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Die Ressourcenuniversität. Seit 1765.

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Zentrum für Umweltforschung

Introduction to OpenGeoSys (OGS) and Basics of Multiphysics Simulations

Norbert Grunwald, Olaf Kolditz & OpenGeoSys Team

Part I: Exploring OGS and Project Setup

29.08.2023, Liège, Belgium

Discovering the Project Website

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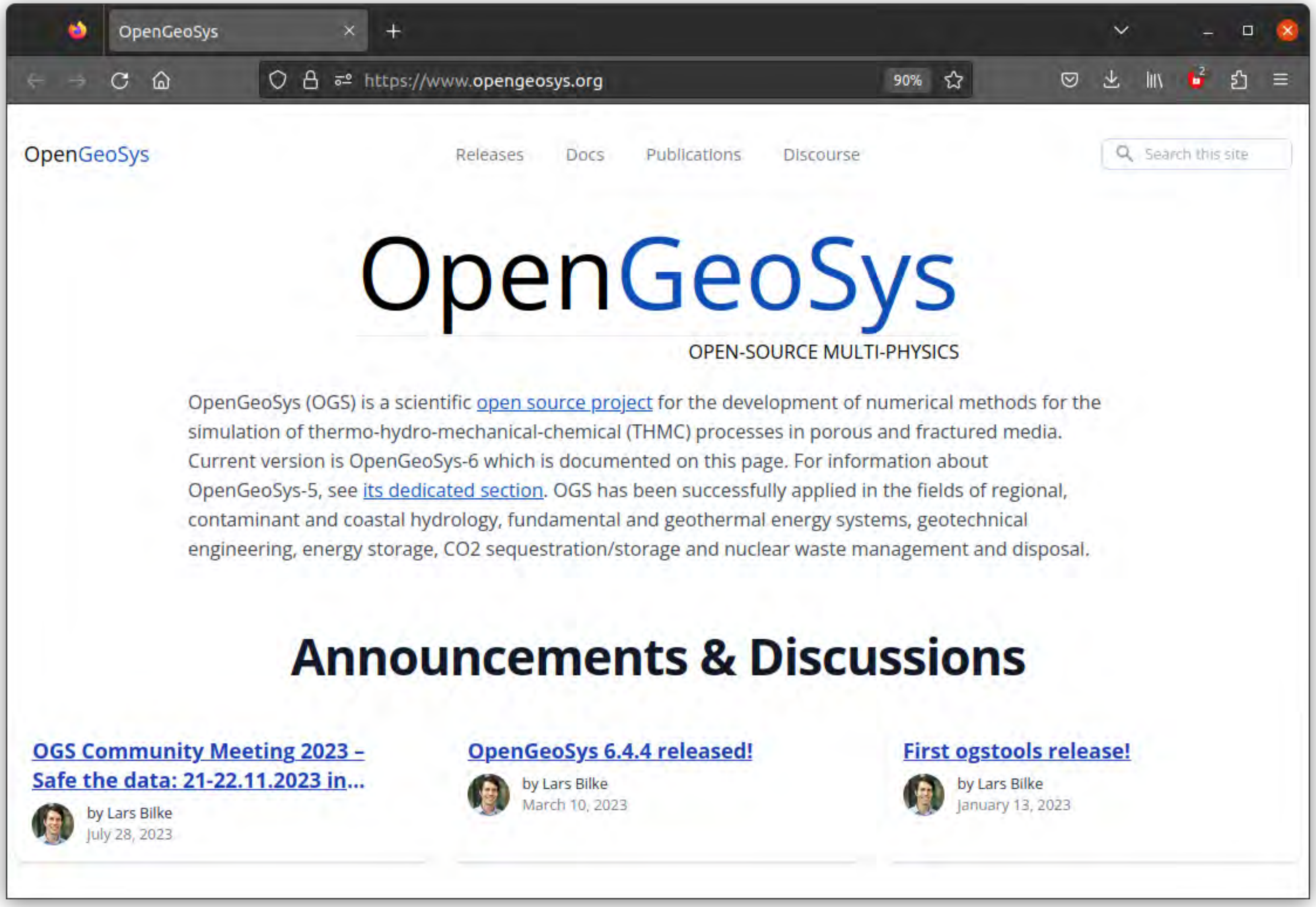
PROJECT WEBSITE

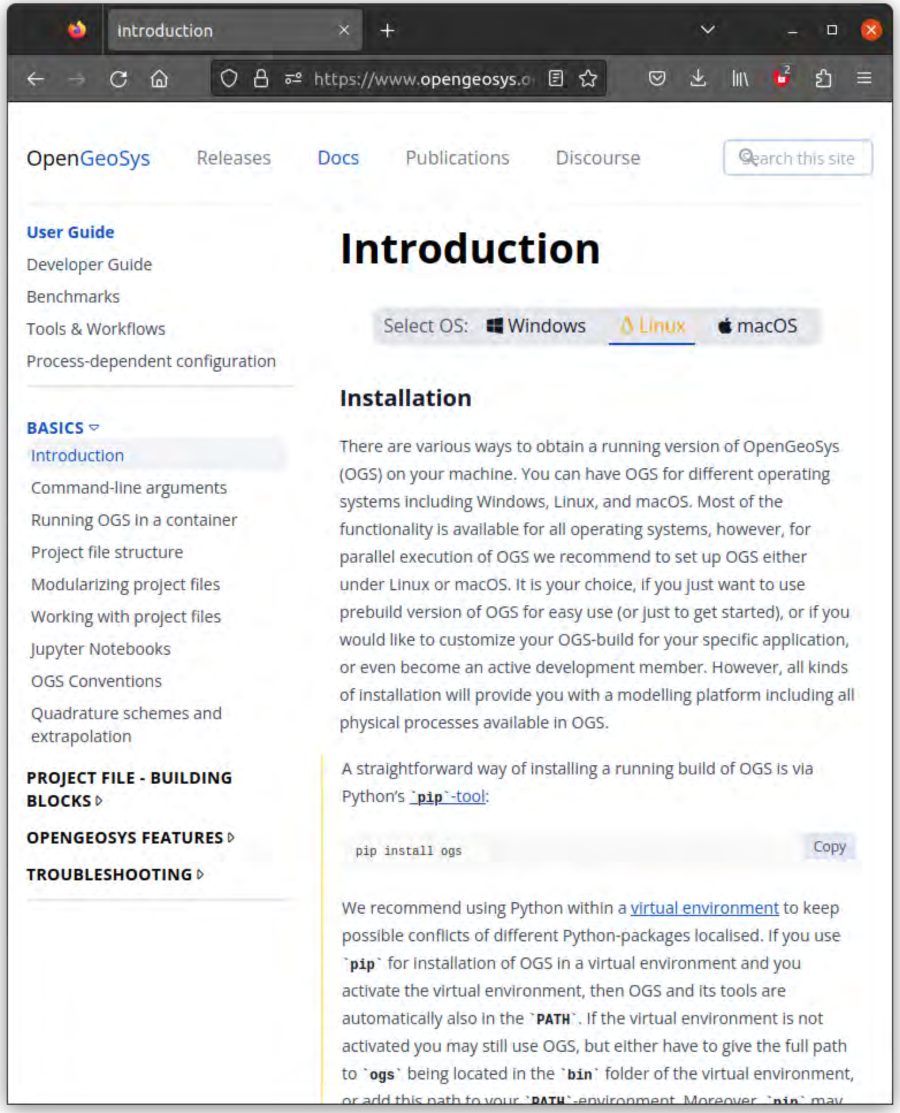
https://www.opengeosys.org/

- features
  - Releases & Downloads
  - Documentation
  - Guides
  - Benchmarks
  - OGS-Community
  - Publications



GETTING STARTED WITH OpenGeoSyS

- ***Download and Install:***
  - **Precompiled Version:**
    - **Visit website:** `https://www.opengeosys.org/`
    - **Go to Docs -> User Guide**
    - **Follow the provided steps for installation**
- **Contribute and Customize**
  - **Source Code on GitLab:**
    - **Access GitLab repository:** `https://gitlab.opengeosys.org/`
    - **Docs -> Developer Guide contains compilation instructions**
- **Start Using OGS:**
  - **Grab an Example Benchmark Test: Explore our sample benchmark tests in the software package**
  - **Use them as templates for your own projects**



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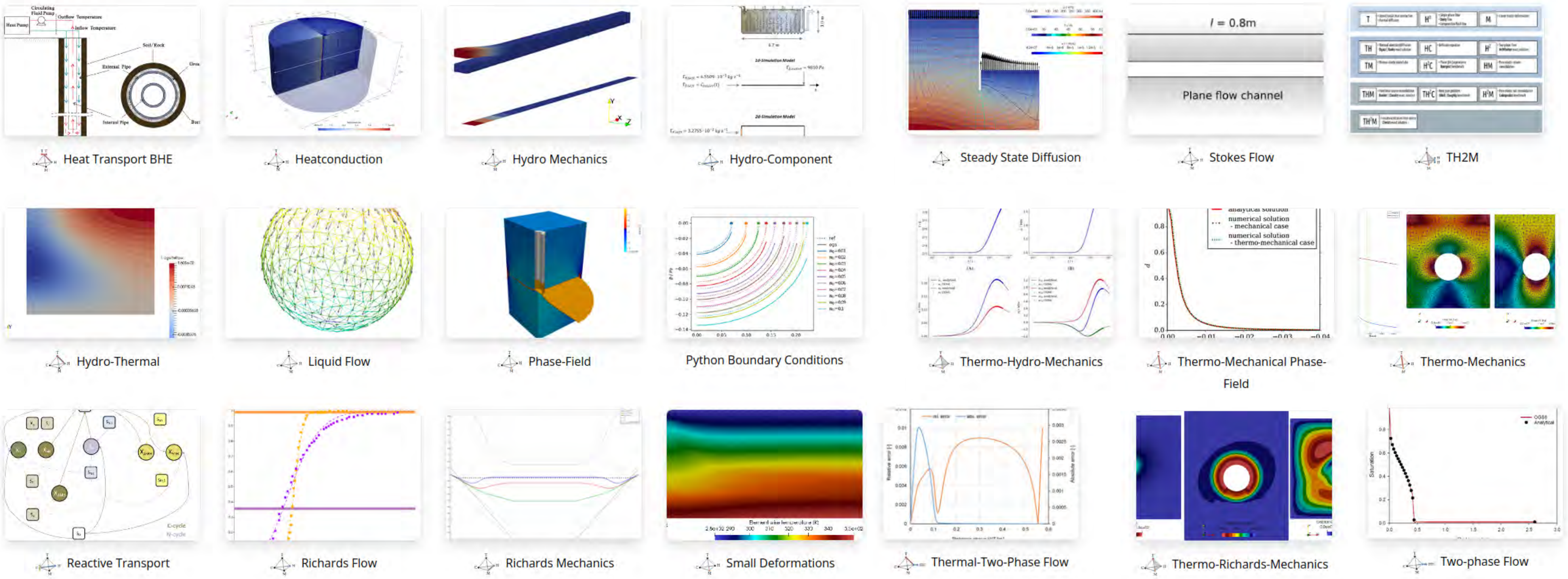
BENCHMARK GALLERY

