Using MFront Generic Behaviours for Swelling Geomaterials in OpenGeoSys

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Outline

- For which materials are we interested in GenericBehaviours?
- Integration with OGS
- Illustrative examples

What is Bentonite ?

- Natural material, generally mined in open pits.
- Bentonite is a plastic clay that is frequently generated from the alteration of volcanic ash.
- Bentonite is a clay material that consists primarily of montmorillonite
- The mineral material is mixed, ground, dried, and processed into different products.

Bentonite properties and applications.

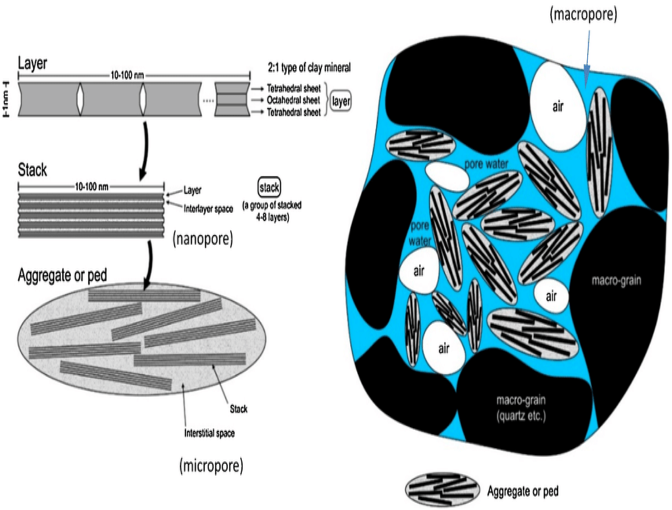
Physical Properties

- Very fine-grained clay (particle size $< 2\,\mu m$).
- High plasticity (moldable when wet) .
- Swelling capacity: absorbs water and expands.
- High cation exchange capacity.
- Very low permeability (10^{-18} to 10^{-20} m^2 when saturated).
- Thixotropy: forms gel with water and liquefies when stirred.

Applications

- **Environmental:** landfill liners, slurry walls, contaminant barriers
- **Nuclear waste disposal:** buffer and backfill sealing material
- **Geotechnical:** soil stabilization, cut-off walls, tunnel sealing
- **Oil & Gas:** drilling muds (lubrication, borehole stability, cooling)
- **Industrial:** iron ore pelletizing, foundry sands, purification processes
- **Everyday:** cosmetics, cat litter, wine clarification, pharmaceuticals

Microstructure, Unsaturated State and Dual Porosity in Bentonite



Microstructure of Bentonite [Li et al. 2020].

Microstructure (Hierarchical Levels)

- **Layer (nm):** 2:1 montmorillonite sheet with interlayer space
- **Stack (10–100 nm):** group of 4–8 layers stacks of layers (nanopores inside)

Unsaturated Condition

- Pores contain both **water** and **air**
- Suction controls water retention and swelling
- Nanopores usually remain water-filled, larger pores may drain

Dual Porosity Concept

- **Micropores / Nanopores:** inside stacks and aggregates, retain water → swelling & low permeability
- **Macropores:** between aggregates, may contain air and water → control flow and storage.

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Why is Bentonite Difficult to Model?

- **Unsaturated material:** simultaneous presence of air and water
- **Swelling/shrinkage:** large volume change with water content
- **Hydro-mechanical coupling:** suction $\leftrightarrow$ volume change $\leftrightarrow$ permeability
- **Dual porosity:**
  - Micropores retain water
  - Macropores allow flow
- **Non-linear and time-dependent response**
- **Widely used models:**
  - Barcelona Basic Model (BBB) models unsaturated soils.
  - Barcelona Expansive Model (BExM) extends BBM for expansive clays(double structure micro and macro).

