



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



TECHNISCHE UNIVERSITÄT
BERGAKADEMIE FREIBERG

Die Ressourcenuniversität. Seit 1765.



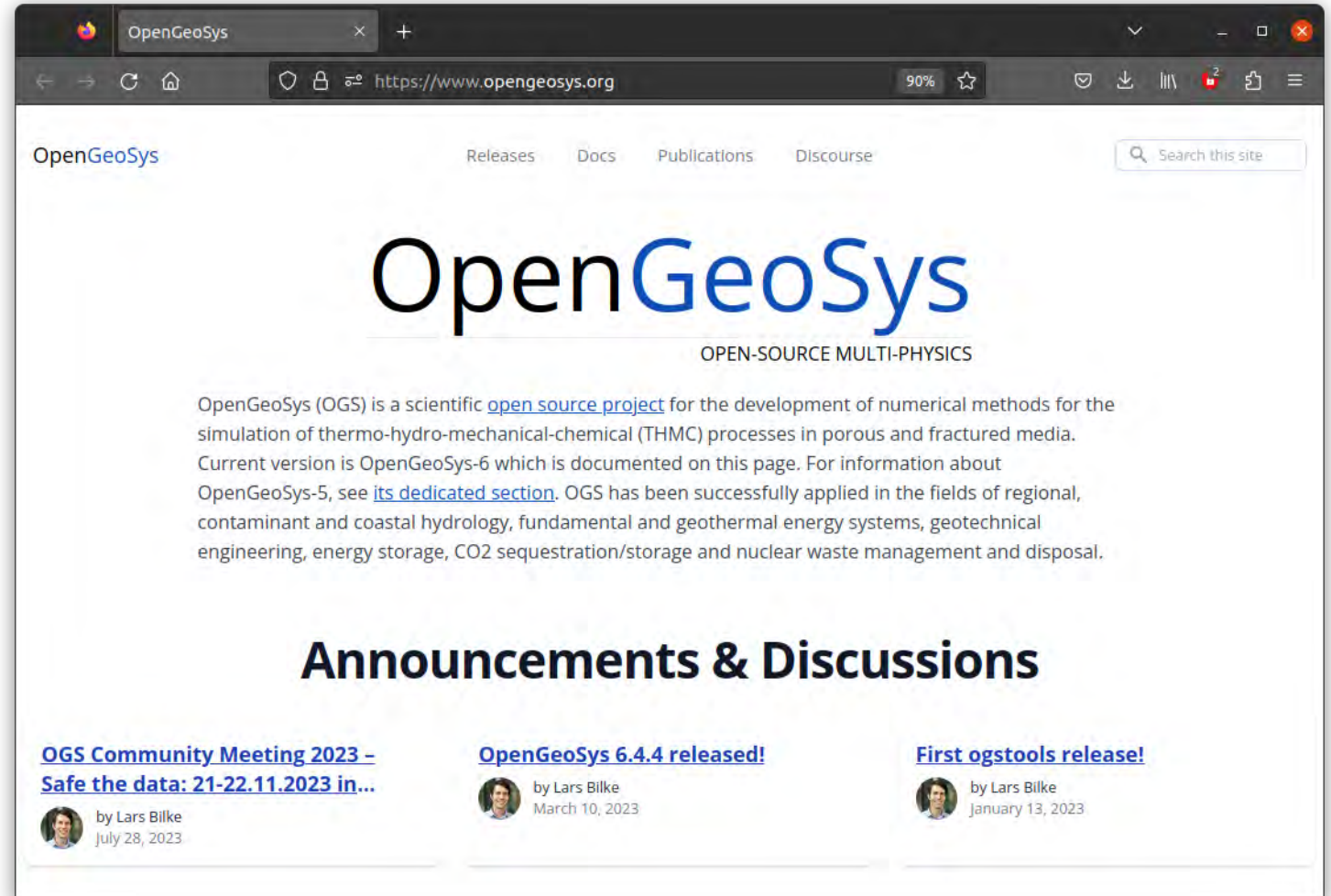
Discovering the Project Website

PROJECT WEBSITE

- **features**

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

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



The screenshot shows the OpenGeoSys website in a browser window. The browser's address bar displays the URL <https://www.opengeosys.org/>. The website header includes the OpenGeoSys logo, navigation links for Releases, Docs, Publications, and Discourse, and a search bar. The main content area features the OpenGeoSys logo and the tagline "OPEN-SOURCE MULTI-PHYSICS". Below this, a paragraph describes the project as a scientific open source project for developing numerical methods for simulating thermo-hydro-mechanical-chemical (THMC) processes in porous and fractured media. It mentions the current version is OpenGeoSys-6 and provides a link to a dedicated section for OpenGeoSys-5. The page also includes a section titled "Announcements & Discussions" with three recent posts: "OGS Community Meeting 2023 - Safe the data: 21-22.11.2023 in..." by Lars Bilke (July 28, 2023), "OpenGeoSys 6.4.4 released!" by Lars Bilke (March 10, 2023), and "First ogstools release!" by Lars Bilke (January 13, 2023).

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**



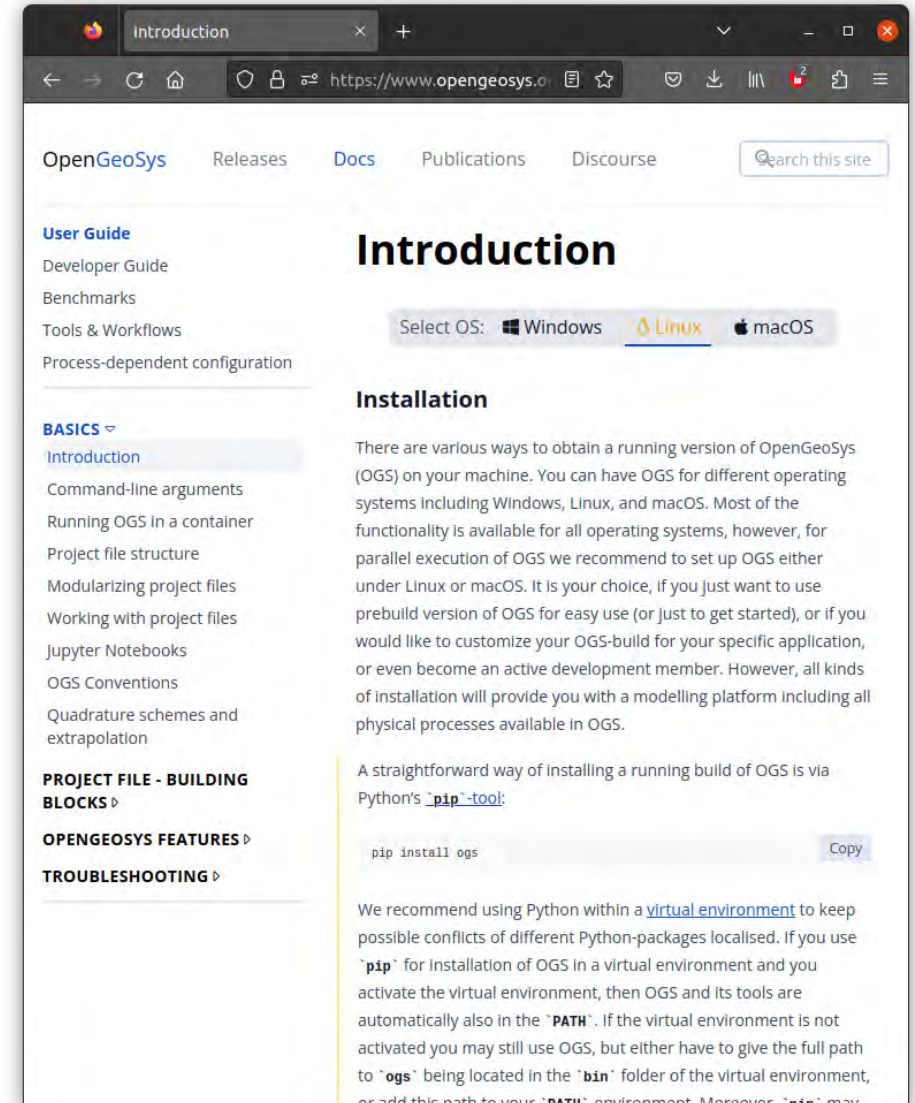
– **Source Code on GitLab:**

- **Access GitLab repository:**
<https://gitlab.opengeosys.org/>
- **Docs -> Developer Guide contains compilation instructions**

• **Start Using OGS:**



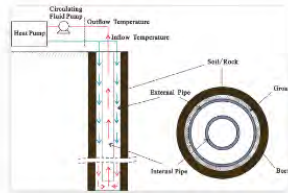
- **Grab an Example Benchmark Test: Explore our sample benchmark tests in the software package**
- **Use them as templates for your own projects**



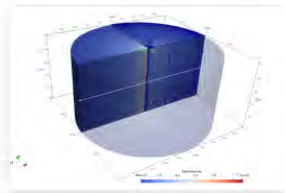
The screenshot shows the OpenGeoSys website's introduction page. The browser address bar shows the URL <https://www.opengeosys.org/>. The page has a navigation menu with links for OpenGeoSys, Releases, Docs, Publications, and Discourse. A search bar is located in the top right corner. The main content area is titled "Introduction" and includes a "Select OS:" dropdown menu with options for Windows, Linux (selected), and macOS. Below this, there is an "Installation" section with text explaining how to obtain a running version of OpenGeoSys (OGS) on different operating systems. A code block shows the command `pip install ogs` with a "Copy" button. The page also features a sidebar with a "User Guide" section containing links to Developer Guide, Benchmarks, Tools & Workflows, and Process-dependent configuration. Other sections include "BASICS" (Introduction, Command-line arguments, Running OGS in a container, Project file structure, Modularizing project files, Working with project files, Jupyter Notebooks, OGS Conventions, Quadrature schemes and extrapolation), "PROJECT FILE - BUILDING BLOCKS", "OPENGEOSYS FEATURES", and "TROUBLESHOOTING".