https://www.opengeosys.org/docs/benchmarks/



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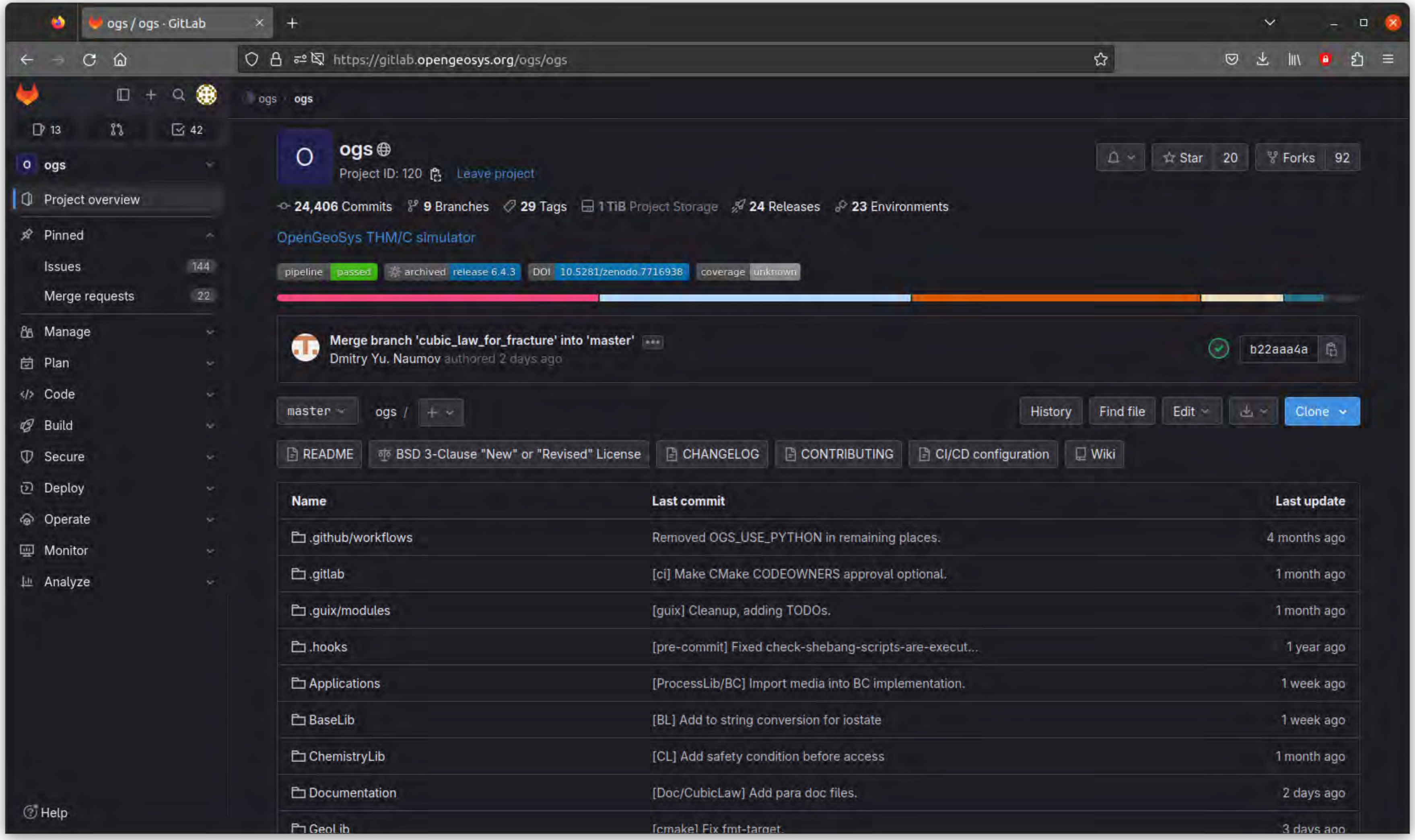
EXPLORING GITLAB REPOSITORY



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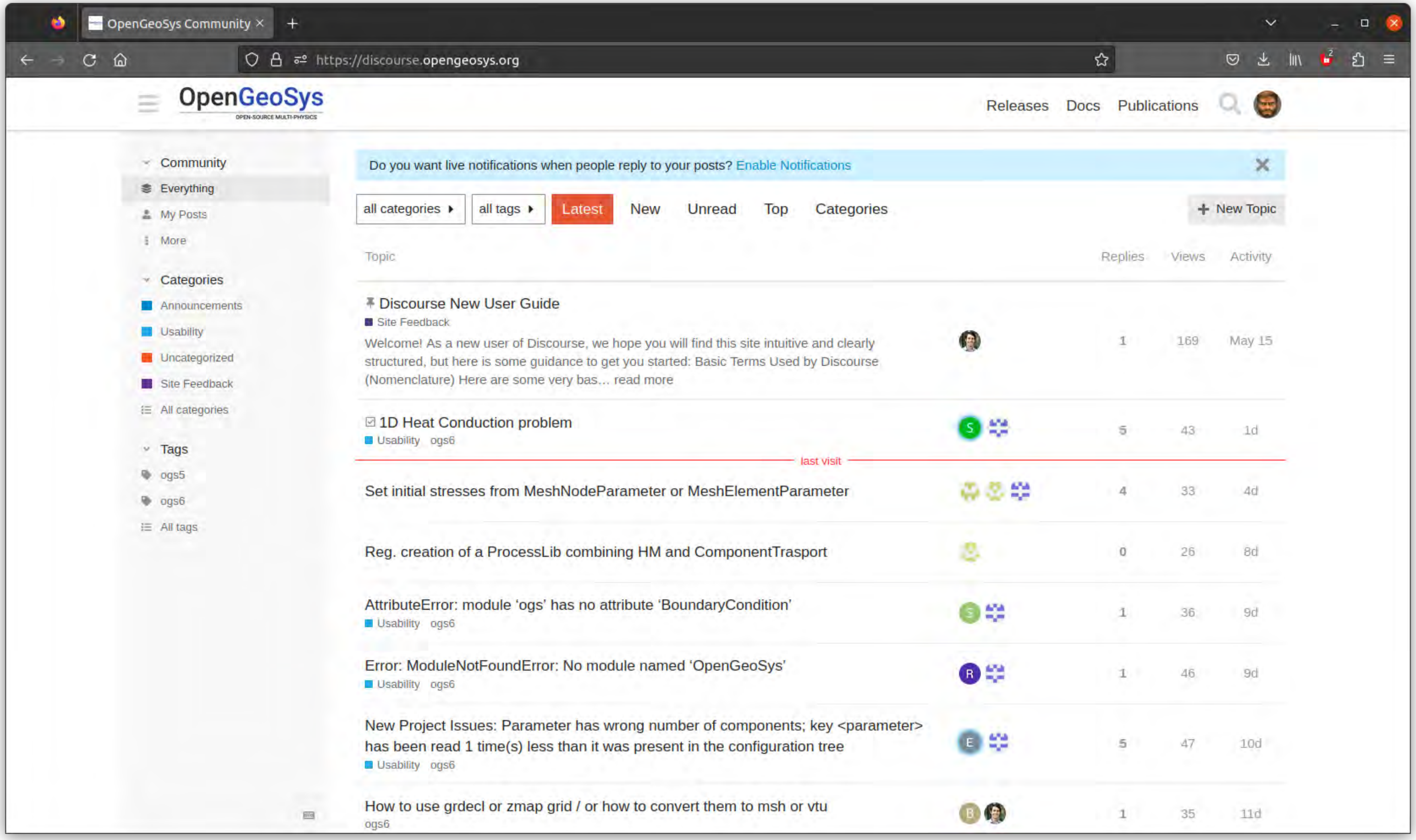
ENGAGE WITH THE DEVS ON OUR DISCOURSE



Configuring a OGS Project

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INPUT FILE STRUCTURE

*XML-based
**VTK-based

INPUT FILE STRUCTURE

Project File *.prj

1. Define XML version and encoding

2. Start a new OpenGeoSys - project

```
<?xml version="1.0" encoding="ISO-8859-1"?>
<OpenGeoSysProject>

...

</OpenGeoSysProject>
```

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INPUT FILE STRUCTURE

Project File *.prj

3. Define the domain/bulk mesh
4. Define BC/ST-meshes
5. Specify process(es)
6. Specify material properties/ constitutive laws
7. Time Control
8. Set up BC/IC
9. Set solver properties/ convergence criteria

```
<meshes>
    <mesh axially_symmetric="true">domain_quad.vtu</mesh>
    <mesh axially_symmetric="true">boundary_axis.vtu</mesh>
    <mesh axially_symmetric="true">boundary_top.vtu</mesh>
    <mesh axially_symmetric="true">boundary_bottom.vtu</mesh>
    <mesh axially_symmetric="true">boundary_borehole.vtu</mesh>
</meshes>
```

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```
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    <mesh axially_symmetric="true">domain_quad.vtu</mesh>
    <mesh axially_symmetric="true">boundary_axis.vtu</mesh>
    <mesh axially_symmetric="true">boundary_top.vtu</mesh>
    <mesh axially_symmetric="true">boundary_bottom.vtu</mesh>
    <mesh axially_symmetric="true">boundary_borehole.vtu</mesh>
</meshes>
```

DETOUR – *.gml FILE

Geometry File *.gml

- Legacy geometry file

```xml
<?xml version="1.0" encoding="ISO-8859-1"?>
<OpenGeoSysProject>
    <mesh>square_100x100_quad_1e4.vtu</mesh>
    <geometry>square_100x100.gml</geometry>
```

DETOUR – *.gml FILE

Geometry File *.gml

- Legacy geometry file
- Defines `points`, `polylines` and `surfaces` by coordinates
- Almost obsolete by now*
- Can be used to create boundary meshes from bulk mesh using `constructMeshesFromGeometry`

```xml
<?xml version="1.0" encoding="ISO-8859-1"?>
<?xml-stylesheet type="text/xsl" href="OpenGeoSysGLI.xsl"?>
<OpenGeoSysGLI xmlns:xsi="http://www.w3.org/2001/XMLSchema-instance"
               xmlns:ogs="http://www.opengeosys.org">
    <name>square_1x1_geometry</name>
    <points>
        <point id="0" x="0" y="0" z="0"/>
        <point id="1" x="100" y="0" z="0"/>
        <point id="2" x="100" y="100" z="0"/>
        <point id="3" x="0" y="100" z="0"/>
    </points>
    <polylines>

