







# OVERVIEW OF OPENGEOSYS HIGH-PERFORMANCE-COMPUTING APPLICATIONS

### Thomas Fischer<sup>1</sup> and Tobias Meisel<sup>1</sup> and Dmitri Naumov<sup>1,2</sup> and Keita Yoshioka<sup>1</sup> and Wenqing Wang<sup>1</sup> and Mostafa Mollaali<sup>1</sup> and Vahid Ziaei Rad<sup>1</sup> and Jörg Buchwald<sup>1</sup> and Thomas Kalbacher<sup>1</sup> and Lars Bilke<sup>1</sup> and Olaf Kolditz<sup>1,3</sup>

<sup>1</sup>Department of Environmental Informatics, Helmholtz Centre for Environmental Research - UFZ, Germany

<sup>2</sup> Institute of Soil Mechanics and Foundation Engineering, Faculty of Geosciences, Geoengineering and Mining, Technische Universität Bergakademie Freiberg, Germany <sup>3</sup> Applied Environmental Systems Analysis, Technische Universität Dresden, Germany

**OpenGeoSys:** High-Performance-Computing

**OpenGeoSys** Thermodynamics OpenGeoSys (OGS) is a scientific open source software for the development of numerical methods for the simulation of coupled thermo-**Mechanics** Solid

#### **HPC** Applications

## German Part of Danube Catchment Groundwater Flow Model • 22 stratigraphic layers • Extent: 419 km west-east, 310 km north-south

hydro-mechanical-chemical (THMC) processes in porous and fractured media. OGS is fully parallelized using the distributed memory programming approach MPI (message passing interface).





#### Results for newly implemented XDMF/HDF5 I/O

Simulation of a German groundwater flow process model • model with 141 767 584 nodes / 212 491 596 elements in the mesh, process variable pressure, simulation using 192 cores

XDMF/HDF5 algorithm





#### HPC Model

- mesh: 6 259 100 nodes / 10 918 250 elements
- Transient simulation (853 timesteps with sizes of  $262\,800\,\mathrm{s}$ )
- Parallel simulation with 48 cores: 43 min
- Parallel simulation with 96 cores: 21 min
- Parallel simulation with 144 cores: 14 min
- Parallel simulation with 192 cores: 12 min



Recharge 2.0e-04 0.0005 0.001 0.002 0.005 0.01 0.02 0.05 0.1 0.2 0.5 1 2.0e+00





- Coupled compartments (Geo#Hydro#Eco)
- Hyper-resolution (time-space)

 Case studies • Workflows



- Colors at surface symbolize the amount of recharge
- Blue bars: positive volumetric flaw rate: groundwater feeds the river
- Brown bars: negative volumetric flow rate: river feeds the groundwater

#### Clay–rock fracturing risk assessment under high gas pressures

#### Crack Modeling using Phase Field

- The variational phase-field model was used to model fractures in clay due to high gas pressures
- Gaussian Proxy for the fracture risk was devel-

#### References

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oped based on the time it took for the fracture to reach a length of 1 m

• Proxy Model was then used for parameter estimation and to analyze the fracture risk in terms of sensitivity indices

#### HPC

• Python workflow ran in JupyterLab on JUWELS allowing for direct analysis and subsequent job submission



#### **Contact:** https://www.opengeosys.org

Thomas Fischer (thomas.fischer@ufz.de) Helmholtz Centre of Environmental Research - UFZ, Department Environmental Informatics

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