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PAUL SCHERRER INSTITUT



WIR SCHAFFEN WISSEN – HEUTE FÜR MORGEN



Sergey V. Churakov :: Institute of Geological Sciences :: University of Bern
Laboratory for Waste Management :: Paul Scherrer Institut

Visualisation needs and challenges in geosciences



Coupled phenomena in geosciences

Geodynamics & Tectonics

- Temporal and spatial evolution of large-scale structures
- Geodynamic of Earth Interior

Multi scale modelling of mass transport phenomena

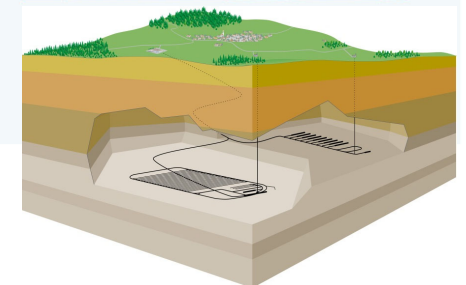
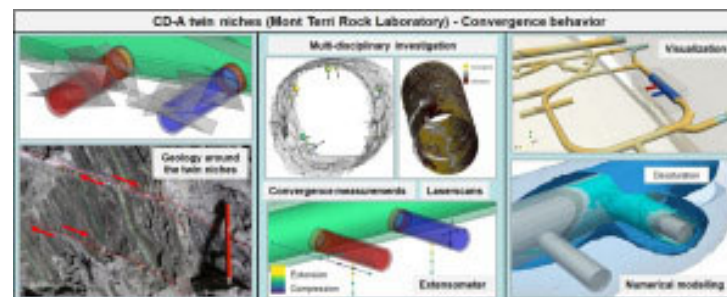
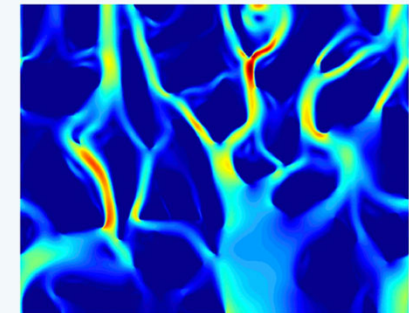
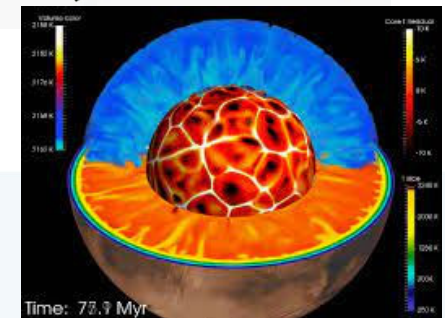
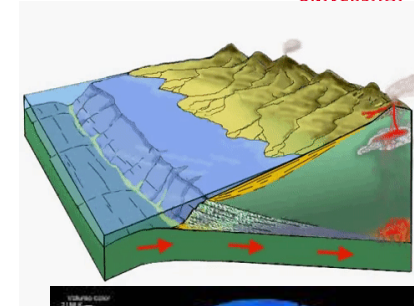
- **Visualisation of rock Microstructure**
- **Fluid transport in porous and fractural media**
- **Molecular scale processes at fluid solid interfaces**

Exploration of natural resources:

- Geothermal energy
- Metal and hydrocarbon deposits
- Sequestration of greenhouse gasses
- **Deep geological disposal of radioactive waste**