        <polyline id="0" name="bottom">
            <pnt>0</pnt>
            <pnt>1</pnt>
        </polyline>
        <polyline id="0" name="right">
            <pnt>1</pnt>
            <pnt>2</pnt>
        </polyline>
        <polyline id="0" name="top">
            <pnt>2</pnt>
            <pnt>3</pnt>
        </polyline>
        <polyline id="0" name="left">
            <pnt>3</pnt>
            <pnt>0</pnt>
        </polyline>

    </polylines>
```

*Although it might be required by some processes(?)

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INPUT FILE STRUCTURE

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```
<processes>
    <process>
        <name>THM</name>
        <type>THERMO_HYDRO_MECHANICS</type>
        <integration_order>3</integration_order>
        <dimension>2</dimension>

        ...

        <process_variables>
            <displacement>displacement</displacement>
            <pressure>pressure</pressure>
            <temperature>temperature</temperature>
        </process_variables>

        <secondary_variables>
            <secondary_variable type="static"
                                internal_name="sigma"
                                output_name="sigma"/>
            <secondary_variable type="static"
                                internal_name="epsilon"
                                output_name="epsilon"/>
        </secondary_variables>

        <specific_body_force>0 -9.81</specific_body_force>
    </process>
</processes>
```

INPUT FILE STRUCTURE

Project File *.prj

3. Define the domain/bulk mesh
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6. **Specify material properties/ constitutive laws**
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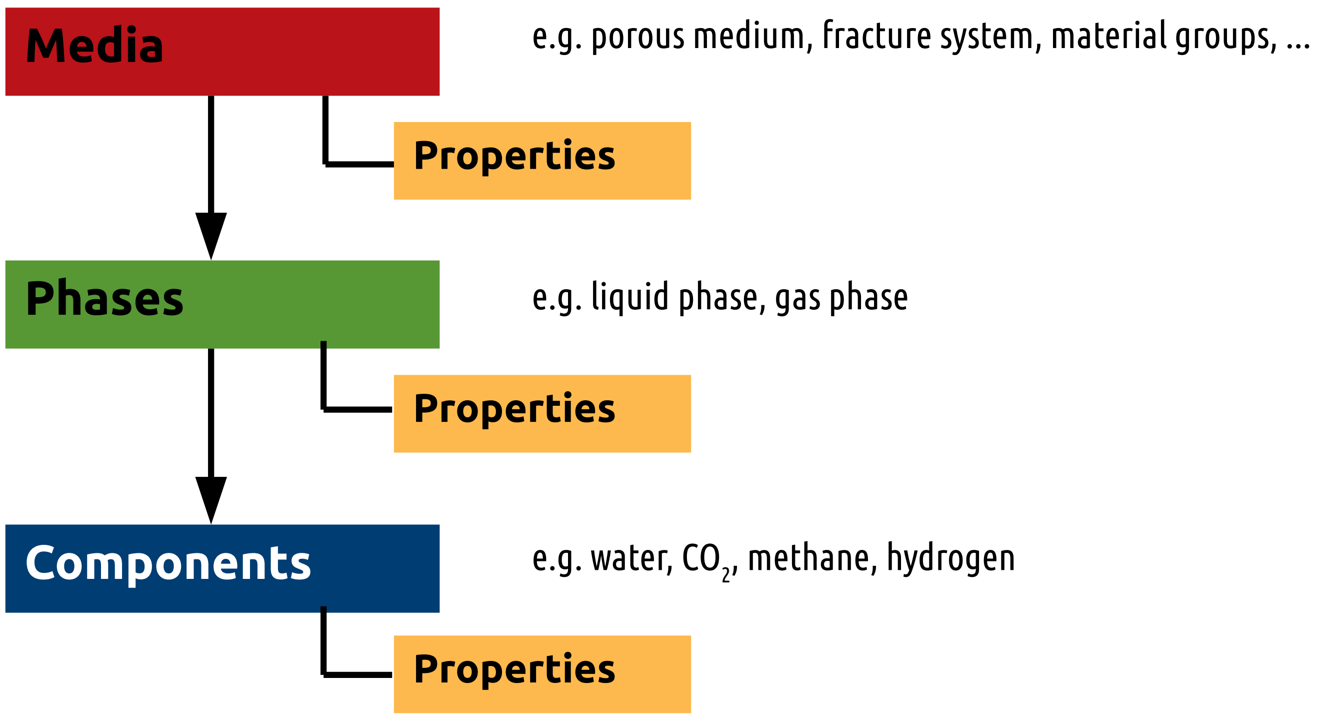
```
<media>
    <medium id="0">
        <phases>
            <phase>
                <type>AqueousLiquid</type>
                <properties>
                    <property>
                        <name>specific_heat_capacity</name>
                        <type>Constant</type>
                        <value>4184.0</value>
                    </property>
                    ...
                </properties>
            </phase>
            <phase>
                <type>Solid</type>
                <properties>
                ...
                </properties>
            </phase>
        </phases>
        <properties>
            <property>
                <property>
                    <name>Permeability</name>
                    <type>Constant</type>
                    <value>1.e-15 0. 0. 1.e-15</value>
                    </property>
                    ...
            </property>
        </properties>
    </medium>
</media>
```

DETOUR - MATERIAL PROPERTY HIERARCHY



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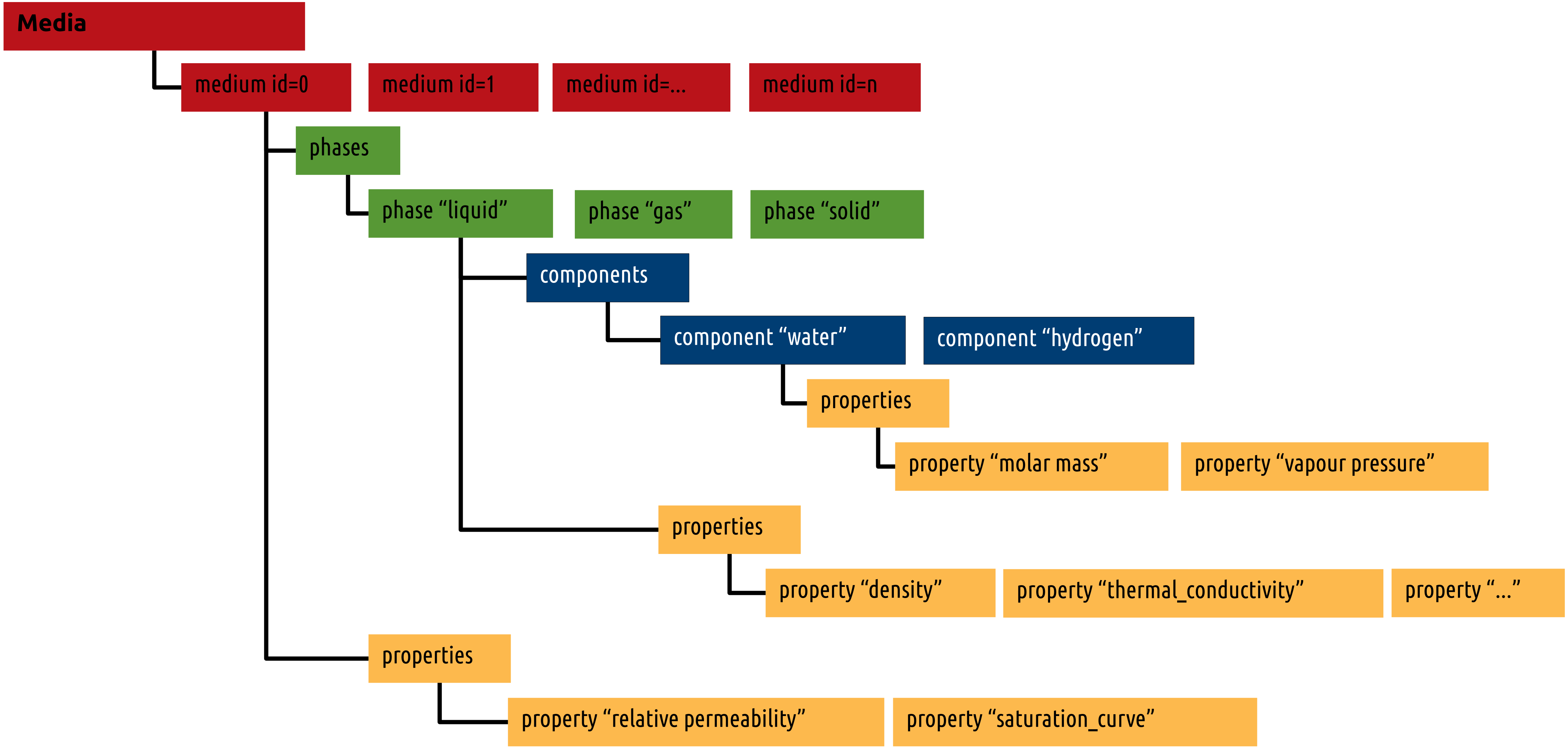
DETOUR - MATERIAL PROPERTY HIERARCHY



INPUT FILE STRUCTURE

Project File *.prj

3. Define the domain/bulk mesh
4. Define BC/ST-meshes
5. Specify process(es)
6. Specify material properties/ constitutive laws
7. **Time Control**
8. Set up BC/IC
9. Set solver properties/ convergence criteria

```xml
<time_loop>
    <processes>
        <process ref="THM">
            <nonlinear_solver>basic_newton</nonlinear_solver>
            <convergence_criterion>
            ...
            </convergence_criterion>
            <time_stepping>
                <type>FixedTimeStepping</type>
                <t_initial>0</t_initial>
                <t_end>2.7e8</t_end>
                <timesteps>
                    <pair><repeat>100</repeat><delta_t>86400</delta_t></pair>
                </timesteps>
            </time_stepping>
        </process>
    </processes>
    <output>
        <type>VTK</type>
        <prefix>result</prefix>
        <timesteps>
            <pair><repeat>1</repeat><each_steps>1</each_steps></pair>
        </timesteps>
        <variables>
            <variable>displacement</variable>
            <variable>temperature</variable>
            <variable>sigma</variable>
            ...
        </variables>
    </output>
</time_loop>
```

INPUT FILE STRUCTURE

Project File *.prj

3. Define the domain/bulk mesh
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5. Specify process(es)
6. Specify material properties/ constitutive laws
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```
<process_variables>
    <process_variable>
        <name>displacement</name>
        <components>2</components>
        <order>2</order>
        <initial_condition>displacement0</initial_condition>
        <boundary_conditions>

            <boundary_condition>
                <mesh>boundary_axis</mesh>
                <type>Dirichlet</type>
                <component>0</component>
                <parameter>dirichlet0</parameter>
            </boundary_condition>

