2 consists (from left to right) of a) transient term, b) quadratic term, c) convective term, d) diffusive term, e) volumetric coupling term and f) leak-off term. Due to their minor contribution to the overall solution terms b) and c) are mostly neglected in numerical investigations. The proposed discrete fracture formulation possesses a high numerical resolution of fracture volume changes and its influence on characteristic diffusion processes.

Results displayed in Fig. 12 indicate the correlation of increasing pressure amplitudes and hydro-mechanically induced non-linearities between pressure and flow transients. The proposed model is capable to consider small volumetric changes of the fracture domain and reproduces their influence on the flow processes in transient settings.

Model-Experiment-Exercises (MEX)

The basic idea of Model-Experiment-Exercises (MEX) is to link modelling and experimental work from the very beginning – i.e. in the conceptual phase of a project. Due to the inherent complexity of each part in the systems analysis, this combination could sometimes not be maintained as planned. Moreover, both models and experiments require highly sophisticated tools and equipment as well as highly specialised professionals. This means that adequate measures and incentives for collaboration across institutions and between experimental as well as modelling personnel are required. GeomInt is introducing the MEX concept exactly for this purpose. Therefore, the following MEX were a dominant part of the GeomInt project work and supply the majority of the publications with research material.

In order to illustrate the MEX concept, Fig. 2 (upper right) depicts the dependencies between laboratory (LAB) and field experiments (URL) as well as modelling work (MOD). Lab experiments (LAB) will be analysed by models (MOD) in order to calibrate parameters and validate the
models [1]. This step in the analysis loop should demonstrate that the models are able to represent the experiments (validation). Validated models will be used for planning experimental work in order to improve the general process understanding [2] (experimental design). Both lab experiments and models must be scaleable to field experiments [3] where it is demonstrated that they can be applied in an engineering-scale context. Finally, the MEX concept was also used as a framework for comparing the different numerical approaches introduced in section “Numerical platform”.

Table 1 lists an overview of the main Model-Experiment-Exercises (MEX) performed in GeomInt combining both theoretical work and experiments at various scales. Model-Experiment-Exercises (MEX) are organised mainly along the projects work packages as well as experiments (EXP: LAB/URL) and various modelling approaches according to the methods of the numerical platform presented in Section “Numerical platform”. Table 1 summarises a matrix of conducted MEX, where processes (WP1 swelling/shrinking, WP2 fluid percolation, WP3 stress redistribution) are arranged in lines and numerical approaches (MOD) in columns. Gray shaded cells indicated research within GeomInt. A full description of MEX can be found in Kolditz et al. (2020).

Here, we present three selected model-experiment-exercises (MEX) which emphasise the following aspects: (i) comparison of various numerical methods against experimental data (section “Three point bending tests (MEX 0-1a)”), (ii) an example with a new numerical approach for shear tests (section “Direct shear tests using a basalt sample (MEX 3-2)”), and (iii) the role of in-situ experiments for model testing and experimental design (section “Model-Experiment-Exercises in Underground Research Laboratories (URL)”).

### Three point bending tests (MEX 0-1a)

Three numerical methods for fracturing - Lattice Element Method (LEM) Sattari et al. (2017), Discrete Element Method (DEM), and Variational Phase-Field model (VPF) discretised by the Finite Element Method Yoshioka et al. (2019) - are compared against three point bending tests performed on Rockville Granite samples. Three point bending tests were conducted by applying a point load on the top of the sample whose rate is controlled by keeping the Crack Mouth Opening Displacement (CMOD) rate fixed at 0.05 µm/s (Fig. 13a). The notch width is 1.2 mm and the ratio of notch length to sample height is 0.2 Tarokh et al. (2017).

The thickness (w), the span (L), and the height (H) of the sample, and Young’s modulus (E), Poisson’s ratio (μ), the uniaxial compressive strength (UCS), the uniaxial tensile strength (σT), and the fracture toughness (Gc) are listed in Table 2.

![Fig. 12 Pressure and flow transients (left) showing an increasing non-linear p – q relationship obtained by numerical investigations of the proposed boundary value problem (right)](image)

Experimental force-displacement results from two samples are shown together with the simulation results in Fig. 13b. The test results exhibit a predominantly linear elastic response until the onset of the failure where they show hardening behaviour followed by softening. All the simulation results reproduce the linear elastic responses. For the variational phase-field model, this is straightforward as it takes the elastic properties directly. However, for lattice element and discrete element methods, these bulk properties need to be derived from the micromechanical properties. The main difference between the lattice/discrete element methods and the variational phase-field model is observed in the post-failure behaviour. While the variational phase-field model used in this study is based on brittle fracture and not equipped with a ductile softening behaviour, lattice/discrete element methods are capable of simulating a gradual softening behaviour of the bulk material.
Direct shear tests using a basalt sample (MEX 3-2)

At the rock mechanical laboratory of TU Bergakademie Freiberg, direct shear tests using a constant normal stiffness (CNS) have been conducted on samples with pre-existing discontinuities. Large-size intact drill cores with diameter of approximately 150 mm where split parallel to their axis in preparation for shear testing. After removing strips at the boundaries of the discontinuities where irregular and non-typical fracture patterns were observed due to the proximate splitting impact, net shear planes of approximately 125 x 175 mm could be generated. A scheme of a CNS test and a photograph of the shear testing device can be seen in Fig. 14.