BENCHMARK GALLERY

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



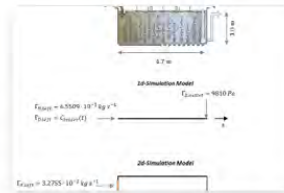
Heat Transport BHE



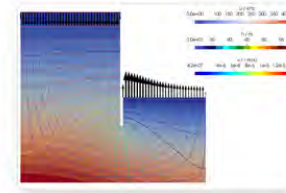
Heatconduction



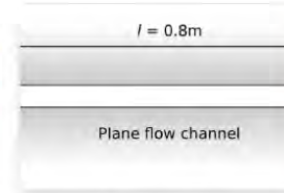
Hydro Mechanics



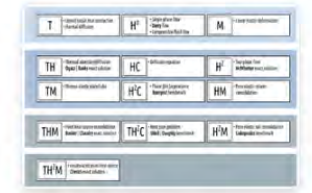
Hydro-Component



Steady State Diffusion



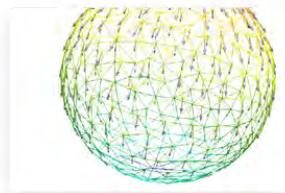
Stokes Flow



TH2M



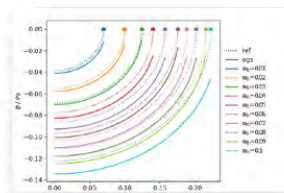
Hydro-Thermal



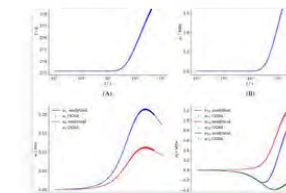
Liquid Flow



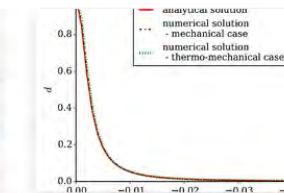
Phase-Field



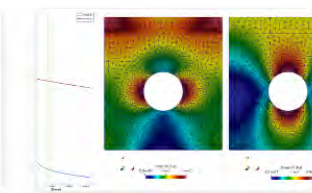
Python Boundary Conditions



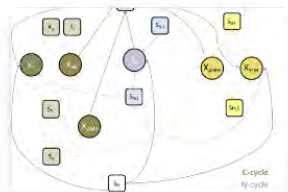
Thermo-Hydro-Mechanics



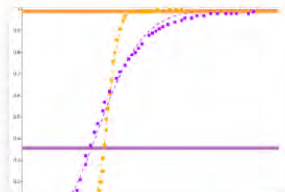
Thermo-Mechanical Phase-Field



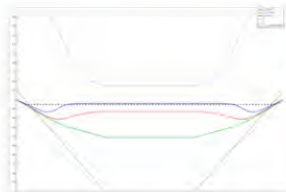
Thermo-Mechanics



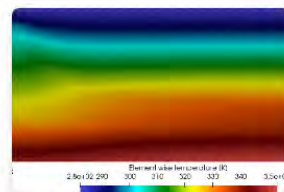
Reactive Transport



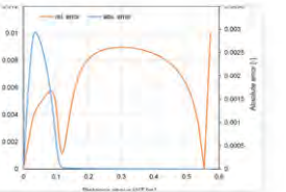
Richards Flow



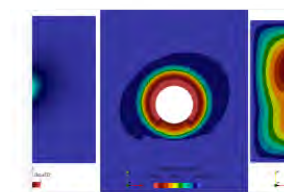
Richards Mechanics



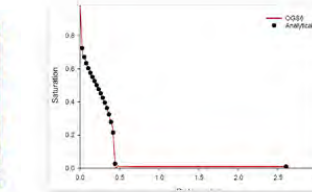
Small Deformations



Thermal-Two-Phase Flow



Thermo-Richards-Mechanics



Two-phase Flow

EXPLORING GITLAB REPOSITORY

The screenshot shows the GitLab web interface for the repository 'ogs/ogs'. The browser address bar shows the URL <https://gitlab.openeosys.org/ogs/ogs>. The repository page includes a sidebar with navigation options like 'Project overview', 'Issues', 'Merge requests', 'Code', 'Build', 'Secure', 'Deploy', 'Operate', 'Monitor', and 'Analyze'. The main content area displays the repository name 'ogs', project ID '120', and statistics: 24,406 Commits, 9 Branches, 29 Tags, 1 TiB Project Storage, 24 Releases, and 23 Environments. A merge request is visible, titled 'Merge branch 'cubic_law_for_fracture' into 'master'', authored by Dmitry Yu. Naumov 2 days ago. Below the merge request, there are buttons for 'History', 'Find file', 'Edit', and 'Clone'. A table lists the repository's files and their last commit details.

Name	Last commit	Last update
<code>.github/workflows</code>	Removed OGS_USE_PYTHON in remaining places.	4 months ago
<code>.gitlab</code>	[ci] Make CMake CODEOWNERS approval optional.	1 month ago
<code>.guix/modules</code>	[guix] Cleanup, adding TODOs.	1 month ago
<code>.hooks</code>	[pre-commit] Fixed check-shebang-scripts-are-execut...	1 year ago
<code>Applications</code>	[ProcessLib/BC] Import media into BC implementation.	1 week ago
<code>BaseLib</code>	[BL] Add to string conversion for iostate	1 week ago
<code>ChemistryLib</code>	[CL] Add safety condition before access	1 month ago
<code>Documentation</code>	[Doc/CubicLaw] Add para doc files.	2 days ago
<code>Geolib</code>	[cmake] Fix fml-target	3 days ago

ENGAGE WITH THE DEVS ON OUR DISCOURSE

The screenshot shows the OpenGeoSys Discourse forum interface. The browser address bar displays `https://discourse.opengeosys.org`. The forum header includes the OpenGeoSys logo and navigation links for Releases, Docs, and Publications. A notification banner at the top asks, "Do you want live notifications when people reply to your posts? Enable Notifications". Below this, there are filters for "all categories", "all tags", and a "Latest" button. A table of topics is displayed with columns for Topic, Replies, Views, and Activity.

Topic	Replies	Views	Activity
<p>Discourse New User Guide</p> <p>Site Feedback</p> <p>Welcome! As a new user of Discourse, we hope you will find this site intuitive and clearly structured, but here is some guidance to get you started: Basic Terms Used by Discourse (Nomenclature) Here are some very bas... read more</p>	1	169	May 15
<p>1D Heat Conduction problem</p> <p>Usability ogs6</p>	5	43	1d
— last visit —			
Set initial stresses from MeshNodeParameter or MeshElementParameter	4	33	4d
Reg. creation of a ProcessLib combining HM and ComponentTrasport	0	26	8d
AttributeError: module 'ogs' has no attribute 'BoundaryCondition'	1	36	9d
Error: ModuleNotFoundError: No module named 'OpenGeoSys'	1	46	9d
New Project Issues: Parameter has wrong number of components; key <parameter> has been read 1 time(s) less than it was present in the configuration tree	5	47	10d
How to use grdecl or zmap grid / or how to convert them to msh or vtu	1	35	11d



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Configuring a OGS Project

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>
```

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>
```

INPUT FILE STRUCTURE

Project File *.prj

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  <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 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`