            <boundary_condition>
                <mesh>boundary_bottom</mesh>
                <type>Dirichlet</type>
                <component>1</component>
                <parameter>dirichlet0</parameter>
            </boundary_condition>

        </boundary_conditions>
    </process_variable>
    ...
</process_variables>
```

INPUT FILE STRUCTURE

Project File *.prj

3. Define the domain/bulk mesh
4. Define BC/ST-meshes
5. Specify process(es)
6. Specify material properties/ constitutive laws
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```
<nonlinear_solvers>
    <nonlinear_solver>
        <name>basic_newton</name>
        <type>Newton</type>
        <max_iter>50</max_iter>
        <linear_solver>general_linear_solver</linear_solver>
    </nonlinear_solver>
</nonlinear_solvers>

<linear_solvers>
    <linear_solver>
        <name>general_linear_solver</name>
        <lis>-i bicgstab -p ilu -tol 1e-16 -maxiter 10000</lis>
        <eigen>
            <solver_type>BiCGSTAB</solver_type>
            <precon_type>ILUT</precon_type>
            <max_iteration_step>10000</max_iteration_step>
            <error_tolerance>1e-16</error_tolerance>
        </eigen>
    </linear_solver>
</linear_solvers>
```

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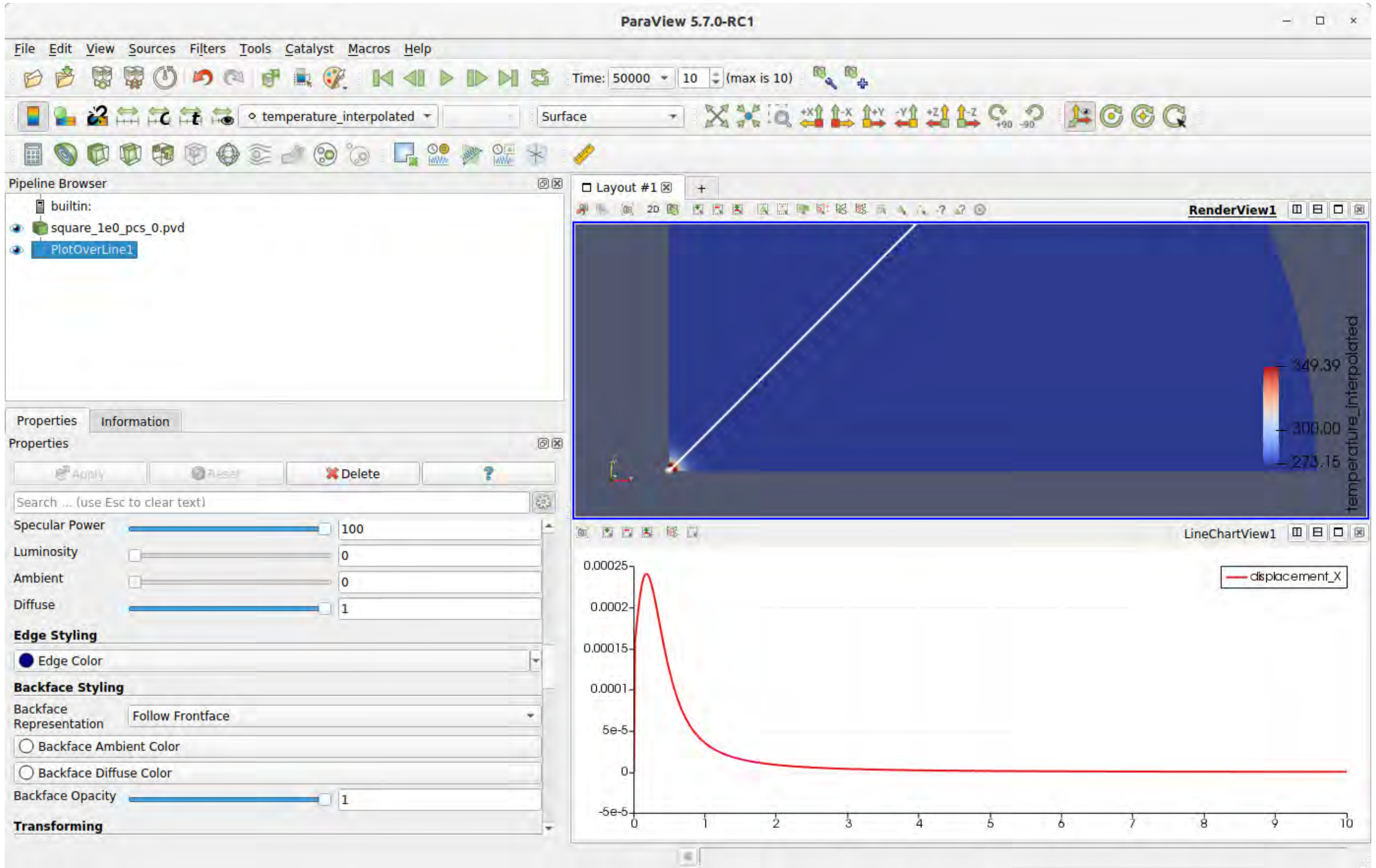
Example Project File

POST-PROCESSING

- Evaluate Results using ParaView



Grunwald, N., Nagel, T., Pitz, M., Kolditz, O. "Extended analysis of benchmarks for gas phase appearance in low-permeable rocks". Under Review at Geomechanics and Geophysics for Geo-Energy and Geo-Resources, 2023.

PYTHON API FOR OGS

ENHANCED WORKFLOW WITH AUTOMATION AND POST-PROCESSING

ogs6py:

- Automating input file generation and modification.
- Change parameters and configurations programmatically.
- Ideal for scenario studies and sensitivity analyses.

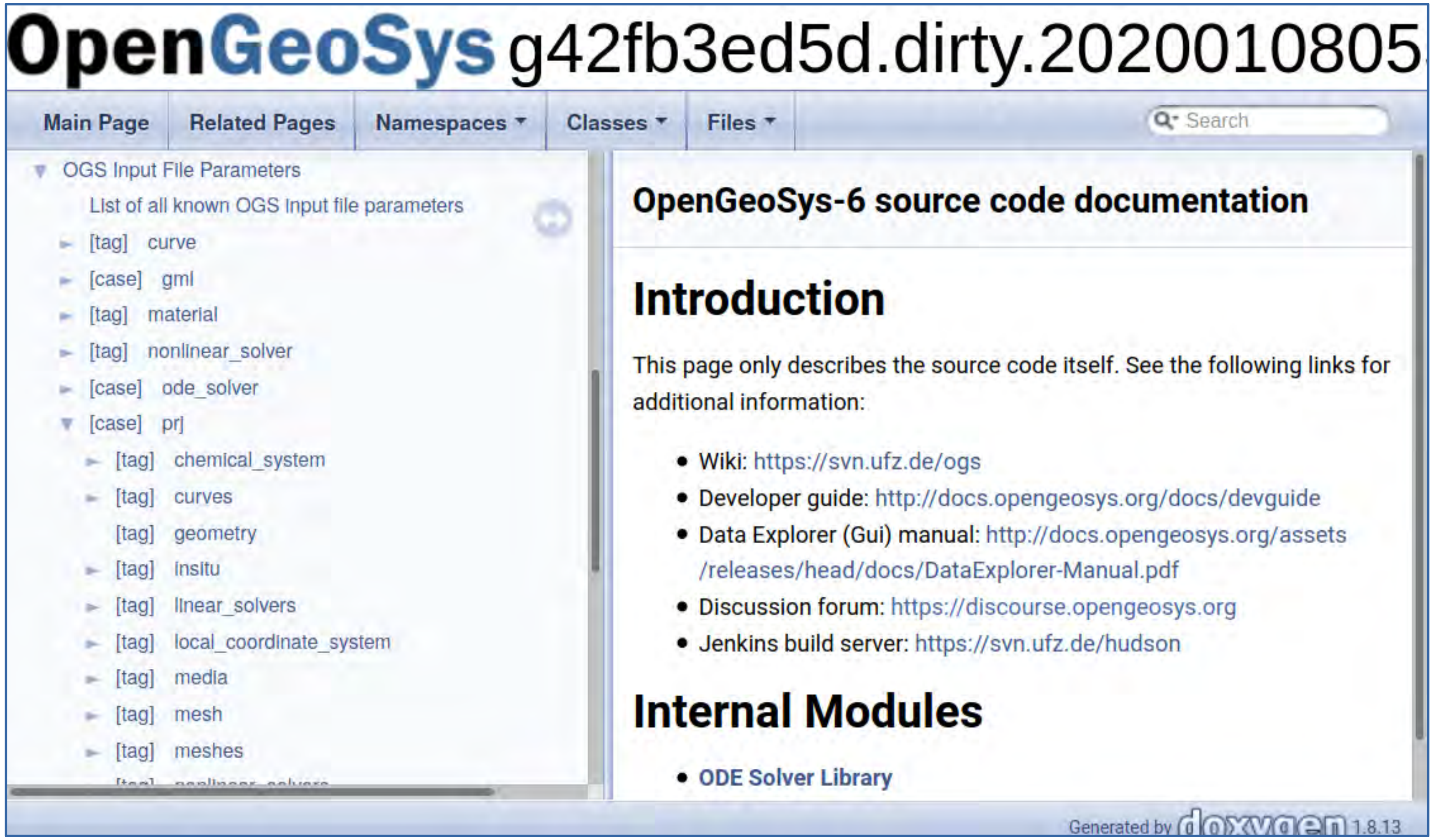
vtuIO

- Advanced post-processing and visualization.
- Reads VTU files from the Visualisation Toolkit.
- Enables result investigation, further calculations, and plotting.