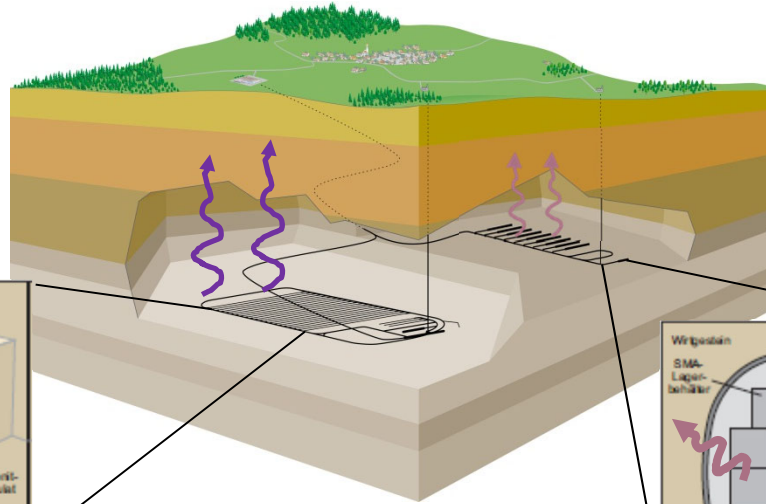
Geological Education

- Virtual laboratories
- Virtual excursions

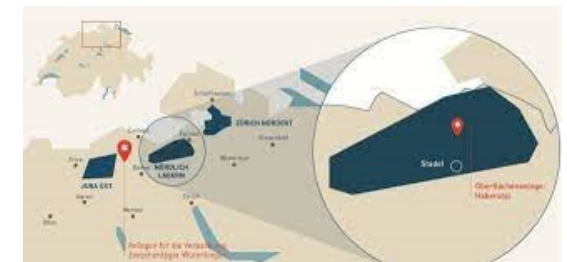
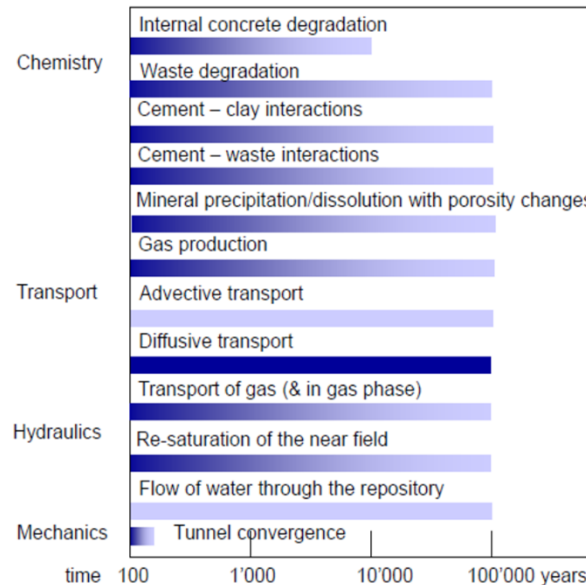
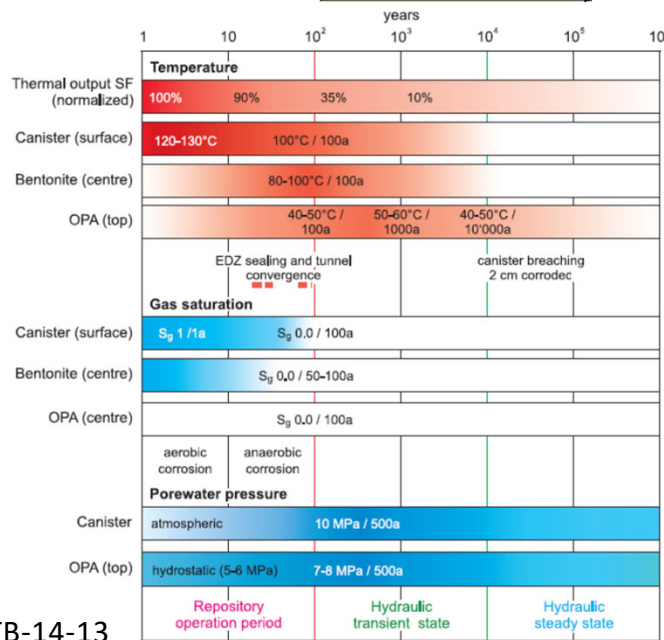
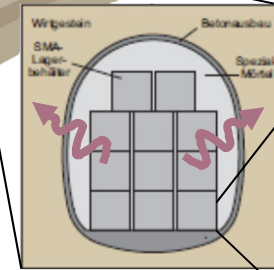
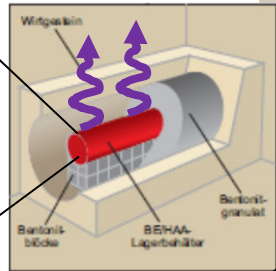
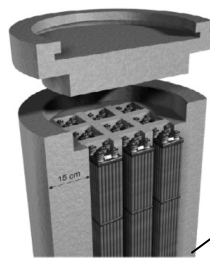


Geological Disposal of Radioactive waste

Thermal pulse
De-/re-saturation
Backfill degradation
Canister corrosion
Radionuclides release



Waste degradation
Cement-clay interaction
Release of Gas & Radionuclides



THMC coupled processes modelling

Heat transport

$$c\rho\frac{\partial T}{\partial t} = -\nabla(-K\nabla T + \sum_{\beta} h_{\beta}\vec{F}_{\beta}) + q$$

Thermodynamics

Mechanics

Deformation

$$\nabla\vec{\sigma} - \rho\vec{g} = 0$$

$$\nabla \cdot (\sigma - (S^L p^L + S^D p^D)\mathbf{I} - \beta_T \Delta T \mathbf{I}) + \rho \mathbf{g} = 0$$

Hydraulics

Fluid flow

$$\frac{\partial}{\partial t} \int_{V_n} M^{\kappa} dV_n = \int_{\Gamma_n} \vec{F}^{\kappa} \vec{n} d\Gamma_n + \int_{V_n} q^{\kappa} dV_n$$

$$M^{\kappa} = \Phi \sum_{\beta} \rho_{\beta} S_{\beta} X_{\beta}^{\kappa}$$

$$\vec{F}_{\beta}^{\kappa} = -\rho_{\beta} \frac{\vec{k} k_{r\beta}}{\mu_{\beta}} (\nabla P_{\beta} - \rho_{\beta} \vec{g})$$