Barcelona Basic Model

- Constitutive model for unsaturated soils developed by Eduardo E Alonso et al. 1990.
- Based on Modified Cam Clay, extended to account for suction effects.
- The yield surface expands with suction (suction acts as an apparent preconsolidation pressure).
- Captures both mechanical loading and wetting/drying effects.

$$0 = f_1(p, q, s, p_0^*) = q^2 - M^2\,(p + p_\mathrm{s})\,(p_0 - p)$$
$$0 = f_2(s, s_0) = s - s_0$$

where

$$p_\mathrm{s} = k_\mathrm{s}\, s$$
$$\frac{p_0}{p_\mathrm{c}} = \left(\frac{p_0^*}{p_\mathrm{c}}\right)^{\dfrac{\lambda(0)-\kappa}{\lambda(s)-\kappa}}$$
$$\lambda(s) = \lambda(0)\left[(1-r)\,\mathrm{e}^{-\beta s} + r\right]$$

Hardening:

$$\frac{\mathrm{d}p_0^*}{p_0^*} = \frac{\nu}{\lambda(0)-\kappa}\,\mathrm{d}\varepsilon_V^\mathrm{p}, \qquad \frac{\mathrm{d}s_0}{s_0 + p_\mathrm{at}} = \frac{\nu}{\lambda_\mathrm{s}-\kappa_\mathrm{s}}\,\mathrm{d}\varepsilon_V^\mathrm{p}.$$

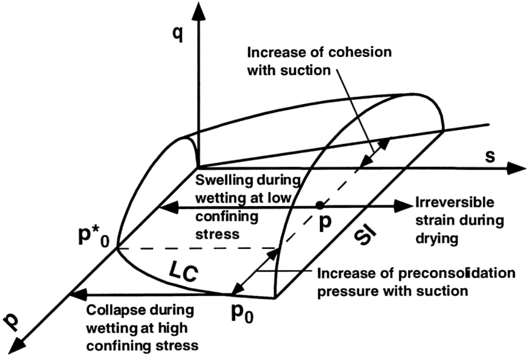

Figure: BBM yield locus in p–q–s plane [E. Alonso et al. 1999].

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Barcelona Expansive Model (BExM)

- Considers two structural levels:
  - **Microstructure:** active clay minerals (assumed saturated)
  - **Macrostructure:** overall soil fabric
- The effective stress concept applies at the microstructural level.
- **Micro–macro strains** are treated as independent.
- **Neutral Line (NL):**

$$p + s = \text{constant}$$

  represents states without microstructural deformation.
- **Above NL:** microstructural swelling $\Rightarrow$ increase in void ratio (e).
- **Below NL:** microstructural shrinkage $\Rightarrow$ decrease in void ratio (e).
- Two yield lines define the limits of reversible behavior:
  - **SI line:** suction increase (shrinkage)
  - **SD line:** suction decrease (swelling)
- **SI** and **SD** are parallel to the **Neutral Line (NL)**; crossing them produces irreversible microstructural strains.

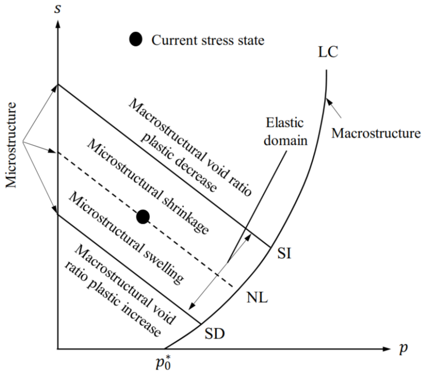

Figure: BExM yield loci in p–s plane [Ghandilou et al. 2024].

Key features and other models

- Strong HM coupling at constitutive level (not just effective stress)
- Hydraulic properties can depend on mechanics and interact with stress formulation (see VIBE model, currently used via a wrapper: Simo et al. 2024)
- Allow for ML-based models

→ More robust and general implementation using GenericBehaviour.

Example 1: Weak secondary coupling

Classical implementation (HM, OpenGeoSys):

$$r_u = \int_\Omega \left[\left(\boldsymbol{\sigma}' - \alpha_\mathrm{B}\,\chi(S_\mathrm{L})\,p\boldsymbol{I}\right) : \operatorname{grad}\boldsymbol{v}_u - \boldsymbol{v}_u \cdot \varrho\,\boldsymbol{b}\right]\mathrm{d}\Omega - \int_{\partial\Omega_t} \boldsymbol{v}_u \cdot \bar{\boldsymbol{t}}\,\mathrm{d}\Gamma$$

$$r_p = \int_\Omega \left[v_p(\phi S_\mathrm{L}\varrho_\mathrm{LR})'_\mathrm{S} + v_p\,\phi S_\mathrm{L}\varrho_\mathrm{LR}\operatorname{div}(\boldsymbol{u})'_\mathrm{S} + \operatorname{grad}v_p \cdot \varrho_\mathrm{LR}\frac{k_\mathrm{rel}\boldsymbol{k}}{\mu_\mathrm{FR}}\left[\operatorname{grad}p - \varrho_\mathrm{LR}\,\boldsymbol{g}\right]\right]\mathrm{d}\Omega - \int_{\partial\Omega_w} v_p \dot{m}_\mathrm{L}\,\mathrm{d}\Gamma$$