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

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

INPUT FILE STRUCTURE

Project File *.prj

3. Define the domain/bulk mesh
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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>
```

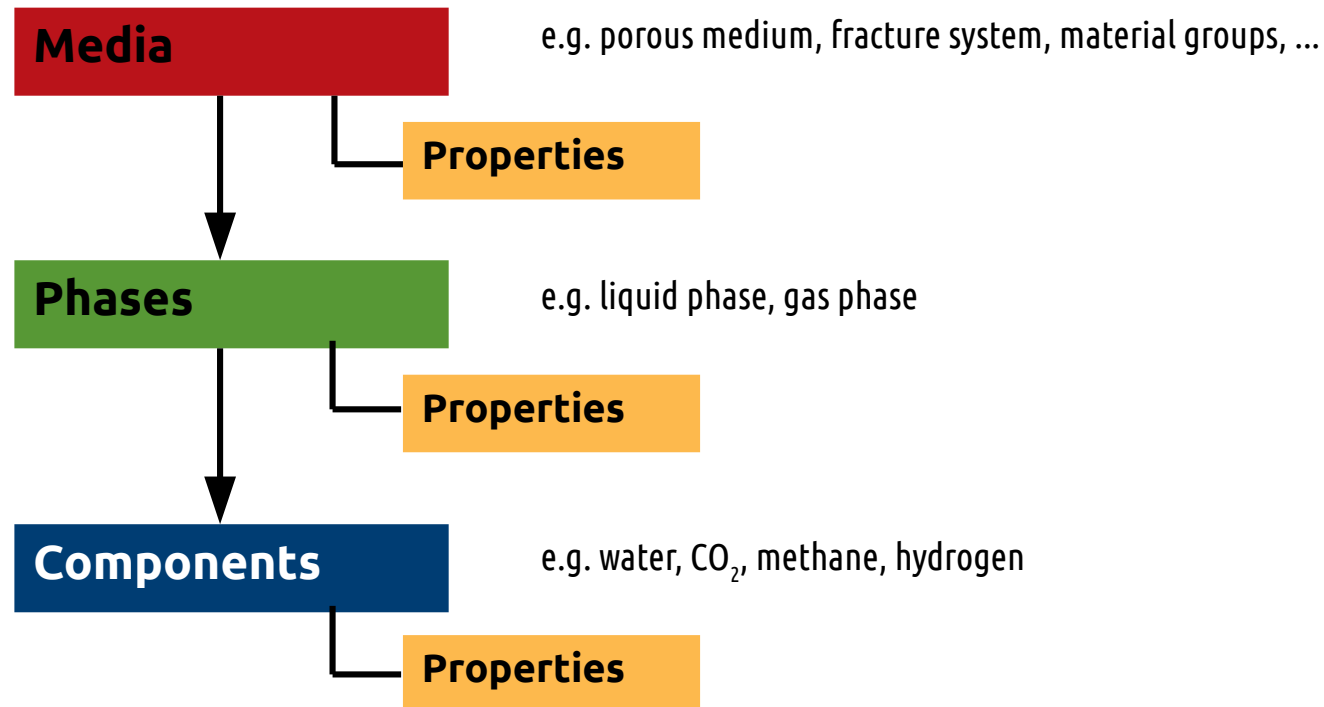
INPUT FILE STRUCTURE

Project File *.prj

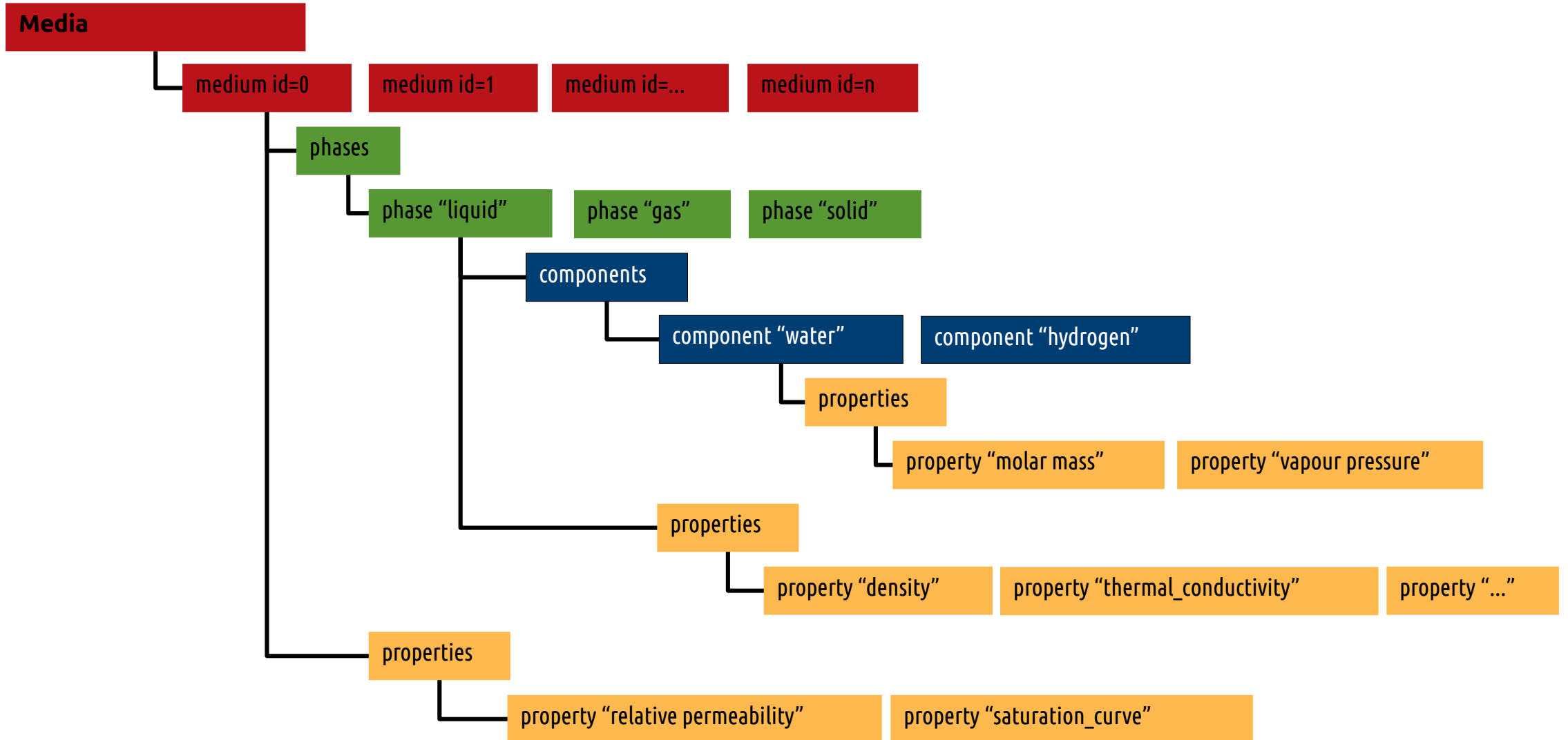
3. Define the domain/bulk mesh
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convergence criteria