$$\sum_{\beta} S_{\beta} = 1$$

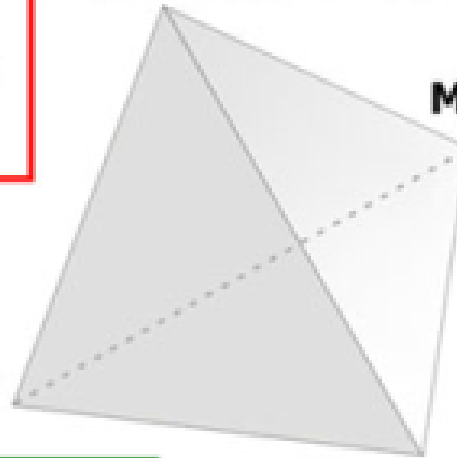
Chemistry

Reactive transport

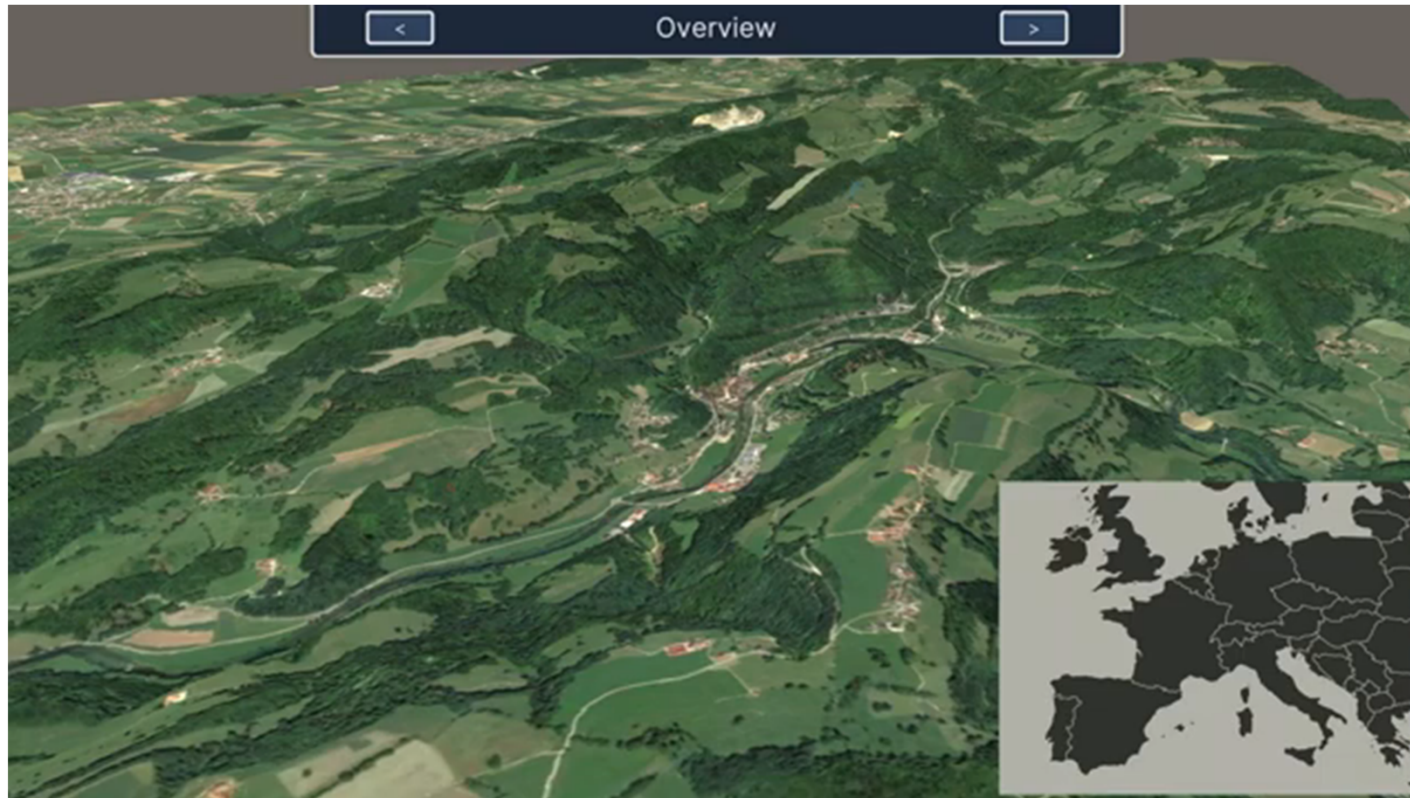
$$\vec{F}^{\kappa} = \sum_{\beta} \left(X_{\beta}^{\kappa} \vec{F}_{\beta} + \rho_{\beta} \vec{D}_{\beta}^{\kappa} \nabla X_{\beta}^{\kappa} \right)$$

$$\ln(K_{P,T}) = \frac{\Delta G_{P,T}^0}{RT}$$

$$K_j = \frac{a_w^{\nu_{w,j}} \prod_i (\gamma_i C_i)^{\nu_{i,j}} \prod_m (a_m)^{\nu_{m,j}} \prod_g (f_g)^{\nu_{g,j}}}{\gamma_j C_j}$$