FURTHER DETAILS – INPUT FILE PARAMETERS

Project File *.prj

https://doxygen.opengeosys.org/



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Introduction to OpenGeoSys (OGS) and Basics of Multiphysics Simulations

Norbert Grunwald, Olaf Kolditz & OpenGeoSys Team

Part II: Basics of Multiphysics Simulations

29.08.2023, Liège, Belgium

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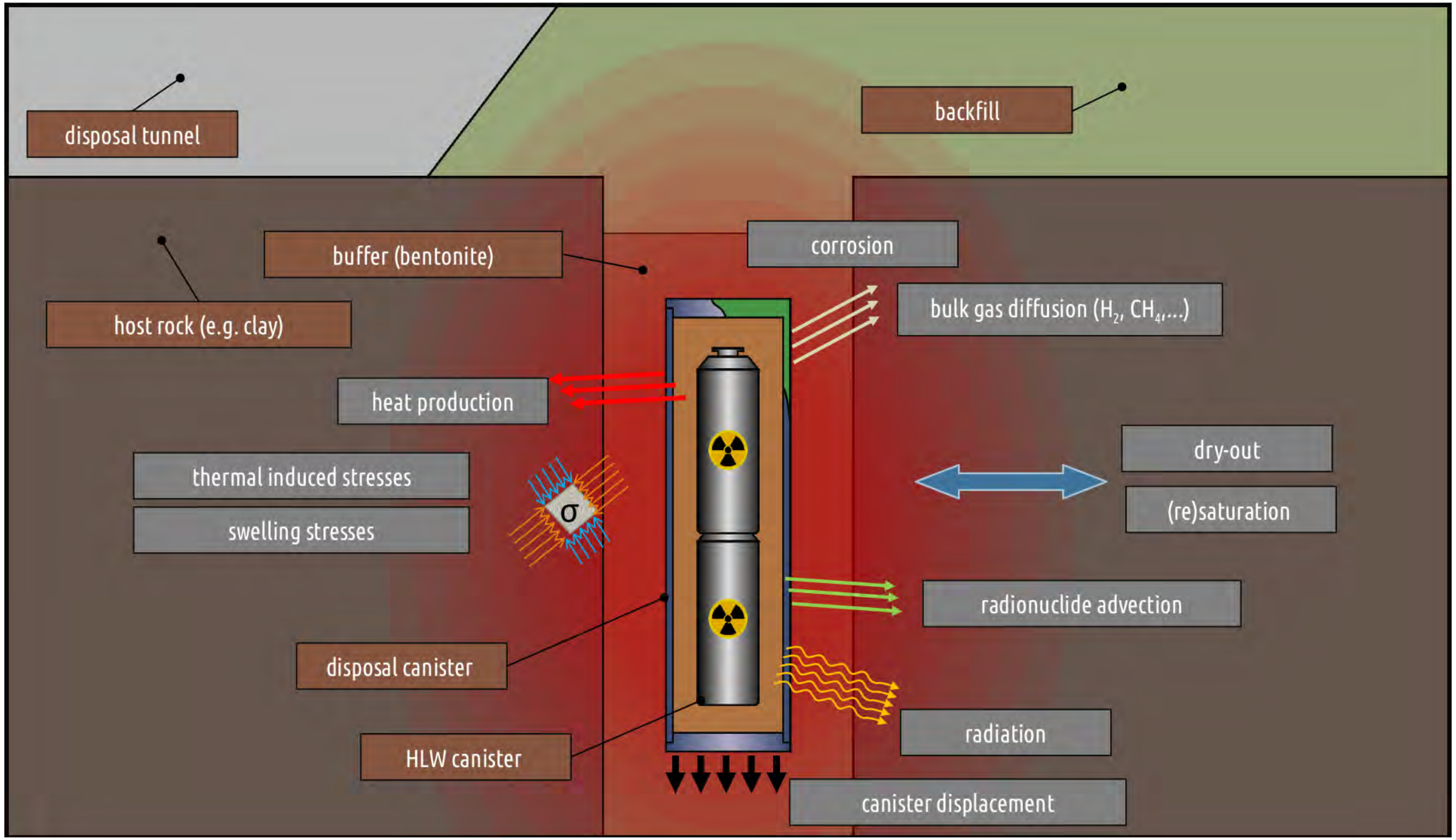
Motivation for TH2M

FOUNDATIONS OF MULTIPHYSICS SIMULATIONS

INTRODUCING THERMO-HYDRAULIC MULTIPHASE MECHANICS (TH2M) SIMULATION



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TH2M Theory

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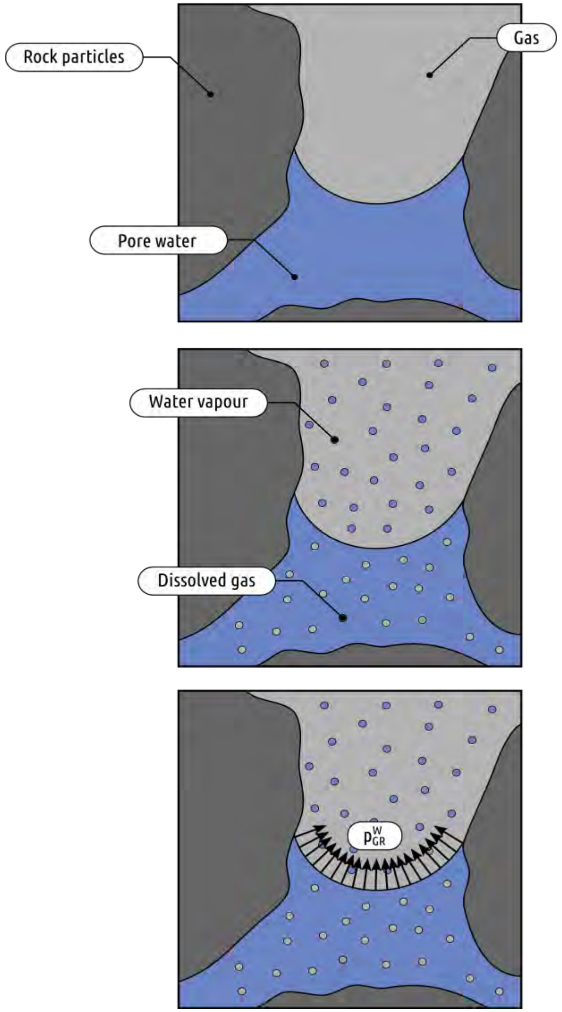
FOUNDATIONS OF MULTIPHYSICS SIMULATIONS

INTRODUCING THERMO-HYDRAULIC MULTIPHASE MECHANICS (TH2M) SIMULATION



Features

- **Two-phase flow in deformable porous media**
- **Phase transitions among fluid phases**
- **Dissolution of gas in water, water evaporation**
- **Heat transport, non-isothermal behaviour due to various factors**
- **Thermodynamically consistent**
- **Fully, monolithically coupled**

Limitations

- **Local thermal equilibrium**
- **Linear elasticity**
- **Small deformations**
- **Quasi-static behavior**

Grunwald, N., Maßmann, J., Kolditz, O., Nagel, T., 2020. Non-iterative phase-equilibrium model of the H2O-CO2-NaCl-system for large-scale numerical simulations. Mathematics and Computers in Simulation, 178, 46-61.

Grunwald, N., Lehmann, C., Maßmann, J., Naumov, D., Kolditz, O., Nagel, T., 2022. Non-isothermal two-phase flow in deformable porous media: Systematic open-source implementation and verification procedure. Geomechanics and Geophysics for Geo-Energy and Geo-Resources, 8, 107. https://doi.org/10.1007/s40948-022-00394-2

TH2M - THEORY

TH2M is based on the 'Theory of Porous Media' (TPM)

Solid Mechanics → TPM ← **Fluid Mechanics**

TPM

- Hybrid combining solid mechanics and fluid mechanics
- "Averaging" of solid and multiple fluid phases with "smeared" properties
- Choice of control volume is essential
- Utilizes volume fractions concept
- Subfields exist in ideal disorder
- Balancing of state variables within the simulation

TH2M - THEORY

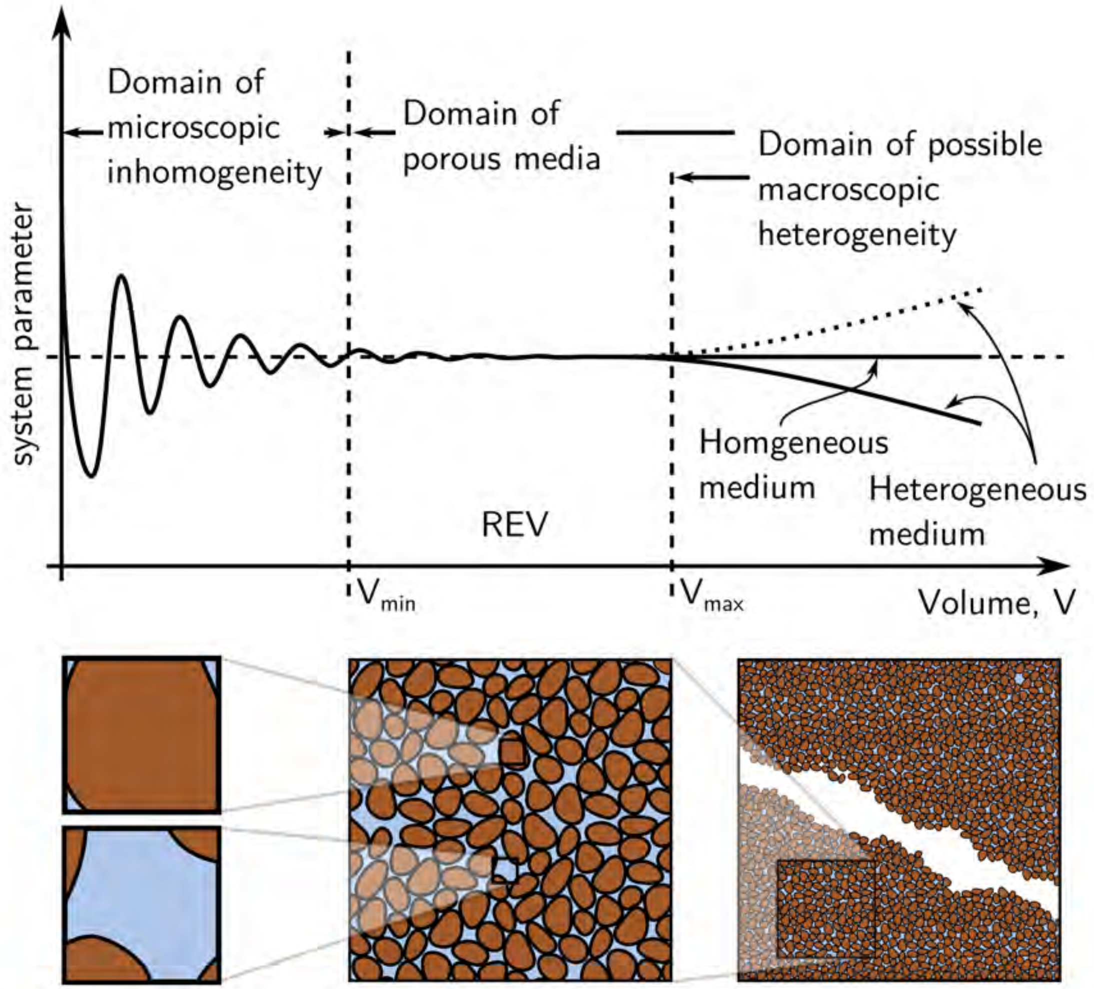
Control volume:

"The smallest volume of a body whose measurable properties are representative of the properties of the entire body."