OGS:

- Fluid EOS $\varrho_\mathrm{LR}(p, T, \dots)$, retention curves $S_\mathrm{L}(p)$, relative permeability $k_\mathrm{rel}(S_\mathrm{L})$, porosity update $(\phi)'_\mathrm{S}$, poro-perm relations $\boldsymbol{k}(\phi)$, ...
- Corresponding linearizations for Newton-Raphson
- Relatively specific residual and Jacobian formulations

MFront:

- Integration of mechanical part of effective stresses: ${}^{t+1}\boldsymbol{\sigma}' \leftarrow ({}^{t+1}\Delta\boldsymbol{\epsilon}_\mathrm{el}, {}^{t}\boldsymbol{\sigma}', {}^{t}\boldsymbol{\kappa})$
- Consistent tangent moduli $\boldsymbol{\mathcal{C}} = \partial_{\Delta\epsilon}\boldsymbol{\sigma}'$

Example 2: Strong secondary coupling

Implementation for porosity-dependent retention and suction-dependent plasticity:

$$r_u = \int_\Omega \left[\boldsymbol{\sigma} : \operatorname{grad} \boldsymbol{v}_u - \boldsymbol{v}_u \cdot \varrho\, \boldsymbol{b} \right] \mathrm{d}\Omega - \int_{\partial\Omega_t} \boldsymbol{v}_u \cdot \bar{\boldsymbol{t}} \mathrm{d}\Gamma$$

$$r_p = \int_\Omega \left[v_p (\phi S_\mathrm{L}\, \varrho_\mathrm{LR})'_\mathrm{S} + v_p\, \phi S_\mathrm{L}\, \varrho_\mathrm{LR} \operatorname{div} (\boldsymbol{u})'_\mathrm{S} + \operatorname{grad} v_p \cdot \varrho_\mathrm{LR} \frac{k_\mathrm{rel} \boldsymbol{k}}{\mu_\mathrm{FR}} \left[\operatorname{grad} p - \varrho_\mathrm{LR}\, \boldsymbol{g} \right] \right] \mathrm{d}\Omega - \int_{\partial\Omega_w} v_p \dot{m}_\mathrm{L} \mathrm{d}\Gamma$$

OGS:

- Reduced set of evaluations and linearizations
- Corresponding linearizations for Newton-Raphson
- Mechanical residual generalized (total stress formulation)

MFront:

- Coupled integration of constitutive sets: ${}^{t+1}(\boldsymbol{\sigma}, S_\mathrm{L}, \phi) \leftarrow ({}^{t+1}\Delta\epsilon_\mathrm{el}, {}^{t+1}p, {}^{t}\boldsymbol{\sigma}, {}^{t}\boldsymbol{\kappa})$
- Block-wise consistent tangent moduli $\partial_{\Delta\epsilon, \Delta p} \{\boldsymbol{\sigma}, S_\mathrm{L}, \phi\}$

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Use of DefaultGenericBehaviour