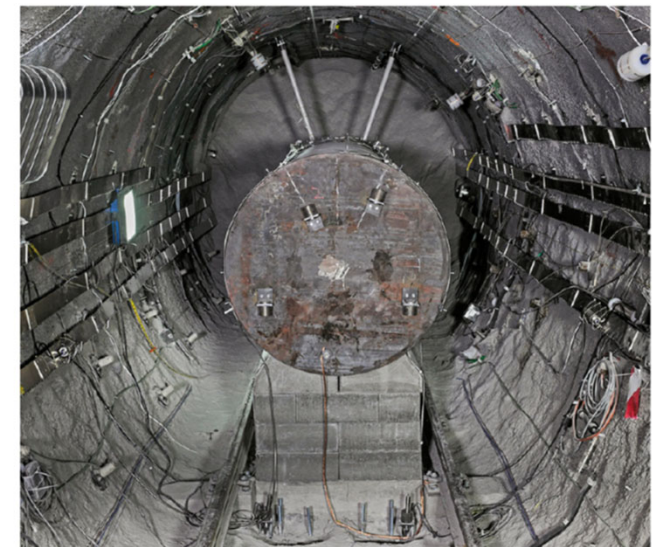
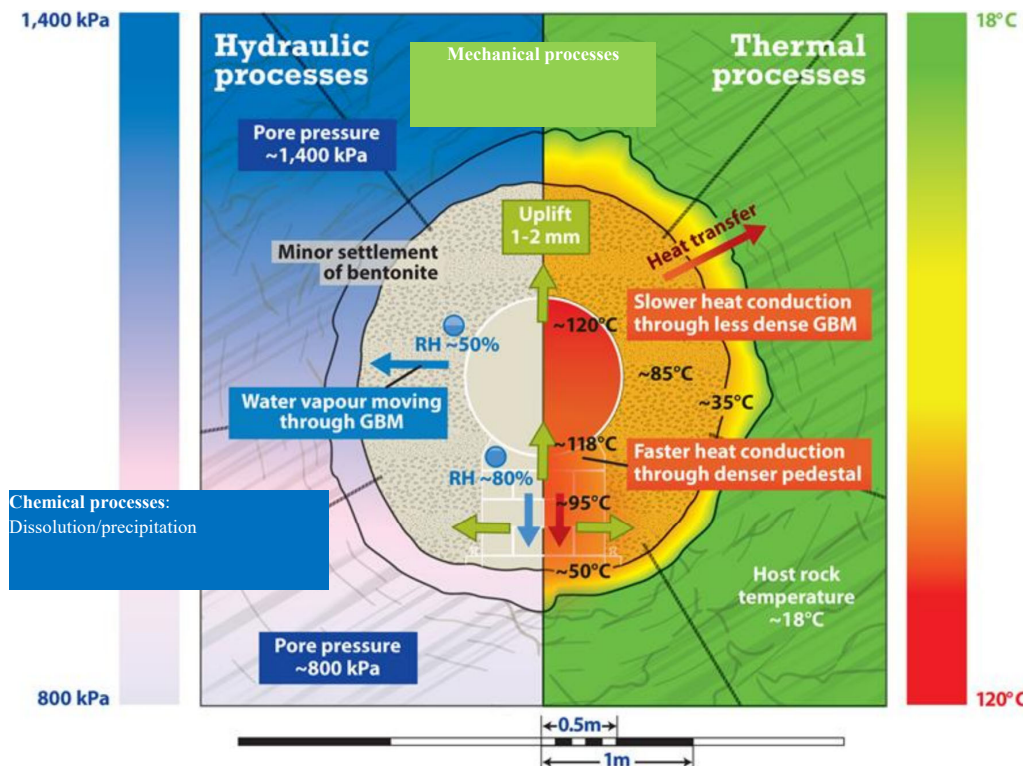
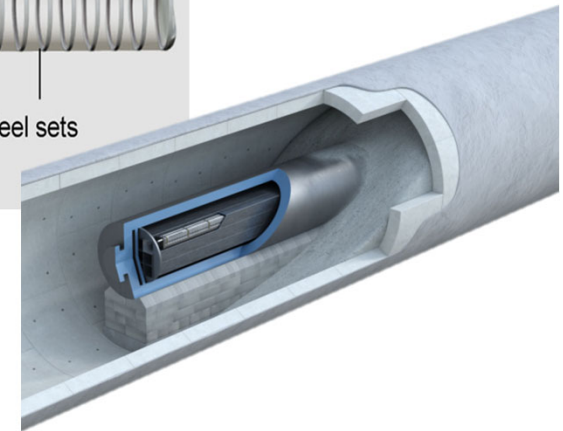
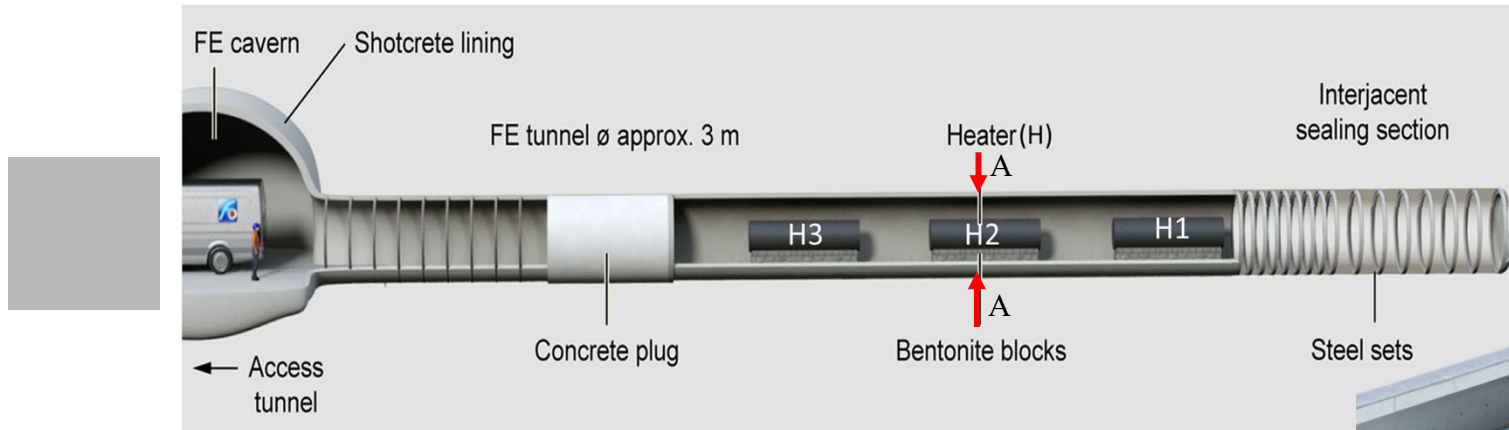
Underground research laboratory Mont Terri