Volume fractions:

- **At each point of the control volume, there are simultaneously material points of all constituents.**
- **The control volume is the sum of all partial volumes.**

$$\phi_\alpha = \frac{d\Omega_\alpha}{d\Omega} \qquad \sum_\alpha \phi_\alpha = 1$$



TH2M - THEORY

General Balance Equation for Single-Phase Bodies:

	Change in Ψ	due to: out/inflow	supply	production
Global form:	$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{B}} \Psi \,\mathrm{d}v =$	$\int_{\mathcal{S}} (\phi \cdot \mathbf{n})\,\mathrm{d}a$	$+ \int_{\mathcal{B}} \sigma \,\mathrm{d}v$	$+ \int_{\mathcal{B}} \hat{\Psi}\,\mathrm{d}v$
	$\frac{\mathrm{d}}{\mathrm{d}t}\int_{\mathcal{B}} \mathbf{\Psi} \,\mathrm{d}v =$	$\int_{\mathcal{S}} (\mathbf{\Phi}\, \mathbf{n})\,\mathrm{d}a$	$+ \int_{\mathcal{B}} \boldsymbol{\sigma} \,\mathrm{d}v$	$+ \int_{\mathcal{B}} \hat{\mathbf{\Psi}}\,\mathrm{d}v$

Local form:

$$\dot{\Psi} + \Psi \operatorname{div} \dot{\mathbf{x}} = \operatorname{div} \phi + \sigma + \hat{\Psi}\,,$$

$$\dot{\mathbf{\Psi}} + \mathbf{\Psi} \operatorname{div} \dot{\mathbf{x}} = \operatorname{div} \mathbf{\Phi} + \boldsymbol{\sigma} + \hat{\mathbf{\Psi}}$$

TH2M - THEORY

Balance Quantities:

Balance	$\Psi, \boldsymbol{\Psi}$	$\phi, \boldsymbol{\Phi}$	$\sigma, \boldsymbol{\sigma}$	$\hat{\Psi}, \hat{\boldsymbol{\Psi}}$
mass	ρ	$\mathbf{0}$	0	0
momentum	$\rho\,\dot{\mathbf{x}}$	$\mathbf{T}$	$\rho\,\mathbf{b} + \mathbf{b}_e$	$\mathbf{0}$
m. o. m.	$\mathbf{x} \times (\rho\,\dot{\mathbf{x}})$	$\mathbf{x} \times \mathbf{T}$	$\mathbf{x} \times (\rho\,\mathbf{b} + \mathbf{b}_e) + \mathbf{c}_e$	$\mathbf{0}$
energy	$\rho\,\varepsilon + \frac{1}{2}\,\dot{\mathbf{x}} \cdot (\rho\,\dot{\mathbf{x}})$	$\mathbf{T}^T\,\dot{\mathbf{x}} - \mathbf{q}$	$\dot{\mathbf{x}} \cdot (\rho\,\mathbf{b}) + \rho\,r + \varepsilon_e$	0
entropy	$\rho\,\eta$	$\boldsymbol{\phi}_\eta$	σ_η	$\hat{\eta}$
charge	ρ_e	$-\,\boldsymbol{\mathcal{J}}$	0	0
Gauss's law (elec.)	0	$-\,\mathbf{D}$	ρ_e	0
Gauss's law (magn.)	0	$-\,\mathbf{B}$	0	0
Faraday's law	$\mathbf{B}$	$-\,\boldsymbol{\mathcal{E}}$	$\mathbf{0}$	$\mathbf{0}$
Ampère's law	$-\mathbf{D}$	$-\,\boldsymbol{\mathcal{H}}$	$\boldsymbol{\mathcal{J}}$	$\mathbf{0}$

Ehlers, Wolfgang. "Foundations of multiphasic and porous materials." Porous media: theory, experiments and numerical applications. Berlin, Heidelberg: Springer Berlin Heidelberg, 2002. 3-86.

TH2M - THEORY

- **Formulation of:**
  - **Mass balances for two components (e.g. Water and Hydrogen) and for the solid phase**
  - **Energy balances for solid (S), liquid (L), and gaseous (G) phases**
  - **Momentum balances for S, L, G**
- **Evaluation of the entropy inequality**
- **Selection of *Ansatz* functions:**

$$\psi_\mathrm{S} = \psi_\mathrm{S}(\epsilon_\mathrm{S}, T, \rho_\mathrm{SR}) \quad \psi_\mathrm{L} = \psi_\mathrm{L}(T, \rho_\mathrm{LR}, s_\mathrm{L}) \quad \psi_\mathrm{G} = \psi_\mathrm{G}(T, \rho_\mathrm{GR})$$

- **Selection of primary variables:**
  - **Gas phase pressure: p_G, Capillary pressure: p_{cap},**
    Temperature: T, Displacement: $\underline{u}_S$
- **Develop of weak formulations:**

$$\psi \approx \tilde{\psi} = \mathrm{N}\hat{\psi} \qquad \mathrm{grad}\,\psi \approx \mathrm{grad}\,\tilde{\psi} = \nabla\mathrm{N}\hat{\psi}$$

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TH2M - THEORY

- **Implementation:**
  - Picard formulation
  - Numerical Jacobian in Quasi Newton-Raphson by perturbation of primary variables
- **Quasi Newton-Raphson Method:**
  - Numerical Jacobian computation
  - Perturbation-based approach
  - Avoids manual derivation
  - Increased runtime
- **Benefits and Trade-offs:**
  - Accurate numerical Jacobian
  - Trade-off: Longer runtime

Weak formulation of component mass:

$$
\begin{aligned}
&\underbrace{\int_\Omega \mathbf{N}_p^{\mathrm{T}} \rho_{\mathrm{FR}}^{\zeta} (\alpha_{\mathrm{B}} - \phi)\, \beta_{p,\mathrm{SR}} \mathbf{N}_p \,\mathrm{d}\Omega}_{\mathbf{M}_{\mathrm{pG}}^{\zeta}} (\hat{\boldsymbol{p}}_{\mathrm{GR}})'_{\mathrm{S}} - \underbrace{\int_\Omega \mathbf{N}_p^{\mathrm{T}} \rho_{\mathrm{FR}}^{\zeta} (\alpha_{\mathrm{B}} - \phi)\, \beta_{p,\mathrm{SR}} s_{\mathrm{L}} \mathbf{N}_p \,\mathrm{d}\Omega}_{\mathbf{M}_{\mathrm{pC}}^{\zeta}} (\hat{\boldsymbol{p}}_{\mathrm{cap}})'_{\mathrm{S}} \\
&+ \underbrace{\int_\Omega \nabla \mathbf{N}_p^{\mathrm{T}} \left(\rho_{\mathrm{GR}}^{\zeta} \frac{k_{\mathrm{G}}^{\mathrm{rel}} \boldsymbol{k}_{\mathrm{S}}}{\mu_{\mathrm{GR}}^{\nu}} + \rho_{\mathrm{LR}}^{\zeta} \frac{k_{\mathrm{L}}^{\mathrm{rel}} \boldsymbol{k}_{\mathrm{S}}}{\mu_{\mathrm{LR}}^{\nu}} + \rho_{\mathrm{G}} \boldsymbol{D}_{\mathrm{G}}^{\zeta} \frac{\partial x_{m,\mathrm{G}}^{\zeta}}{\partial p_{\mathrm{GR}}} + \rho_{\mathrm{L}} \boldsymbol{D}_{\mathrm{L}}^{\zeta} \frac{\partial x_{m,\mathrm{L}}^{\zeta}}{\partial p_{\mathrm{GR}}} \right) \nabla \mathbf{N}_p \,\mathrm{d}\Omega}_{\mathbf{L}_{\mathrm{pG}}^{\zeta}} \hat{\boldsymbol{p}}_{\mathrm{GR}} \\
&+ \underbrace{\int_\Omega \nabla \mathbf{N}_p^{\mathrm{T}} \left(\rho_{\mathrm{G}} \boldsymbol{D}_{\mathrm{G}}^{\zeta} \frac{\partial x_{m,\mathrm{G}}^{\zeta}}{\partial p_{\mathrm{cap}}} + \rho_{\mathrm{L}} \boldsymbol{D}_{\mathrm{L}}^{\zeta} \frac{\partial x_{m,\mathrm{L}}^{\zeta}}{\partial p_{\mathrm{cap}}} - \rho_{\mathrm{LR}}^{\zeta} \frac{k_{\mathrm{L}}^{\mathrm{rel}} \boldsymbol{k}_{\mathrm{S}}}{\mu_{\mathrm{LR}}^{\nu}} \right) \nabla \mathbf{N}_p \,\mathrm{d}\Omega\, \hat{\boldsymbol{p}}_{\mathrm{cap}}}_{\mathbf{L}_{\mathrm{pC}}^{\zeta}} + \underbrace{\int_\Omega \mathbf{N}_p^{\mathrm{T}} \rho_{\mathrm{FR}}^{\zeta} \alpha_{\mathrm{B}} \boldsymbol{m}^{\mathrm{T}} \mathbf{B}_u \,\mathrm{d}\Omega}_{\mathbf{M}_{\mathrm{uS}}^{\zeta}} (\hat{\boldsymbol{u}}_{\mathrm{S}})'_{\mathrm{S}} \\
&- \underbrace{\int_\Omega \mathbf{N}_p^{\mathrm{T}} \rho_{\mathrm{FR}}^{\zeta} (\alpha_{\mathrm{B}} - \phi)\, \beta_{T,\mathrm{SR}} \mathbf{N}_p \,\mathrm{d}\Omega}_{\mathbf{M}_{\mathrm{T}}^{\zeta}} (\hat{\boldsymbol{T}})'_{\mathrm{S}} + \underbrace{\int_\Omega \nabla \mathbf{N}_p^{\mathrm{T}} \left(\rho_{\mathrm{G}} \boldsymbol{D}_{\mathrm{G}}^{\zeta} \frac{\partial x_{m,\mathrm{G}}^{\zeta}}{\partial T} + \rho_{\mathrm{L}} \boldsymbol{D}_{\mathrm{L}}^{\zeta} \frac{\partial x_{m,\mathrm{L}}^{\zeta}}{\partial T} \right) \nabla \mathbf{N}_p \,\mathrm{d}\Omega\, \hat{\boldsymbol{T}}}_{\mathbf{L}_{\mathrm{T}}^{\zeta}} \\
&= \underbrace{\int_\Omega \nabla \mathbf{N}_p^{\mathrm{T}} \left(\rho_{\mathrm{GR}}^{\zeta} \frac{k_{\mathrm{G}}^{\mathrm{rel}} \boldsymbol{k}_{\mathrm{S}}}{\mu_{\mathrm{GR}}^{\nu}} \rho_{\mathrm{GR}} + \rho_{\mathrm{LR}}^{\zeta} \frac{k_{\mathrm{L}}^{\mathrm{rel}} \boldsymbol{k}_{\mathrm{S}}}{\mu_{\mathrm{LR}}^{\nu}} \rho_{\mathrm{LR}} \right) \boldsymbol{b} \,\mathrm{d}\Omega}_{f_{\mathrm{I}}^{\zeta}} - \underbrace{\int_\Omega \mathbf{N}_p^{\mathrm{T}} \phi \left[s_{\mathrm{G}} (\rho_{\mathrm{GR}}^{\zeta})'_{\mathrm{S}} + s_{\mathrm{L}} (\rho_{\mathrm{LR}}^{\zeta})'_{\mathrm{S}} \right] \mathrm{d}\Omega}_{f_{\mathrm{II}}^{\zeta}} \\
&- \underbrace{\int_\Omega \mathbf{N}_p^{\mathrm{T}} \left[\phi \left(\rho_{\mathrm{LR}}^{\zeta} - \rho_{\mathrm{GR}}^{\zeta} \right) - \rho_{\mathrm{FR}}^{\zeta} p_{\mathrm{cap}} (\alpha_{\mathrm{B}} - \phi)\, \beta_{p,\mathrm{SR}} \right] (s_{\mathrm{L}})'_{\mathrm{S}} \,\mathrm{d}\Omega}_{f_{\mathrm{III}}^{\zeta}} + \underbrace{\int_{\partial\Omega} \mathbf{N}_p^{\mathrm{T}} \dot{m}_{\mathrm{AJ}}^{\zeta} \,\mathrm{d}\Gamma}_{f_{\mathrm{IV}}^{\zeta}}
\end{aligned}
$$