A basalt sample was sheared multiple times using increasing stiffness values $K_n$. The shear forces and the vertical movement of the sample were recorded. The simulation approach explicitly calculates the forces on the surface geometry. For that purpose, 3D scan data were obtained. Basic rock parameters were investigated in standard tests.

In order to simulate shear behaviour of rock joints in crystalline rock a MATLAB-code using a Forces on Fracture Surfaces (FFS) approach was developed. Its main objective is to simulate shear behaviour by only using physical-founded input parameters and realising minimal calculation times. Starting point of the calculation algorithm is a matrix of the actual surface geometry prior to the direct shear test. A quadratic grid is used which is created from the raw scan data by linear interpolation of measurement data to the neighbouring points. The surface is then duplicated and shearing is done by shifting the matrices against each other at consecutive steps of one pixel.

Thus, the grid constant is the increment of the shear displacement. At each shear step grid contact forces and grid geometry are updated based on classical approaches like Hooke’s formulation for linear elasticity, Coulomb’s friction law and Mohr’s shear strength model.

In Fig. 15, a visual comparison of the damaged areas of the rock surface proves that the code is able to detect areas which are damaged and therefore strongly influence the shear behaviour.

The simulation results for a selected stiffness value can be seen in Fig. 16. In this case, the destroyed edge of the sample was removed before starting the simulation. The overall quality of the numerical result is considered fair. It clearly can be seen that the dilatation and shear stress curves are tightly correlated. This implies that the key for adequate results is a good approach to model the vertical movements of the sample. In laboratory tests, a negative normal displacement at the first stage of the shear tests is measured which can be explained by not perfectly matching sample halves. The code is so-far not able to simulate this behaviour as it considers a perfect match.

Finally it can be said that the simple, physically motivated approach works properly in terms of detecting the zones of importance. A general trend for the shape of the shear curves can be displayed but the difference to the laboratory data can be significant. The mentioned perfectly matching parts and the inability to destroy larger parts of the sample at...
once are the main limitations at the moment. The code and the input data will be published and a further development focusing on this problems is possible. For further details see Fruehwirt et al. (2020).

**Model-Experiment-Exercises in Underground Research Laboratories (URL)**

The Underground Research Laboratory Mont Terri plays an extraordinary role for model testing and experimental design Bossart and Milnes (2018). Figure 17a illustrates some of the ongoing model-experiment activities which are also integrated into a virtual reality context (VR Task) Rink et al. (2020). As an example, the study concerning the CD/CD-A experiments are briefly presented in the following (Fig. 17b).

**Cyclic-Deformation experiment (MEX 1-4)**

The Cyclic-Deformation (CD/LP) experiment focuses on the deformation of a niche, caused by seasonally influenced desaturation of the Opalinus Clay. This experiment was used twofold: (i) for code verification and (ii) for experimental design of the planned CD-A follow-up experiment (see below). In particular, it has been used for the verification of a newly implemented model within the open-source finite element code OpenGeoSys 6 (OGS-6) for strongly hydro-mechanically coupled problems with consideration of desaturation by comparison against the former weakly-coupled version in OGS-5 Ziefle et al. (2017). Hereby, the new implementation in OGS-6 has proven its practical applicability under real conditions and its capacity for high performance computing. It was thus used for further validation against observations.

The CD-A experiment has been prepared in recent years, to distinguish between deformation processes due to stress redistribution and seasonal variations in air humidity that cause saturation (swelling) and desaturation (shrinkage) of the rock and stress redistribution alone. To this end, two identical niches were excavated, one sealed towards the gallery and with a high humidity inside to minimise desaturation and one open to the general air circulation of the rock laboratory. The measurement campaign was started in October 2019 Ziefle et al. (2019). Pre-calculations with OGS-5 have been a major factors for the dimensioning of

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**Table 2** Parameters used for the simulation of three point bending tests

| w  | L    | H    | E     | ν     | UCS  | σ_T  | G_c |
|----|------|------|-------|-------|------|------|-----|
| 30 mm | 127 mm | 50.8 mm | 27.5 GPa | 0.175 | 106 MPa | 8.1 MPa | 100 Pa-m |

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**Fig. 13** Three-point-bending test: numerical interpretation on experimental data

**Fig. 14** Schematic (left) and laboratory view (right) of a direct shear test with constant normal stiffness boundary conditions. One part of the sample is fixed and the other part sheared off. (from Nguyen et al. (2014), Konietzky et al. (2012))
the experimental design, e.g. the distance between the two
niches (Fig. 17b). Currently, a numerical 3D model of the
CD-A experiment for OGS-6 has been set up and is being
evaluated, cf. Fig. 18. The high-performance computing
capacity of OGS-6 will assure a reasonable run-time even
for this problem taking into account the complex non-linear
deformation behaviour of the hydro-mechanically coupled
system.