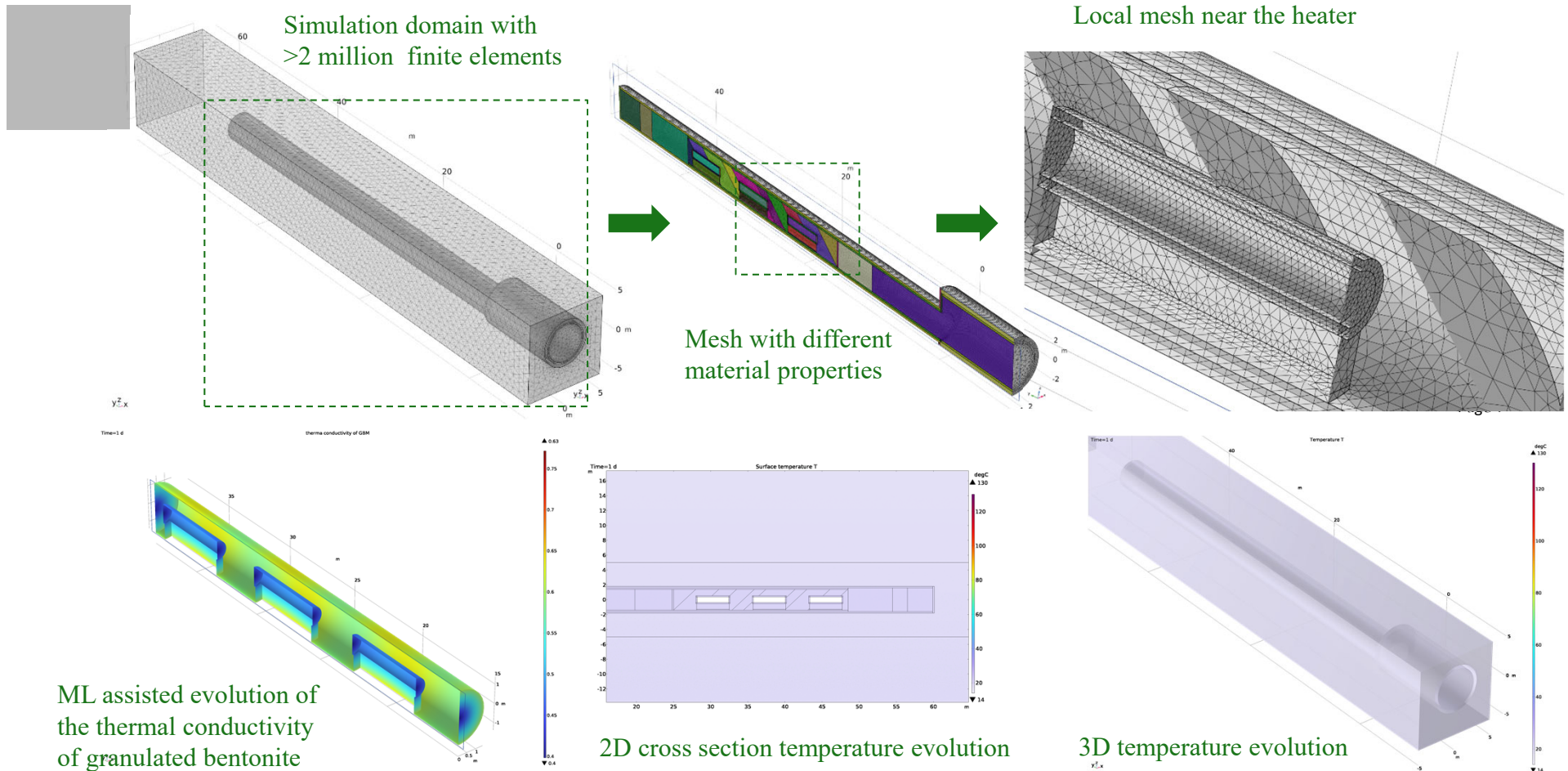
<https://www.youtube.com/watch?v=VH9I1iaeAiM>

Mont Terry Consortium / OpenGeoSys (O. Kolditz (UFZ))