```
<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



DETOUR - MATERIAL PROPERTY HIERARCHY



INPUT FILE STRUCTURE

Project File *.prj

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

```

<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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```
<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
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5. Specify process(es)
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9. Set solver properties/
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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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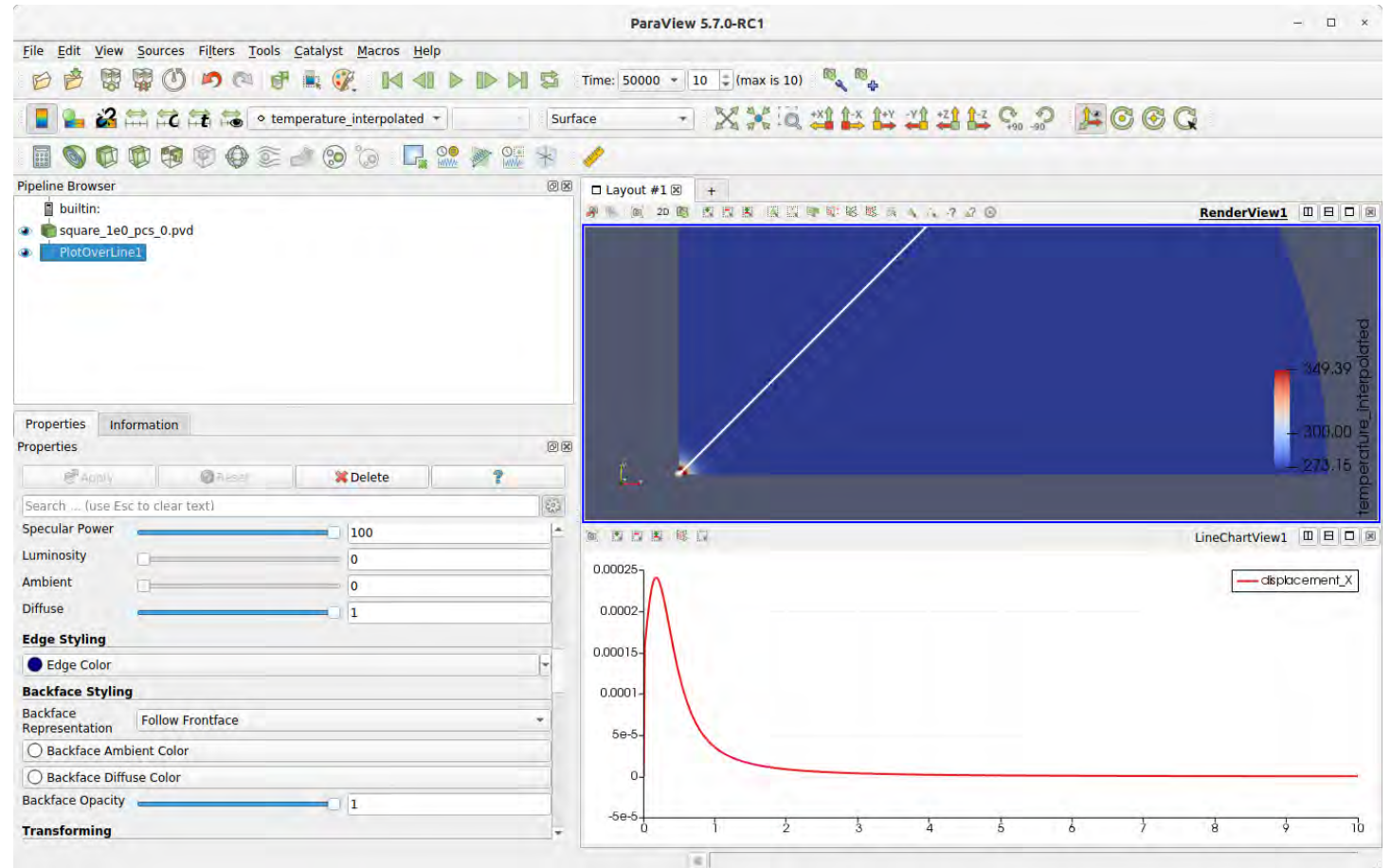
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Example Project File

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.

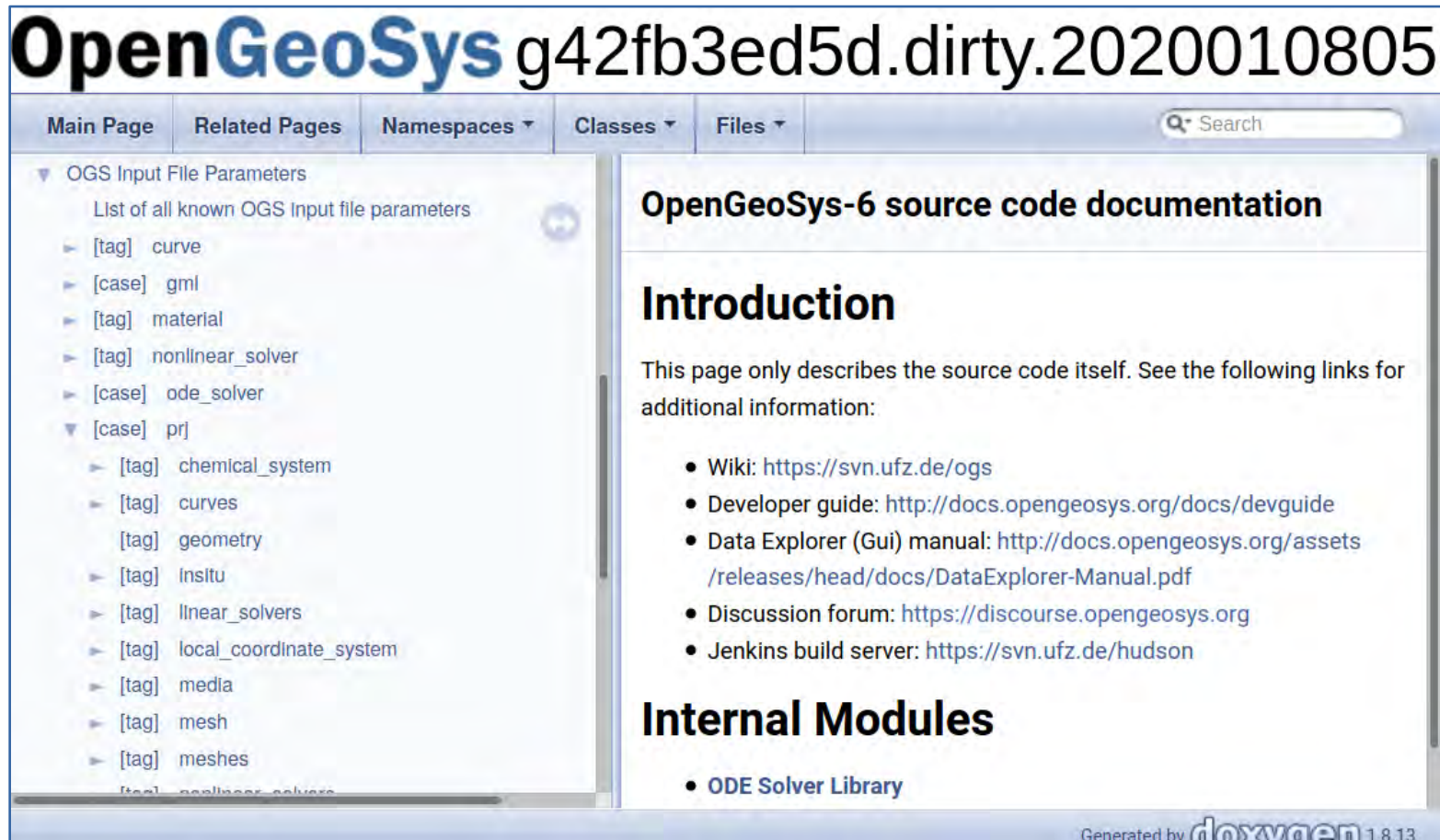
vtuIO

- 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/>



OpenGeoSys g42fb3ed5d.dirty.2020010805

Main Page | Related Pages | Namespaces ▾ | Classes ▾ | Files ▾ | Search

▼ OGS Input File Parameters
List of all known OGS Input file parameters

- ▶ [tag] curve
- ▶ [case] gml
- ▶ [tag] material
- ▶ [tag] nonlinear_solver
- ▶ [case] ode_solver
- ▼ [case] prj
 - ▶ [tag] chemical_system
 - ▶ [tag] curves
 - [tag] geometry
 - ▶ [tag] Insitu
 - ▶ [tag] linear_solvers
 - ▶ [tag] local_coordinate_system
 - ▶ [tag] media
 - ▶ [tag] mesh
 - ▶ [tag] meshes
 - [tag] nonlinear_solvers

OpenGeoSys-6 source code documentation

Introduction

This page only describes the source code itself. See the following links for additional information:

- Wiki: <https://svn.ufz.de/ogs>
- Developer guide: <http://docs.opengeosys.org/docs/devguide>
- Data Explorer (Gui) manual: <http://docs.opengeosys.org/assets/releases/head/docs/DataExplorer-Manual.pdf>