- **Inputs (gradients):** strain increment $\Delta\varepsilon$, liquid pressure increment Δp_{LR} (and ΔT if used).
- **Main ingredients:**
  - Linear isotropic thermo-elasticity: λ, μ, K, α.
  - Retention: van Genuchten $S_{\mathrm{L}}(p_{\mathrm{cap}})$ with residual saturations $S_{\mathrm{L}}^{\mathrm{r}}$, $S_{\mathrm{G}}^{\mathrm{r}}$, bubble pressure p^{b}, exponent m.
  - Bishop's parameter $\chi(S_{\mathrm{L}})$: supports *power law* ($\chi = S_{\mathrm{L}}^{n}$) *or saturation cutoff* (threshold S_{cut}).
  - Total-stress formulation; Biot-type partition handled inside the constitutive update.
  - Optional isotropic saturation-dependent swelling contribution.
- **Outputs (fluxes):** updated total stress and liquid-saturation $\{\boldsymbol{\sigma}, S_{\mathrm{L}}\}$ and **block-consistent tangents** $\partial_{\Delta\varepsilon}\{\cdot\}$, $\partial_{\Delta p}\{\cdot\}$ (and $\partial_{\Delta T}\{\cdot\}$ if thermal).

```
@DSL DefaultGenericBehaviour;
@Behaviour ThermoPoroElasticitySwelling;
// ... Rest of the code ...
@Gradient StrainStensor εᵗᵒ; εᵗᵒ.setGlossaryName("Strain");
@Gradient real p_LR;         p_LR.setEntryName("LiquidPressure");
@Flux StressStensor σ;       σ.setGlossaryName("Stress");
@Flux real S_L;              S_L.setEntryName("Saturation");
@StateVariable StressStensor swelling_stress;
swelling_stress.setEntryName("swelling_stress");
@TangentOperatorBlocks{∂σ/∂Δεᵗᵒ, ∂σ/∂ΔT, ∂σ/∂Δp_LR, ∂S_L/∂Δp_LR};
// ... Rest of the code ...
@Integrator {
// ... Rest of the code ...
  σ = σ + λ ⋅ trace(Δεᵗᵒ) ⋅ I₂ + 2 ⋅ μ ⋅ Δεᵗᵒ - 3 ⋅ K ⋅ α ⋅ ΔT ⋅ I₂ -
      αᵇ ⋅ (χ ⋅ (p_LR + Δp_LR) - x_prev ⋅ p_LR) ⋅ I₂ -
      swelling_contribution ⋅ I₂;

  if (computeTangentOperator_) {
    ∂σ/∂Δεᵗᵒ = λ ⋅ (I₂ ⊗ I₂) + 2 ⋅ μ ⋅ I₄;
    ∂σ/∂Δp_LR = -αᵇ ⋅ (
        χ - (p_LR + Δp_LR) ⋅ ∂χ/∂S_L ⋅ ∂S_L/∂p_cap(-(p_LR + Δp_LR))) ⋅ I₂
        + swelling_pressure * dphi_dS * ∂S_L/∂p_cap( -(p_LR+Δp_LR)) ⋅ I₂;
    ∂σ/∂ΔT = -3 ⋅ K ⋅ α ⋅ I₂;
    ∂S_L/∂Δp_LR = - ∂S_L/∂p_cap( -(p_LR+Δp_LR));
  }
}
```


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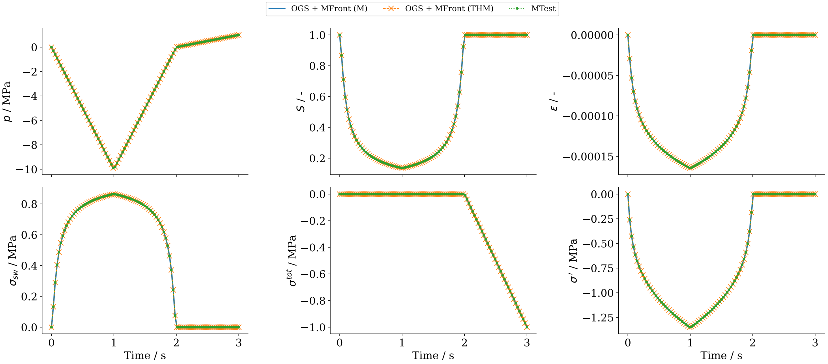
Uniaxial drainage and imbibition test with swelling using DefaultGenericBehaviour