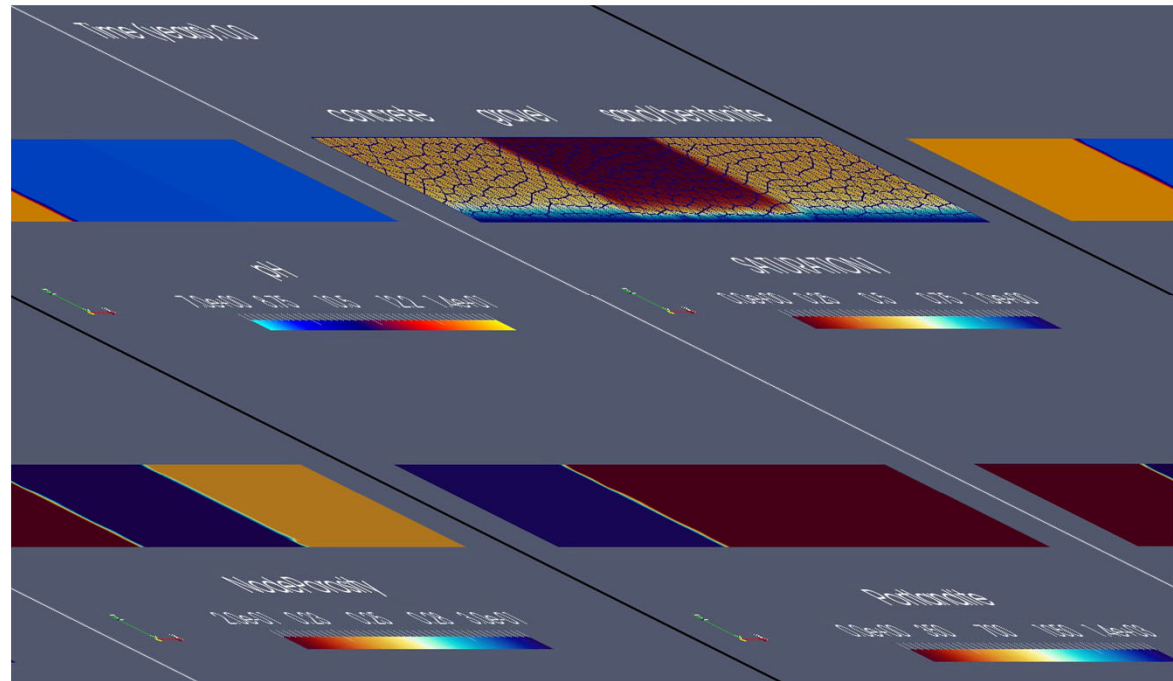
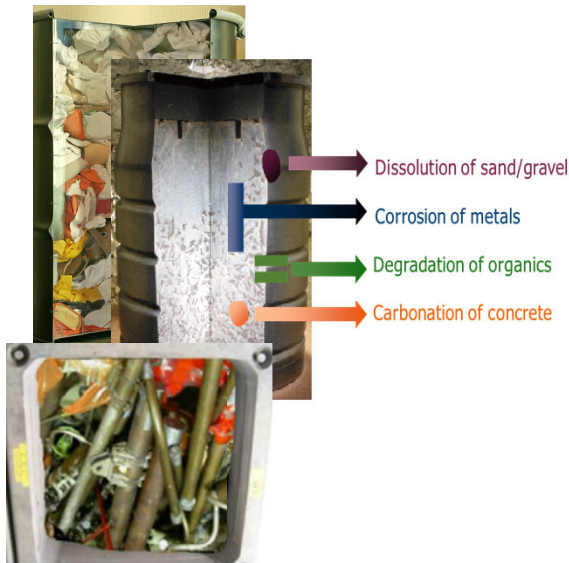
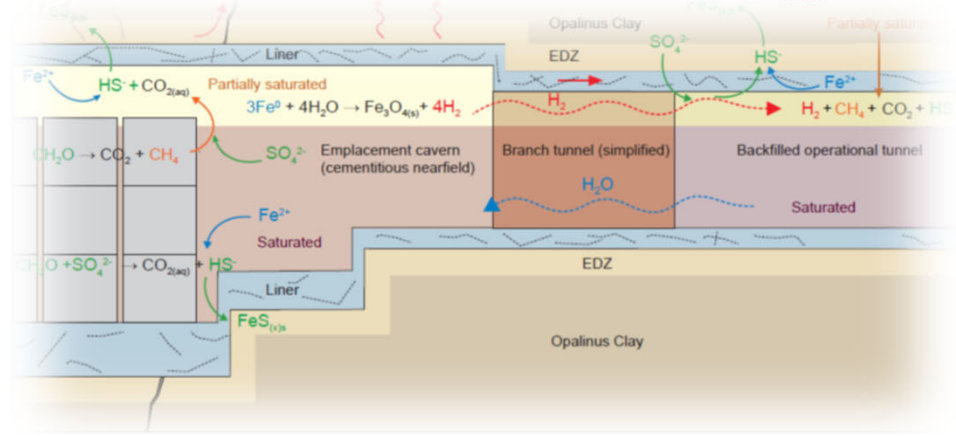
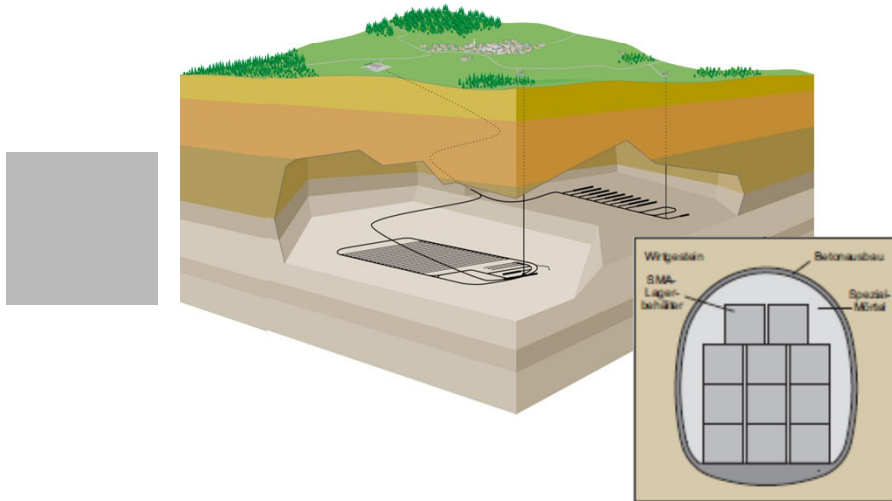
FE-experiment at Mont Terri