- Discussion forum: <https://discourse.opengeosys.org>
- Jenkins build server: <https://svn.ufz.de/hudson>

Internal Modules

- ODE Solver Library

Generated by **doxygen** 1.8.13



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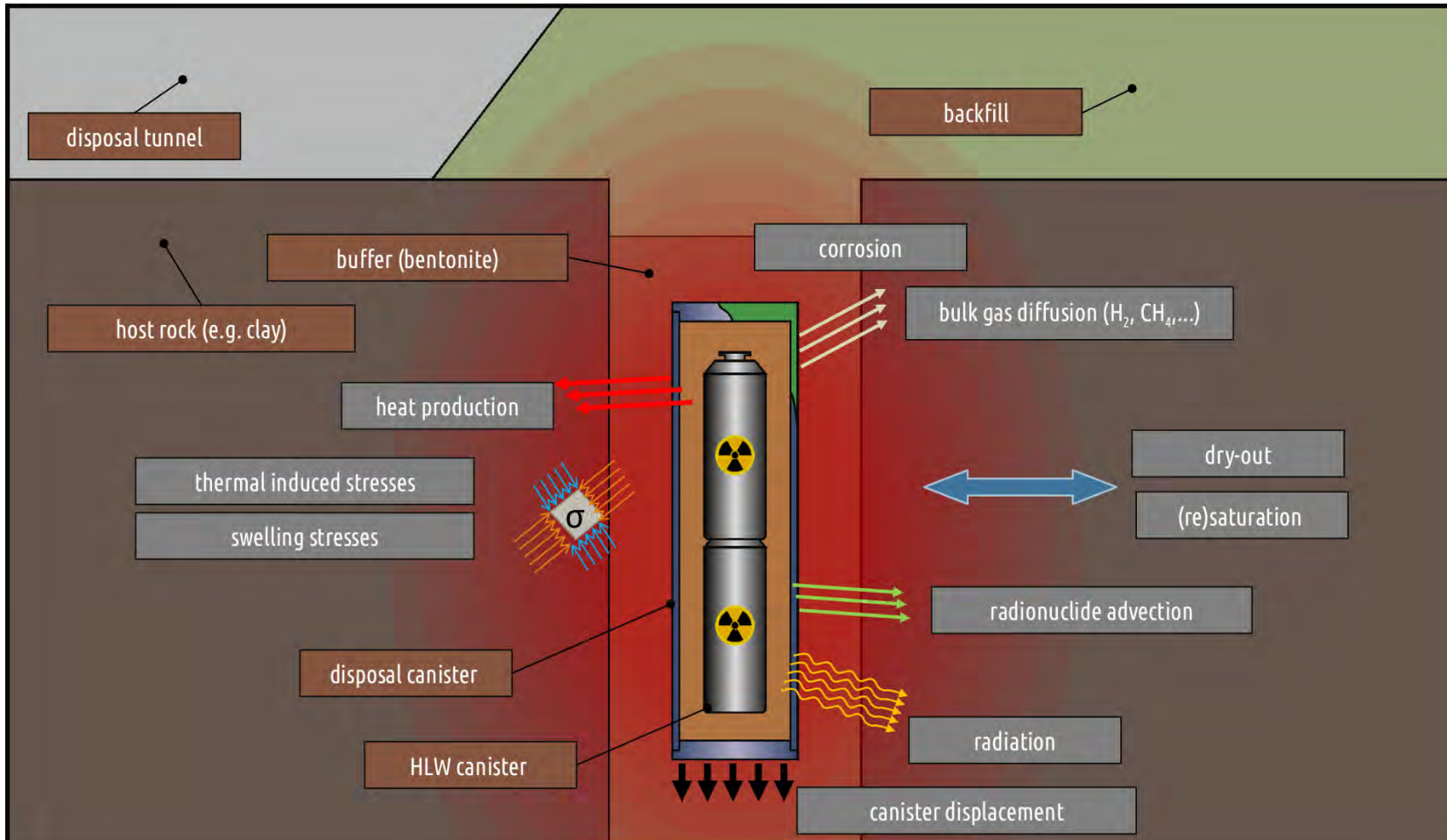
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Motivation for TH2M

FOUNDATIONS OF MULTIPHYSICS SIMULATIONS

INTRODUCING THERMO-HYDRAULIC MULTIPHASE MECHANICS (TH2M) SIMULATION





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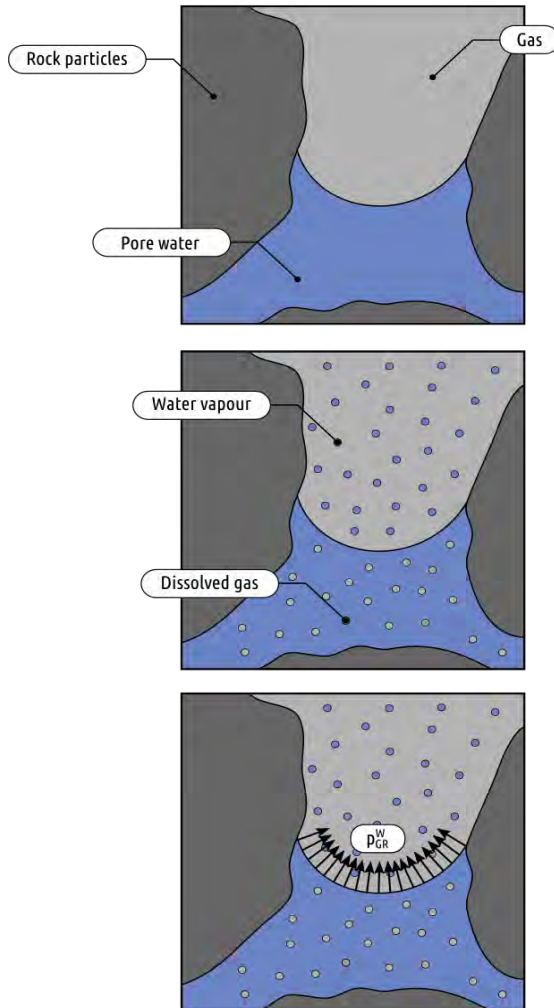
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TH2M Theory

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

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

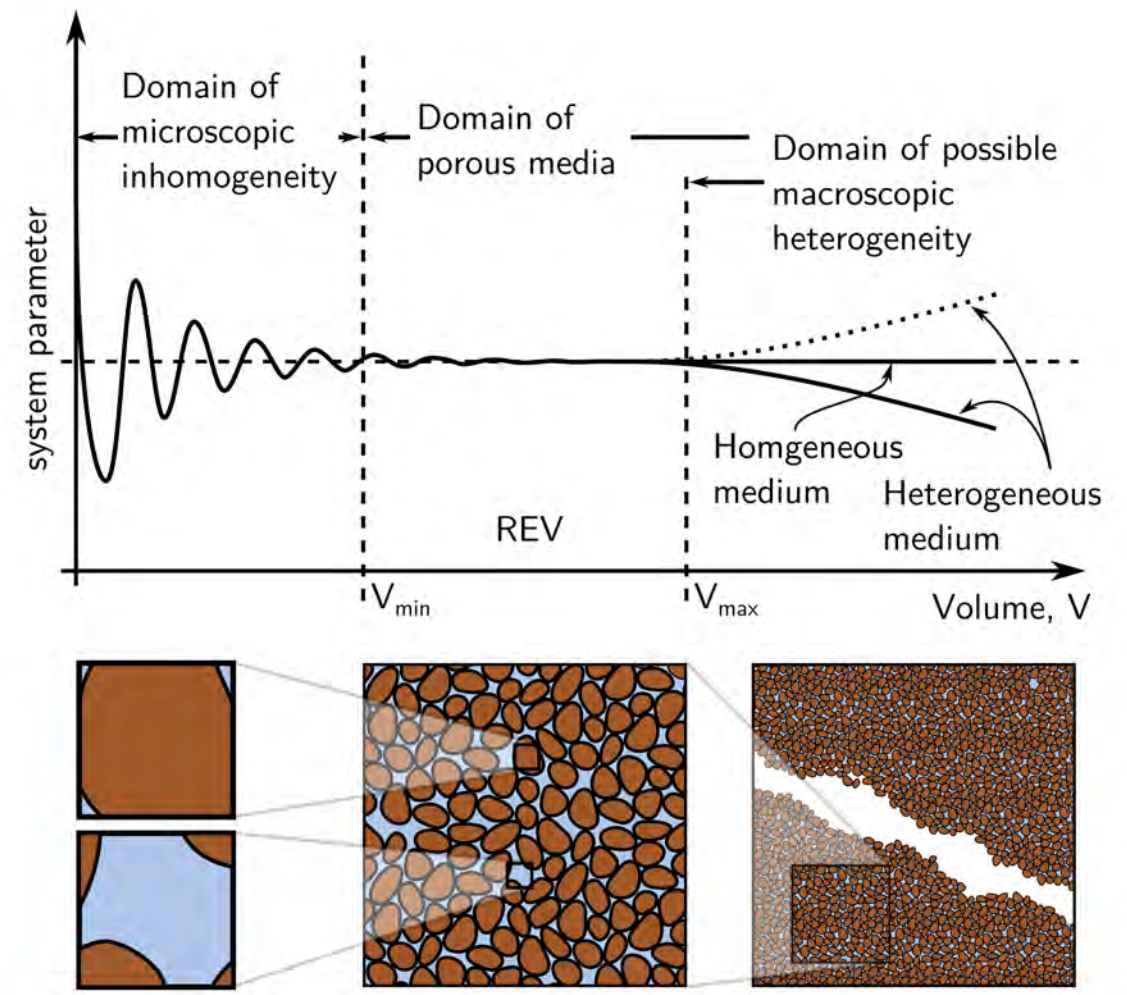
Control volume:

"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.

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



TH2M - THEORY

General Balance Equation for Single-Phase Bodies:

Change in Ψ	due to: out/inflow	supply	production
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Global form:

$$\frac{d}{dt} \int_{\mathcal{B}} \psi \, dv = \int_{\mathcal{S}} (\phi \cdot \mathbf{n}) \, da + \int_{\mathcal{B}} \sigma \, dv + \int_{\mathcal{B}} \hat{\psi} \, dv$$

$$\frac{d}{dt} \int_{\mathcal{B}} \Psi \, dv = \int_{\mathcal{S}} (\Phi \mathbf{n}) \, da + \int_{\mathcal{B}} \sigma \, dv + \int_{\mathcal{B}} \hat{\Psi} \, dv$$

Local form:

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

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

TH2M - THEORY

Balance Quantities:

Balance	Ψ, Ψ	ϕ, Φ	σ, σ	$\hat{\Psi}, \hat{\Psi}$
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	$\rho \eta$	ϕ_η	σ_η	$\hat{\eta}$
charge	ρ_e	$-\mathcal{J}$	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}	$-\mathcal{E}$	0	0