TH2M Benchmarking

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TH2M BENCHMARK HIERARCHY

1 Primary variable	T • Linear/ radial heat conduction • thermal diffusion	H^a • Single-phase flow • **Darcy** flow • Compressible fluid flow	M • Linear-elastic deformation
2 Primary variables	TH • Thermal advection/diffusion **Ogata** | **Banks** exact solution	HC • Diffusion equation	H^2 • Two-phase flow: **McWhorter** exact solution
	TM • Thermo-elastic plate/cube	H^2C • Phase (dis-)appearance **Bourgeat** benchmark	HM • Poro-elastic column consolidation
3 Primary variables	THM • Point heat source consolidation **Booker** | **Chaudry** exact solution	TH^2C • Heat pipe problem **Udell** | **Doughty** benchmark	H^2M • Poro-elastic soil consolidation **Liakopoulos** benchmark
4 Primary variables	TH^2M • unsaturated point heat source **Cherati** exact solution		

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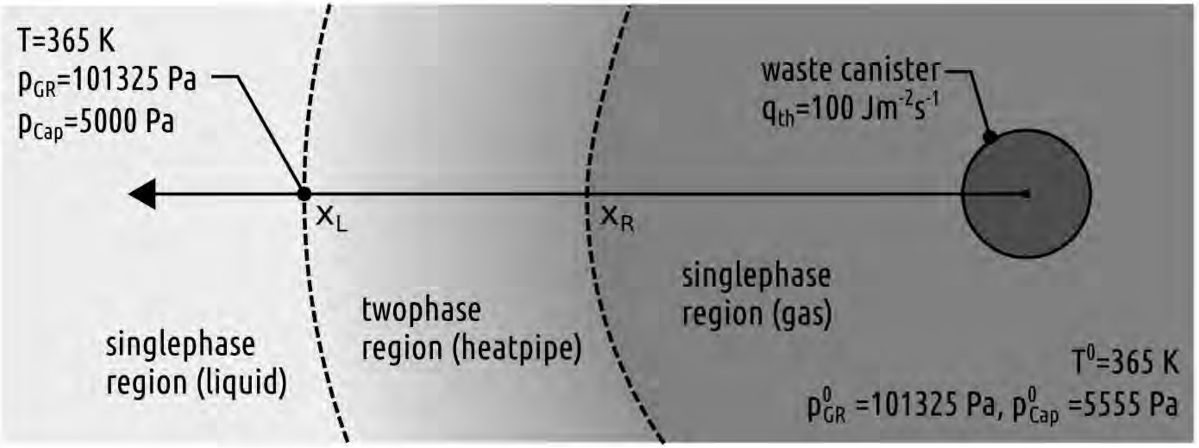
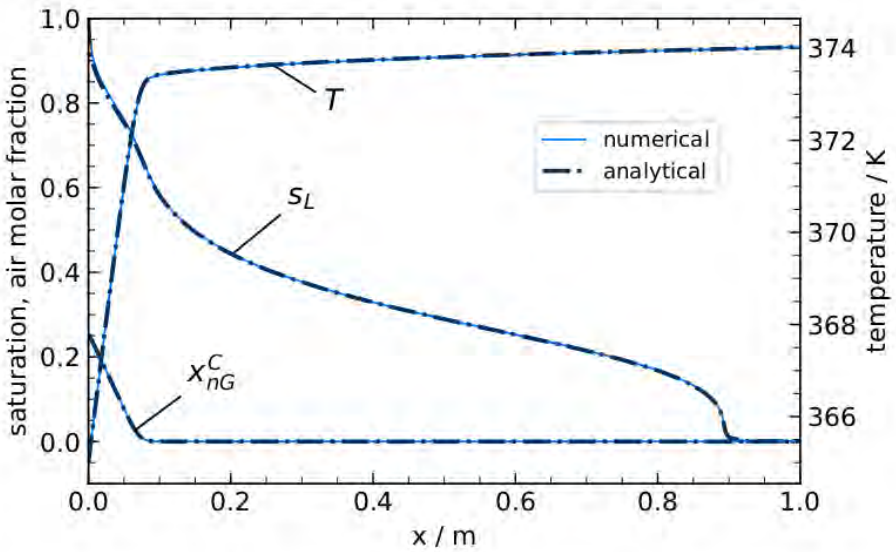
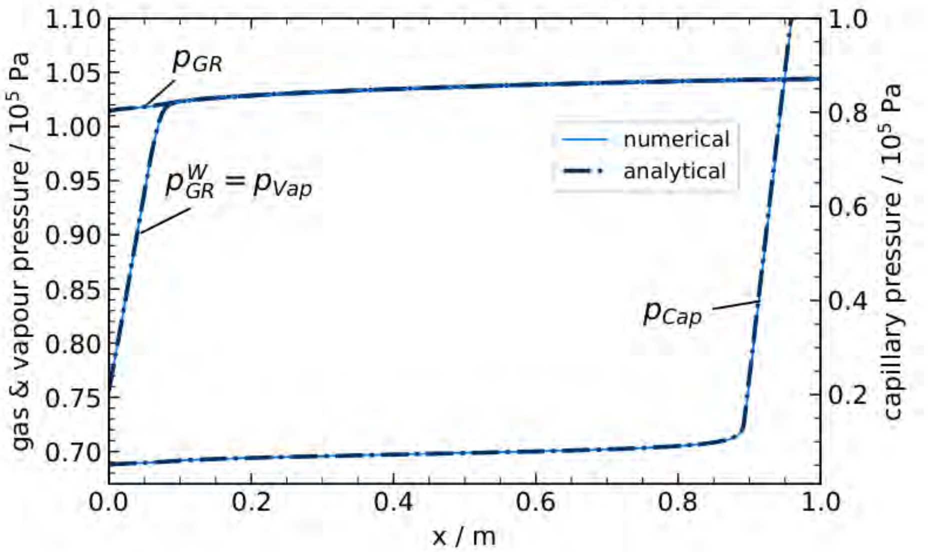
BENCHMARK TEST: HEATPIPE PROBLEM

Heatpipe effect, steady state analytical solution (Udell, 1985)

- Water evaporates at the right edge
- Steam flows to the left edge and condenses, giving off energy in the form of enthalpy of condensation
- The condensate flows back to the right edge.
- High rate of heat transport



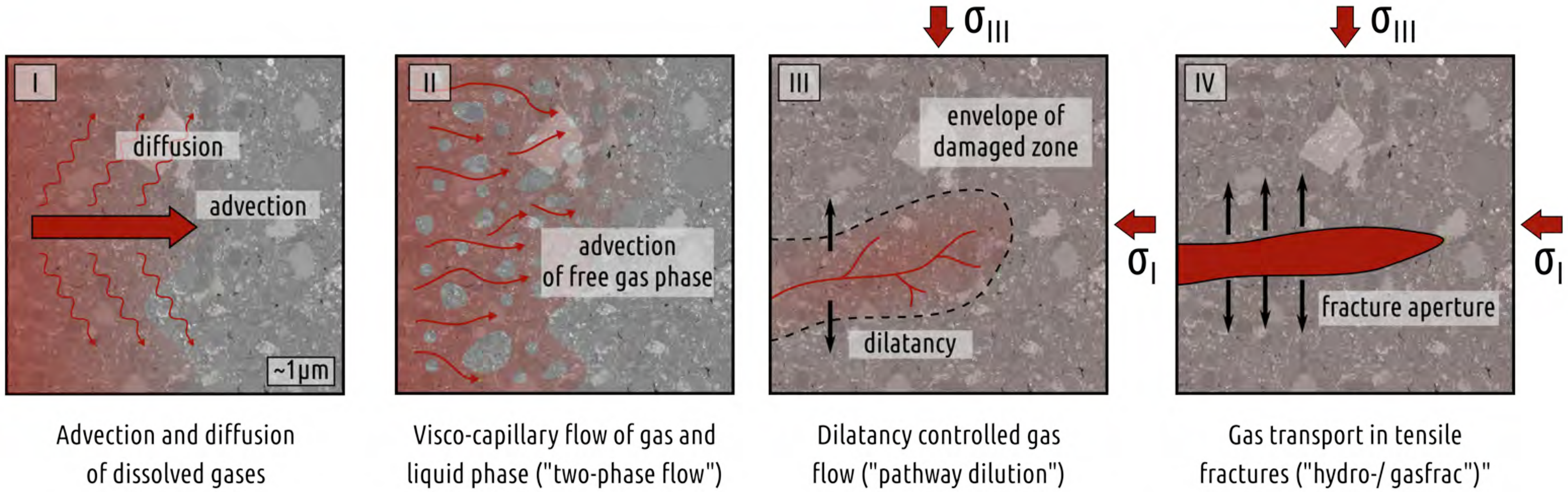




Udell, Kent S. “Heat transfer in porous media considering phase change and capillarity—the heat pipe effect.” International Journal of Heat and Mass Transfer 28.2 (1985): 485-495.