Digital twin of Full emplacement FE experiment



Interaction of repository barriers



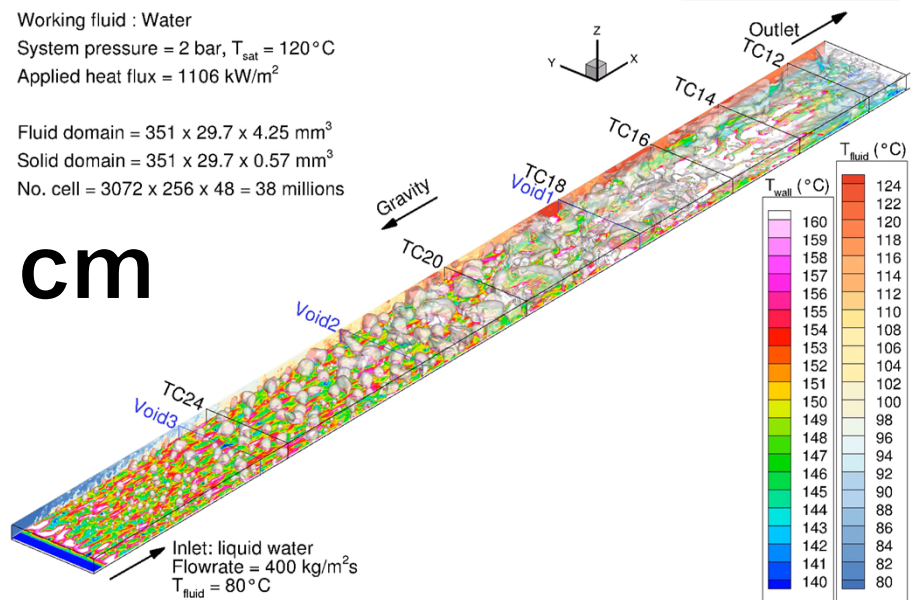
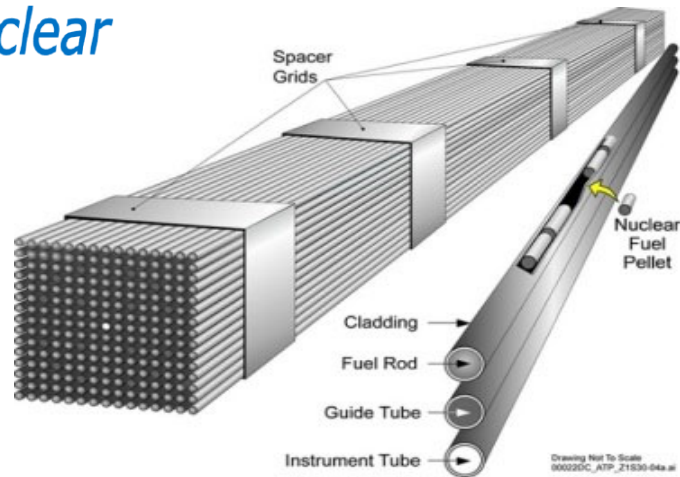
Multiscale Boiling Phenomena (LES-LSM)

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PSI-BOIL Sato & Niceno (LSM/NES)

Working fluid : Water
 System pressure = 2 bar, $T_{sat} = 120^\circ\text{C}$
 Applied heat flux = 1106 kW/m^2

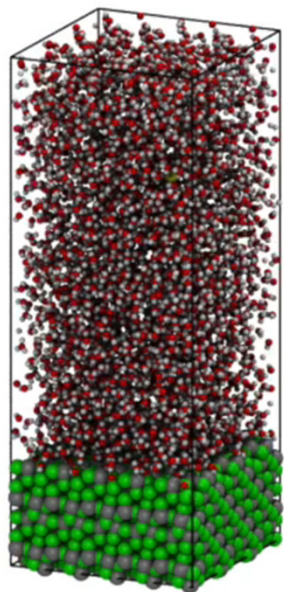
Fluid domain = $351 \times 29.7 \times 4.25 \text{ mm}^3$
 Solid domain = $351 \times 29.7 \times 0.57 \text{ mm}^3$
 No. cell = $3072 \times 256 \times 48 = 38 \text{ millions}$