Ampère's law	$-\mathbf{D}$	$-\mathcal{H}$	\mathcal{J}	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:**

$$\psi_S = \psi_S(\epsilon_S, T, \rho_{SR}) \quad \psi_L = \psi_L(T, \rho_{LR}, s_L) \quad \psi_G = \psi_G(T, \rho_{GR})$$

- **Selection of primary variables:**

- Gas phase pressure: p_G , Capillary pressure: p_{cap}
Temperature: T , Displacement: \underline{u}_S

- **Develop of weak formulations:**

$$\psi \approx \tilde{\psi} = N\hat{\psi} \quad \text{grad } \psi \approx \text{grad } \tilde{\psi} = \nabla N\hat{\psi}$$

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^T \rho_{FR}^{\zeta} (\alpha_B - \phi) \beta_{p,SR} \mathbf{N}_p \, d\Omega}_{M_{pG}^{\zeta}} (\hat{\mathbf{p}}_{GR})'_S - \underbrace{\int_{\Omega} \mathbf{N}_p^T \rho_{FR}^{\zeta} (\alpha_B - \phi) \beta_{p,SR^S L} \mathbf{N}_p \, d\Omega}_{M_{pC}^{\zeta}} (\hat{\mathbf{p}}_{cap})'_S \\
 & + \underbrace{\int_{\Omega} \nabla \mathbf{N}_p^T \left(\rho_{GR}^{\zeta} \frac{k_G^{rel} \mathbf{k}_S}{\mu_{GR}^v} + \rho_{LR}^{\zeta} \frac{k_L^{rel} \mathbf{k}_S}{\mu_{LR}^v} + \rho_G D_G^{\zeta} \frac{\partial x_{m,G}^{\zeta}}{\partial p_{GR}} + \rho_L D_L^{\zeta} \frac{\partial x_{m,L}^{\zeta}}{\partial p_{GR}} \right) \nabla \mathbf{N}_p \, d\Omega}_{L_{pG}^{\zeta}} \hat{\mathbf{p}}_{GR} \\
 & + \underbrace{\int_{\Omega} \nabla \mathbf{N}_p^T \left(\rho_G D_G^{\zeta} \frac{\partial x_{m,G}^{\zeta}}{\partial p_{cap}} + \rho_L D_L^{\zeta} \frac{\partial x_{m,L}^{\zeta}}{\partial p_{cap}} - \rho_{LR}^{\zeta} \frac{k_L^{rel} \mathbf{k}_S}{\mu_{LR}^v} \right) \nabla \mathbf{N}_p \, d\Omega}_{L_{pC}^{\zeta}} \hat{\mathbf{p}}_{cap} + \underbrace{\int_{\Omega} \mathbf{N}_p^T \rho_{FR}^{\zeta} \alpha_B \mathbf{m}^T \mathbf{B}_u \, d\Omega}_{M_{us}^{\zeta}} (\hat{\mathbf{u}}_S)'_S \\