TH2M Test Case

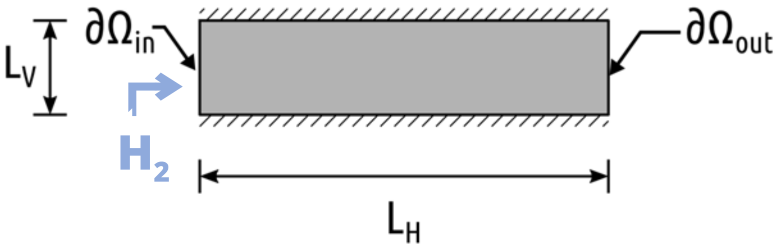
GAS TRANSPORT REGIMES
IN LOW PERMEABLE MEDIA



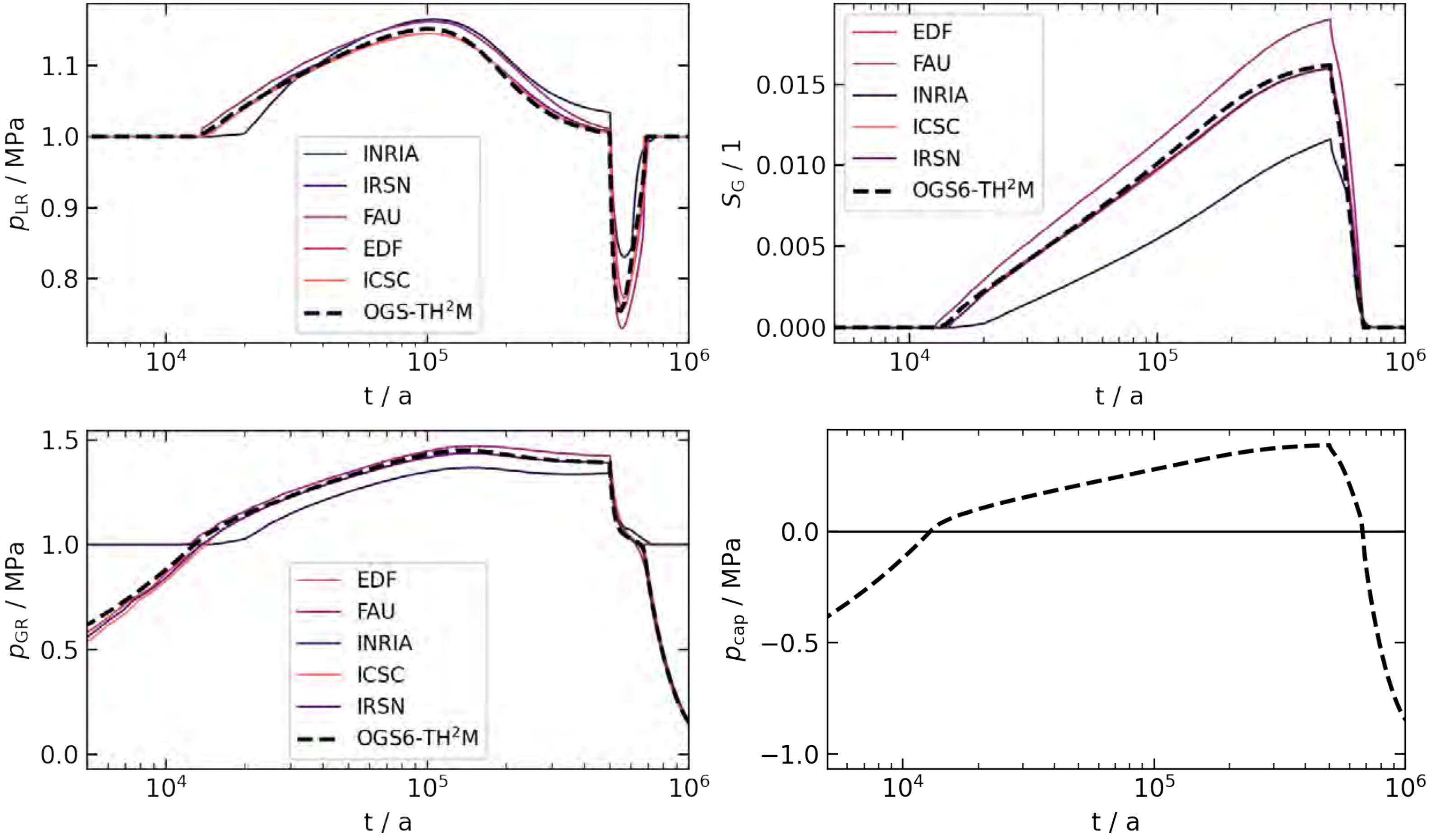
Classification of gas transport regimes in clay rock, adapted and modified from Marschall et al. [2005]

Grunwald, N., Nagel, T., Pitz, M., Kolditz, O. "Extended analysis of benchmarks for gas phase appearance in low-permeable rocks". Under Review at Geomechanics and Geophysics for Geo-Energy and Geo-Resources, 2023. in

PHASE APPEARANCE / DISAPPEARANCE



- Benchmark (Bourgeat et al.)
- Continuous H_2-injection at $\partial\Omega_{in}$ at $0 \leq t \leq 500{,}000$a
- Gas phase appears at t≈15,000a
- At t=500,000a rapid drop in water pressure
- Gas phase disappears at t≈700,000a7



A. **Bourgeat** et al. ”Compositional two-phase flow in saturated-unsaturated porous media: benchmarks for phase appearance/ disappearance“. In: Simulation of flow in porous media 12 (2013), S. 81–106.

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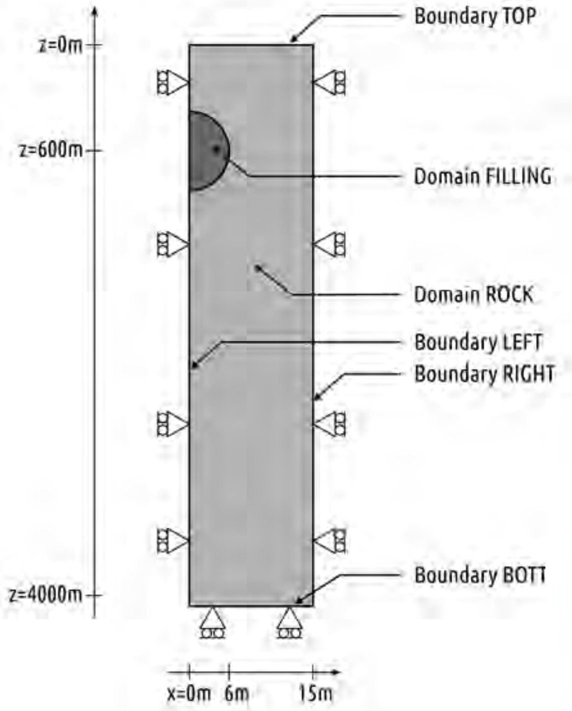
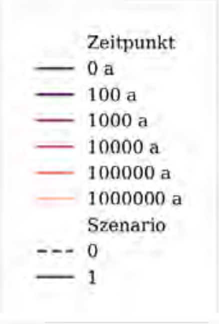
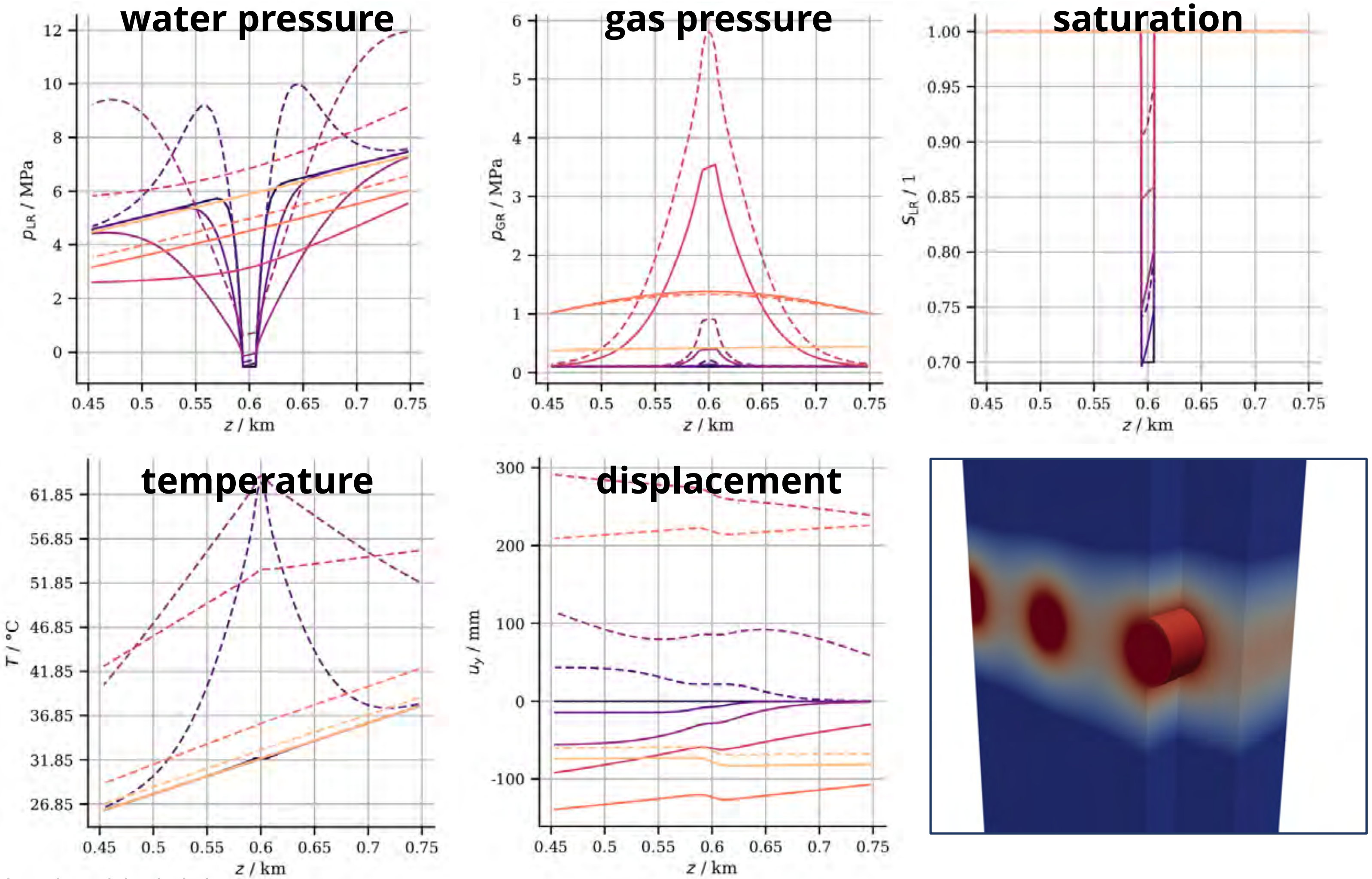
APPLICATION: HLWR-SCALE TH2M-SIMULATION I

Motivated by ANSICHT-II* project
created within a cooperation with BGR







Entry-point for eurad HITEC

*Jobmann, M. et al. (2022, in review): ANSICHT-II: Methodik und Beispiele für eine Sicherheitsbewertung von Endlagersystemen im Tongestein in Deutschland. Synthesebericht. BGR, BGETEC, GRS

APPLICATION: HLWR-SCALE TH2M-SIMULATION II