Synthesis and outlook

As a result of the GeomInt research project a broad com-
bined experimental and numerical platform for the inves-
tigation of discontinuities due to swelling and shrinkage
processes, pressure-driven percolation and stress redistri-
bution for important reservoir and barrier rocks (clay, salt,
crystalline) has been developed. Model comparisons for
damage and fracture phenomena driven by different physi-
cal processes provide information on the optimal areas of
application of the numerical methods as well as their limita-
tions (see Section “Numerical platform”).

A comprehensive validation of the platforms (“Proof-of-
Concept”) and in particular their integration across institu-
tions and work groups was carried out by “Model-Experiment-
Exercises” (MEX). Each MEX targeted damage and
fracture processes driven by different mechanisms along the
lines of each work package (see section “Model-Experiment-
Exercises (MEX)”). The MEX concept is the central syn-
thesis element of GeomInt as it is directly linking models
(MOD) with lab experiments (LAB) and paving the way
towards the analysis of in-situ experiments (URL) which
has been started in the current project phase and will be
continued in future activities (see section “Outlook–Future
directions”).

The project results published in dedicated articles allow
an improved understanding of the processes, the methods
used and their application-oriented relevance on appropri-
ate time and length scales in order to make the planning
and implementation of geotechnical uses of the underground
safer, more reliable and efficient. An important part of future
work is the demonstration of transferability of the experi-
mental-numerical concepts and methods to other geotechn-
ological applications (e.g. deep geothermal energy, energy
storage, repository problems, methods for hydraulic stimula-
tion, conventional and unconventional resource extraction or
tunnel construction). Ongoing activities also aim at intensi-
fying the internationalisation started in the current project
in cooperation with complementary research projects (e.g.
EURAD, DECOVALEX 2023, Mont Terri project).

Synthesis–Numerical methods capabilities

Significant emphasis in GeomInt was directed on the
development of numerical methods for modelling of dis-
continuities in various rock types as well as the analysis of
advantages / disadvantages of particular methods for specific fracture pattern at various scales. The numerical methods are described in more detail in the GeomInt book Kolditz et al. (2020). Here the capabilities of the numerical methods used will be compactly summarised in the following tables.

Table 3 provides an overview of the capabilities of the numerical methods for simulation of fracturing processes, i.e. (i) crack representation by elements explicitly/separative or by damage variables, (ii) failure criteria, (iii) used mesh types and (iv) fracture aperture calculation.

An evaluation of the capabilities of all used methods concerning the analysis of discontinuities is provided in Table 4. An important part of the MEX concept was the application of multiple methods to these exercises (e.g. for MEX 0-1A three methods, LEM, DEM and FEM-VPF have been applied). For the analysis of lab-scale experiments all present methods (discontinuous and continuous) could be applied successfully. The advantages of the discontinuous methods (LEM, DEM) lies in the simulation of small scale processes, e.g. fracture initiation and propagation, and because they rely on fundamental fracture mechanical phenomena. Discontinuous methods exhibit some difficulties when it comes to coupled processes and at larger scales where continuum methods (FEM#) are rather strong. We also added 3D capabilities and HPC implementation status to the table.

Benchmarking is a typical method in geosciences for evaluating and assessing the validity of experimental and modelling approaches. Related projects and initiatives e.g. are DECOVALEX Birkholzer et al. (2018, 2019), SeS Bench Steefel et al. (2015), InterComp Maxwell et al. (2014), and recently BenVaSim to mention a few. Those benchmarking initiatives have been focused on providing a best fit between measured data and simulated results. GeomInt follows the proven path but providing a systematic study of fracture mechanics methods at different scales, additionally.
Outlook – Future directions

The main concept of a unified modelling framework for various rock type will be pursued also in the future. After a strongly methodically oriented first phase, the continuation is intended to demonstrate practical applicability under in-situ conditions. In this context, the focus of experimental investigations will shift significantly to the realisation and evaluation of in-situ experiments in various underground laboratories (URLs). For this purpose, the international cooperation with the Mont Terri project and DECOVALEX-2023 will be further intensified. Focused laboratory experiments will be performed particularly where knowledge gaps limit the ability to study the URL experiments.

In addition, aspects of digitalisation will be emphasised in two regards, computation and virtualisation. For the efficient numerical simulation of coupled mechanical, thermal and hydraulic processes in the formation and development of discontinuities on the scale under consideration, the adaptation of models and algorithms will be further developed in future using high-performance computing (HPC) capabilities. The descriptive presentation of structural, experimental and model results in the real context (e.g. URLs) is to be carried out within the framework of an integrated visual data analysis (virtualisation).

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