 & - \underbrace{\int_{\Omega} \mathbf{N}_p^T \rho_{FR}^{\zeta} (\alpha_B - \phi) \beta_{T,SR} \mathbf{N}_p \, d\Omega}_{M_T^{\zeta}} (\hat{\mathbf{T}})'_S + \underbrace{\int_{\Omega} \nabla \mathbf{N}_p^T \left(\rho_G D_G^{\zeta} \frac{\partial x_{m,G}^{\zeta}}{\partial T} + \rho_L D_L^{\zeta} \frac{\partial x_{m,L}^{\zeta}}{\partial T} \right) \nabla \mathbf{N}_p \, d\Omega}_{L_T^{\zeta}} \hat{\mathbf{T}} \\
 & = \underbrace{\int_{\Omega} \nabla \mathbf{N}_p^T \left(\rho_{GR}^{\zeta} \frac{k_G^{rel} \mathbf{k}_S}{\mu_{GR}^v} \rho_{GR} + \rho_{LR}^{\zeta} \frac{k_L^{rel} \mathbf{k}_S}{\mu_{LR}^v} \rho_{LR} \right) \mathbf{b} \, d\Omega}_{f_I^{\zeta}} - \underbrace{\int_{\Omega} \mathbf{N}_p^T \phi \left[s_G (\rho_{GR}^{\zeta})'_S + s_L (\rho_{LR}^{\zeta})'_S \right] \, d\Omega}_{f_{II}^{\zeta}} \\
 & - \underbrace{\int_{\Omega} \mathbf{N}_p^T \left[\phi (\rho_{LR}^{\zeta} - \rho_{GR}^{\zeta}) - \rho_{FR}^{\zeta} p_{cap} (\alpha_B - \phi) \beta_{p,SR} \right] \langle s_L \rangle'_S \, d\Omega}_{f_{III}^{\zeta}} + \underbrace{\int_{\partial\Omega} \mathbf{N}_p^T \dot{m}_{AJ}^{\zeta} \, d\Gamma}_{f_{IV}^{\zeta}}
 \end{aligned}$$



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TH2M Benchmarking

TH2M BENCHMARK HIERARCHY

1 Primary variable

T	<ul style="list-style-type: none"> • Linear/ radial heat conduction • thermal diffusion 	H^a	<ul style="list-style-type: none"> • Single-phase flow • Darcy flow • Compressible fluid flow 	M	<ul style="list-style-type: none"> • Linear-elastic deformation
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2 Primary variables

TH	<ul style="list-style-type: none"> • Thermal advection/diffusion Ogata Banks exact solution 	HC	<ul style="list-style-type: none"> • Diffusion equation 	H²	<ul style="list-style-type: none"> • Two-phase flow: McWhorter exact solution
TM	<ul style="list-style-type: none"> • Thermo-elastic plate/cube 	H²C	<ul style="list-style-type: none"> • Phase (dis-)appearance Bourgeat benchmark 	HM	<ul style="list-style-type: none"> • Poro-elastic column consolidation