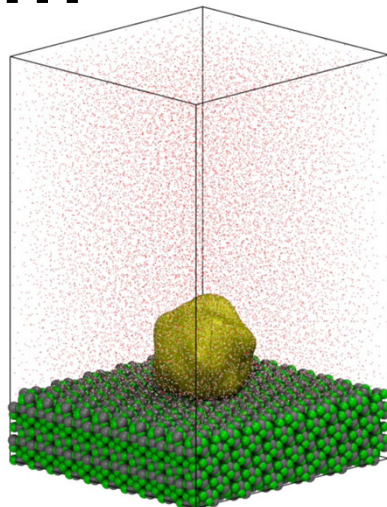
cm

Molecular Dynamics of vapor nucleation (LES):

www.nature.com/articles/s41598-021-99229-5



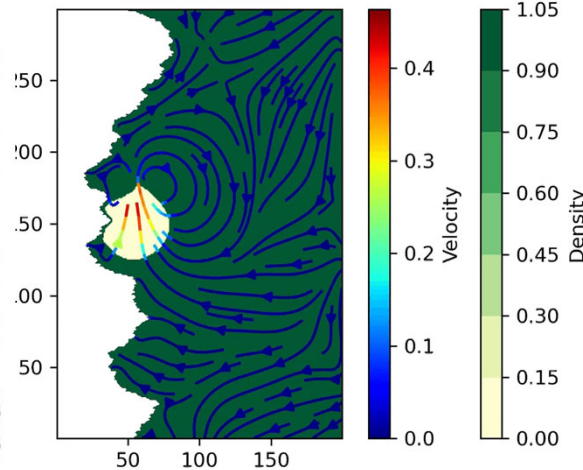
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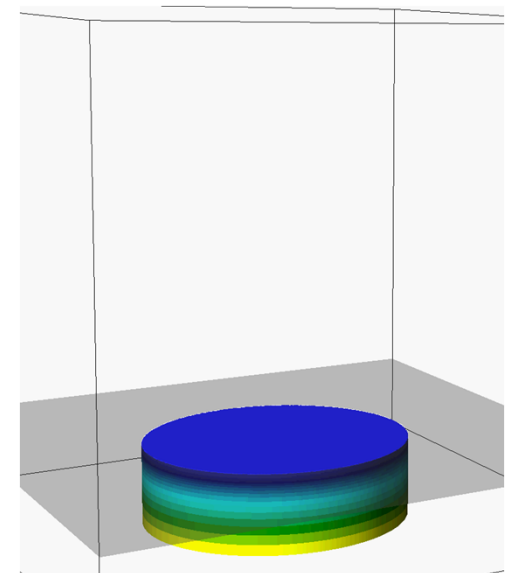
Lattice Boltzmann(LES):

μm

Time:500.0



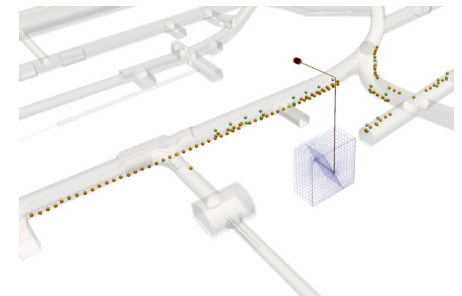
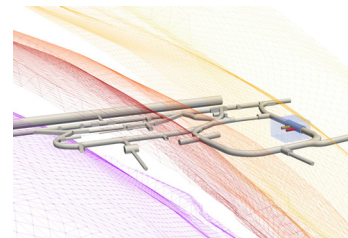
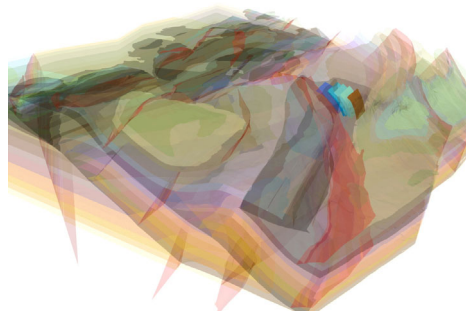
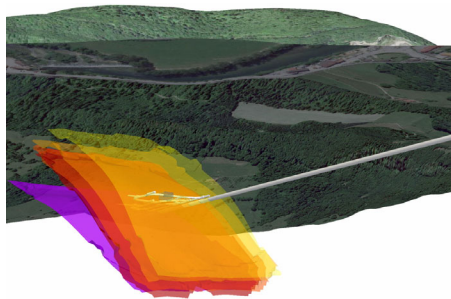
mm



Visualization needs

Digital twins:

- BIM of laboratory / field experiments and disposal systems
- Visualization of process simulations data (multi-field analysis)
- Virtual laboratories / Lab on a chip experiments



Thank you for your
attention!

Acknowledgments to
Nagra for a
longstanding
partnership!