Use of ImplicitGenericBehaviour

- Modified Cam Clay with THM coupling.
- Use of `@DSL Implicit;` is not possible.
- **Main ingredients:**
  - MCC yield & hardening; parameters $M,\ \kappa,\ \lambda$.
  - **Pressure-dependent bulk modulus** $K = K(p)$ $\Rightarrow$ **non-constant** Young's modulus $E = 3K(1-2\nu)$ with constant ν.
  - Retention $S_\mathrm{L}(p_\mathrm{cap})$ (van Genuchten).
  - Bishop $\chi(S_\mathrm{L})$: *power law* or *saturation cutoff*.
  - Total-stress formulation; Biot-type partition handled inside the constitutive update.
  - Optional isotropic saturation-dependent swelling contribution.
- **Outputs:** $\{\boldsymbol{\sigma}, S_\mathrm{L}\}$ and **block-consistent tangents** $\partial_{\Delta\boldsymbol{\varepsilon}}\{\cdot\}, \partial_{\Delta p}\{\cdot\}$ (and $\partial_{\Delta T}\{\cdot\}$ if thermal).
- **Next step (toward BBM):** implement suction effects on the yield locus: mean-stress shift $p_\mathrm{s} = k_\mathrm{s}\, s$ and a suction-dependent cap $p_0(s)$.

```
@DSL ImplicitGenericBehaviour;
@Behaviour ModCamClay_semiExpl_coupled;
// ... Rest of the code ...
@Algorithm NewtonRaphson;

@Gradient StrainStensor εᵗᵒ;              εᵗᵒ.setGlossaryName("Strain");
@ThermodynamicForce StressStensor σ;  σ.setGlossaryName("Stress");
@Gradient real pᴸᴿ;                       pᴸᴿ.setEntryName("LiquidPressure");
@ThermodynamicForce real Sᴸ;              Sᴸ.setEntryName("Saturation");
@StateVariable StressStensor σˢʷ;        σˢʷ.setEntryName("swelling_stress");
@StateVariable StrainStensor εᵉˡ;        εᵉˡ.setGlossaryName("ElasticStrain");
@AuxiliaryStateVariable real εᵛₚₗ;       εᵛₚₗ.setEntryName("PlasticVolumetricStrain");
// ... Rest of the code ...
@InitializeLocalVariables
{
    // ... Rest of the code ...
    φ₀ = std::pow((Sᴸ₀ - Sᴸₗ) / (Sᴸₕ - Sᴸₗ) , mˢʷ);
    Δpˢʷ = pˢʷ · (φ - φ₀);
    σ₀ = σ + αᵇ · χ₀ · pᴸᴿ · I₂;
    // ... Rest of the code ...
}
@ComputeThermodynamicForces{
    σ = σ₀ + θ · ∂σ/∂εᵉˡ · Δεᵉˡ - 3 · K · α · ΔT · I₂ - Δpˢʷ · I₂;
}
@Integrator{ ... }
@ComputeFinalThermodynamicForces{
    σ = σ₀ + ∂σ/∂εᵉˡ · Δεᵉˡ
    - 3 · K · α · ΔT · I₂ - αᵇ · χ · pᴸᴿ · I₂ - Δpˢʷ · I₂;}
@UpdateAuxiliaryStateVariables{ ... }

@TangentOperator{ ... }
```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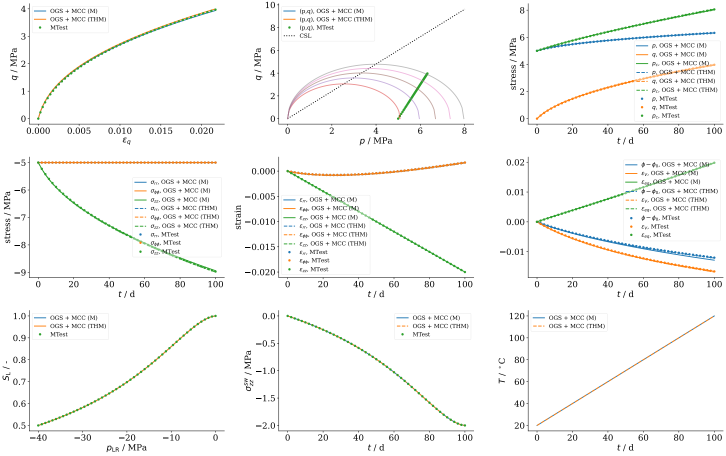
Triaxial test with swelling using ImplicitGenericBehaviour



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Conclusions

- ImplicitGenericBehaviour great step towards complex material models
- Testing coupled load paths: thermal, hydraulic and mechanical loadings on materials
- Allows for cleaner / more general code structure in solvers
- Allows for better split between solver and material knowledge V&V Helfer et al. 2025

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Thank you for your attention!

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