3 Primary variables

THM	<ul style="list-style-type: none"> • Point heat source consolidation Booker Chaudry exact solution 	TH²C	<ul style="list-style-type: none"> • Heat pipe problem Udell Doughty benchmark 	H²M	<ul style="list-style-type: none"> • Poro-elastic soil consolidation Liakopoulos benchmark
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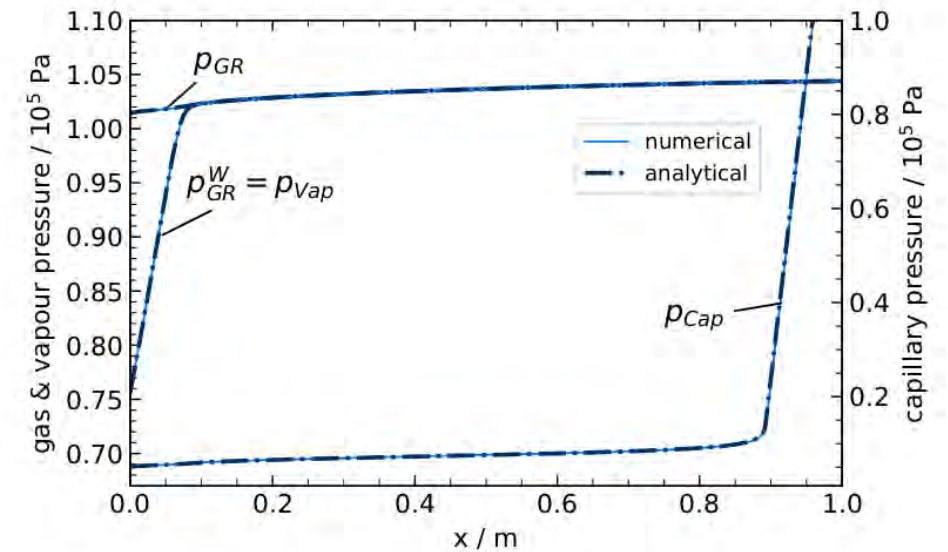
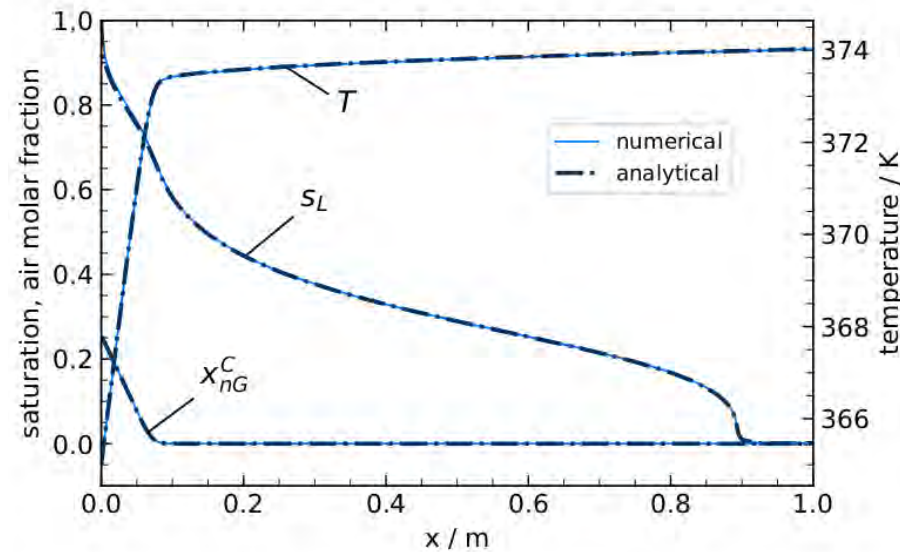
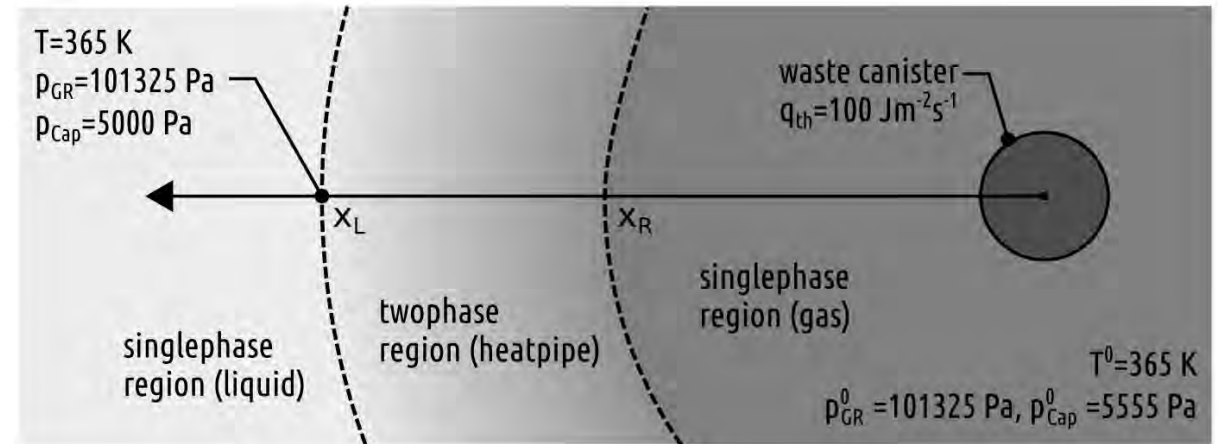
4 Primary variables

TH²M	<ul style="list-style-type: none"> • 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





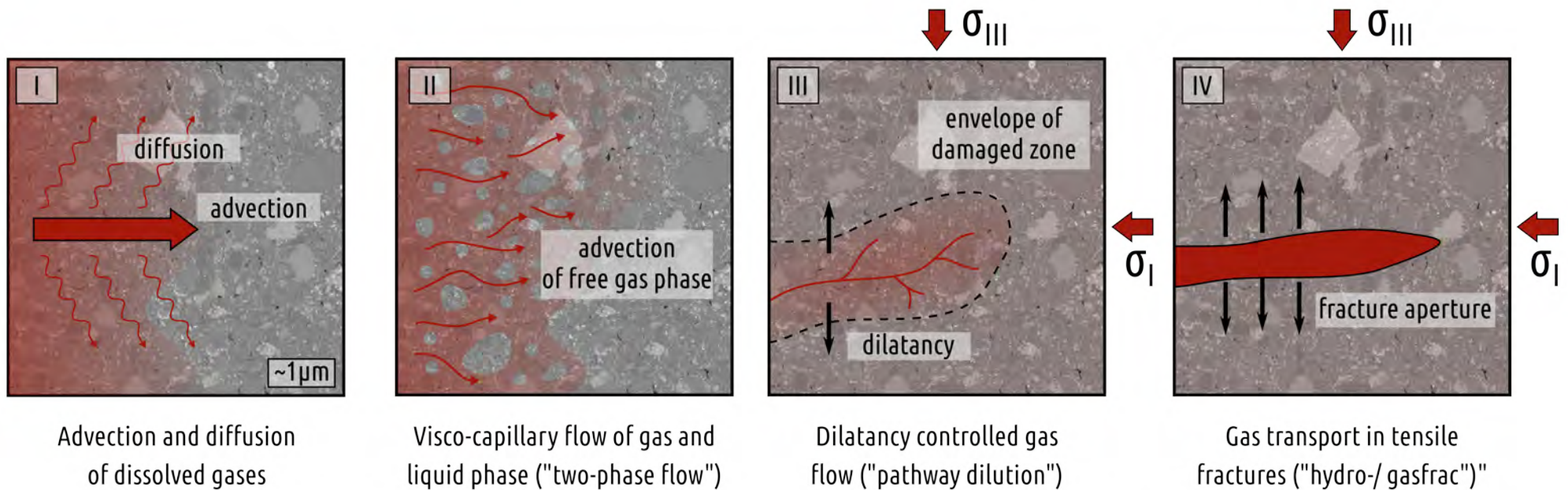
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TH2M Test Case

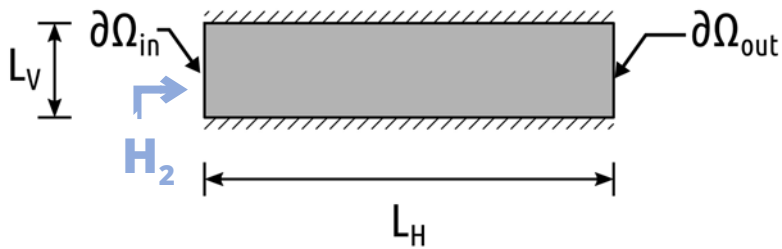
GAS TRANSPORT REGIMES IN LOW PERMEABLE MEDIA



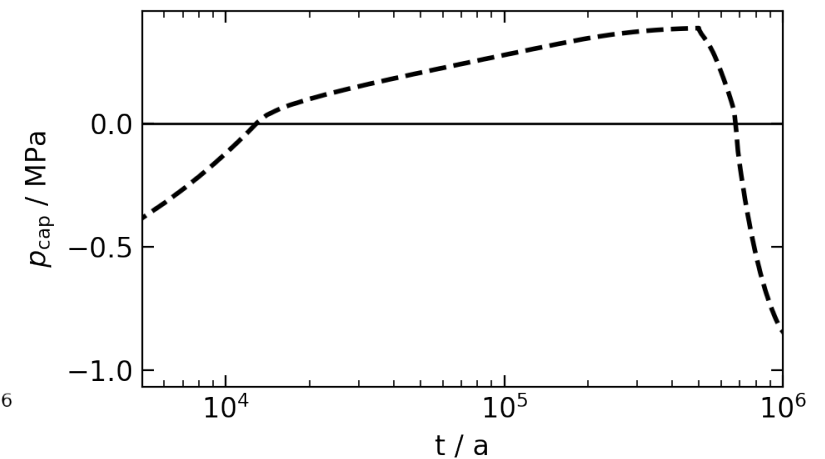
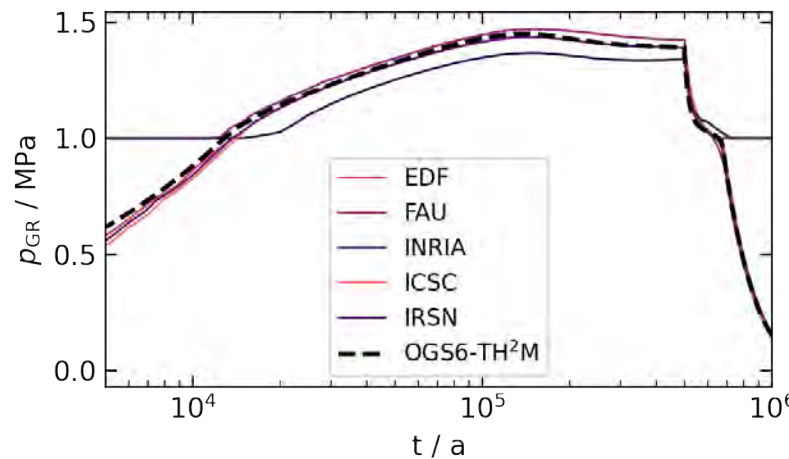
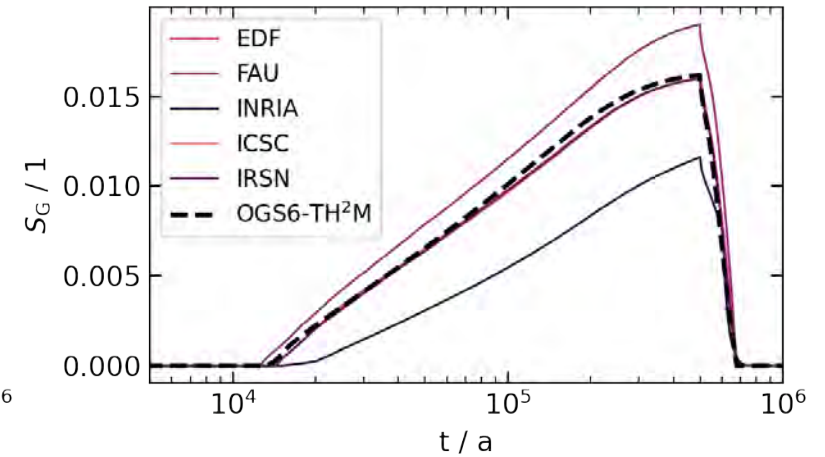
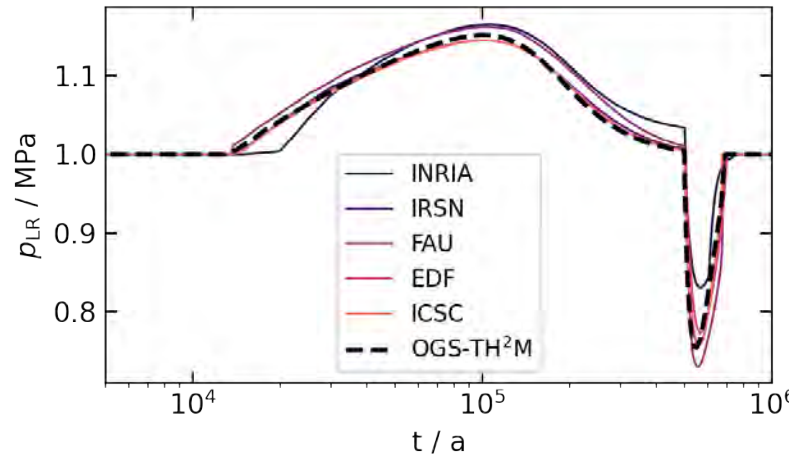
Classification of gas transport regimes in clay rock, adapted and modified from Marschall et al. [2005]

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

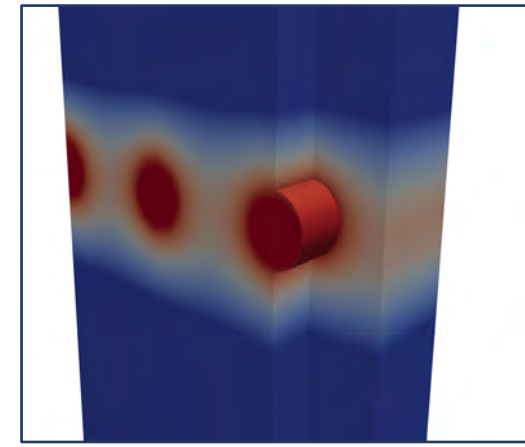
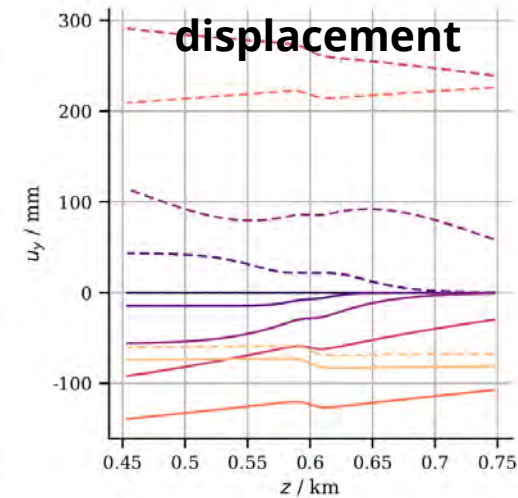
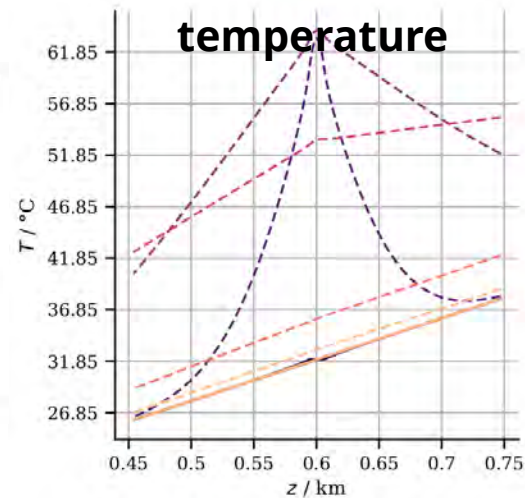
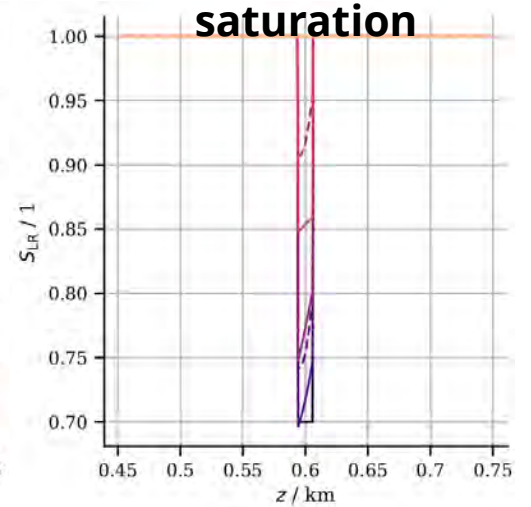
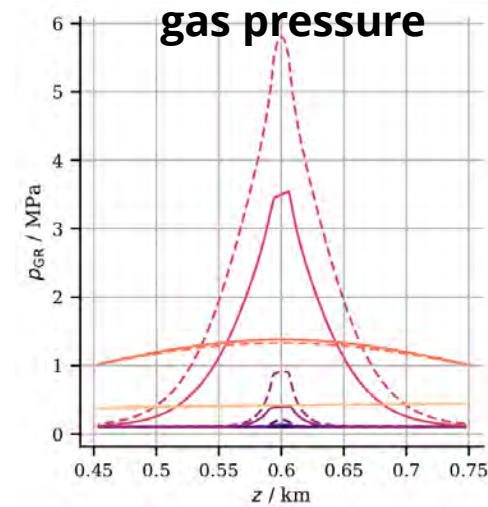
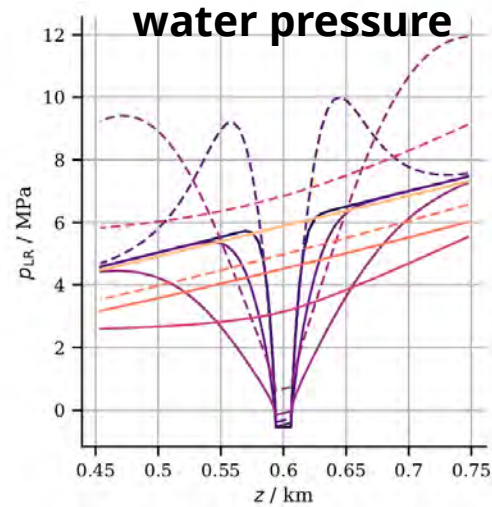
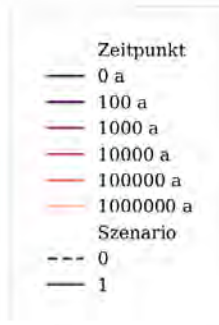
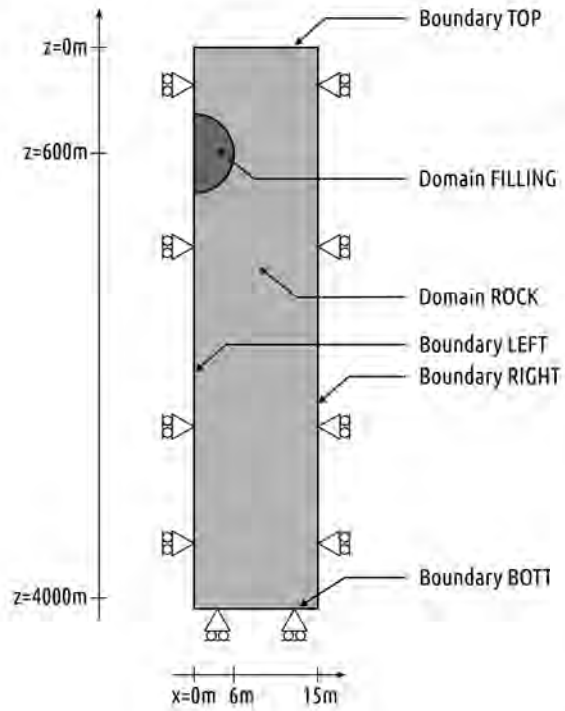


- Benchmark (Bourgeat et al.)
- Continuous H_2 -injection at $\partial\Omega_{in}$ at $0 \leq t \leq 500,000a$
- Gas phase appears at $t \approx 15,000a$
- At $t = 500,000a$ rapid drop in water pressure
- Gas phase disappears at $t \approx 700,000a$



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

