Compatible/equilibrium and incompatible/non-equilibrium initial states in OpenGeoSys

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Preliminary version. Testing in progress.
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1 Preliminary remarks

We distinguish between several concepts:

- **Constitutive reference states**. These are essentially material parameters and only active constitutively. Example: T_{ref}, p_{ref}, ϱ_{ref} in order to calculate

$$\varrho = \varrho_{\text{ref}} + \beta_T (T - T_{\text{ref}}) + \beta_p (p - p_{\text{ref}}) \tag{1}$$

- **Compatible/equilibrium initial states**. These are initial values for primary and secondary variables that enter the weak form and are in equilibrium with the boundary conditions.

- **Incompatible/non-equilibrium initial states**. These are initial states which are not explicitly in equilibrium with any boundary conditions. They are not considered in the weak form but affect the constitutive behaviour of the materials.

2 Small deformation

A total stress is

Discrete linearized weak form (NR scheme):

$$\int_{\Omega} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{C} \boldsymbol{B} \, \mathrm{d}\Omega \, \Delta \hat{\boldsymbol{u}} = \int_{\partial \Omega_{\mathrm{N}}} \boldsymbol{N}^{\mathrm{T}} \bar{\boldsymbol{t}} \, \mathrm{d}\Gamma + \int_{\Omega} \boldsymbol{N}^{\mathrm{T}} \varrho \boldsymbol{b} \, \mathrm{d}\Omega - \int_{\Omega} \boldsymbol{B}^{\mathrm{T}} (\boldsymbol{\sigma} - \boldsymbol{\sigma}_{0\text{neq}}) \, \mathrm{d}\Omega \tag{2}$$

Where the last term has been included to account for incompatible initial states (non-equilibrium states). The constitutive model integration proceeds as follows:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}_{0\text{eq}} + \boldsymbol{\sigma}_{0\text{neq}} + \int_{t_0}^{t} \dot{\boldsymbol{\sigma}}(\dot{\boldsymbol{\epsilon}}, \boldsymbol{\sigma}, \boldsymbol{\kappa}, \dots) \, \mathrm{d}\bar{t} \tag{3}$$

In other words, the constitutive integration always gets the total stress (including initial equilibrium and non-equilibrium contributions) as an argument.

2.1 Case A: Total stress form—compatible/equilibrium initial states

The user supplies an initial state which is in equilibrium with the initial tractions. All subsequent load changes are total loads in equilibrium with the total stress.

$$\int_{\Omega} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{C} \boldsymbol{B} \, \mathrm{d}\Omega \, \Delta \hat{\boldsymbol{u}} = \int_{\partial \Omega_{\mathrm{N}}} \boldsymbol{N}^{\mathrm{T}} \bar{\boldsymbol{t}} \, \mathrm{d}\Gamma + \int_{\Omega} \boldsymbol{N}^{\mathrm{T}} \varrho \boldsymbol{b} \, \mathrm{d}\Omega - \int_{\Omega} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{\sigma} \, \mathrm{d}\Omega \, , \quad \boldsymbol{\sigma}_{0\text{neq}} = 0 \tag{4}$$

such that a deformation-free state at $t = t_0$ requires

$$\int_{\partial \Omega_{\mathrm{N}}} \boldsymbol{N}^{\mathrm{T}} \bar{\boldsymbol{t}}(t = t_0) \, \mathrm{d}\Gamma + \int_{\Omega} \boldsymbol{N}^{\mathrm{T}} \varrho(t = t_0) \boldsymbol{b}(t = t_0) \, \mathrm{d}\Omega - \int_{\Omega} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{\sigma}_{0\text{eq}} \, \mathrm{d}\Omega = \boldsymbol{0} \tag{5}$$

2.2 Case B: Incremental stress form—incompatible/non-equilibrium initial states

The user supplies an initial state which is *not* in equilibrium with the initial tractions. Since these stresses are not considered in the equilibrium formulation, all tractions supplied are considered as *additional* loads

$$\int_{\Omega} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{C} \boldsymbol{B} \, \mathrm{d}\Omega \, \Delta \hat{\boldsymbol{u}} = \int_{\partial \Omega_{\mathrm{N}}} \boldsymbol{N}^{\mathrm{T}} \bar{\boldsymbol{t}} \, \mathrm{d}\Gamma + \int_{\Omega} \boldsymbol{N}^{\mathrm{T}} \varrho \boldsymbol{b} \, \mathrm{d}\Omega - \int_{\Omega} \boldsymbol{B}^{\mathrm{T}} (\boldsymbol{\sigma} - \boldsymbol{\sigma}_{0\mathrm{neq}}) \, \mathrm{d}\Omega \tag{6}$$

such that a deformation-free state at $t = t_0$ requires

$$\int_{\partial \Omega_{\mathrm{N}}} \boldsymbol{N}^{\mathrm{T}} \bar{\boldsymbol{t}}(t = t_0) \, \mathrm{d}\Gamma + \int_{\Omega} \boldsymbol{N}^{\mathrm{T}} \varrho \boldsymbol{b}(t = t_0) \, \mathrm{d}\Omega = \boldsymbol{0} \tag{7}$$

i.e. that no (additional) external loads are acting.

Remark on the body-force term: Typically, the specific body force will be constant, e.g. gravity. Therefore, additional *specific* body forces will not occur. However, density changes can cause changes in the body forces:

$$\varrho \mathbf{b} = (\varrho_0 + \varrho_{\mathrm{incr}})(\mathbf{b}_0 + \mathbf{b}_{\mathrm{incr}}) \quad \text{with} \quad \varrho_{\mathrm{incr}} = \int_{t=t_0}^{t_1} \dot{\varrho} \, \mathrm{d}\bar{t} \tag{8}$$

Thus, even if a constant specific source term (e.g. gravity) is used, i.e. $\mathbf{b}_{\mathrm{incr}} = \mathbf{0}$, one would not have a vanishing body force term in Eq. (6). Instead, the acting force causing deformation beyond the initial state would consist of a specific body-force increment acting on the total density and a body force stemming from the density alteration:

$$\varrho \mathbf{b}_{\mathrm{incr}} + \varrho_{\mathrm{incr}} \mathbf{b}_0 = \varrho \mathbf{b} - \varrho_0 \mathbf{b}_0 \tag{9}$$

This is essential in unsaturated settings where during de-/resaturation strong density changes occur. In the small deformation process we assume this to be negligible. Thus, one would arrive at a typical setting that looks like this:

$$\int_{\Omega} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{C} \boldsymbol{B} \, \mathrm{d}\Omega \, \Delta \hat{\boldsymbol{u}} = \int_{\partial \Omega_{\mathrm{N}}} \boldsymbol{N}^{\mathrm{T}} \bar{\boldsymbol{t}} \, \mathrm{d}\Gamma - \int_{\Omega} \boldsymbol{B}^{\mathrm{T}} (\boldsymbol{\sigma} - \boldsymbol{\sigma}_{0\mathrm{neq}}) \, \mathrm{d}\Omega \tag{10}$$

such that a deformation-free state at $t = t_0$ requires

$$\int_{\partial \Omega_{\mathrm{N}}} \boldsymbol{N}^{\mathrm{T}} \bar{\boldsymbol{t}}(t = t_0) \, \mathrm{d}\Gamma = \boldsymbol{0} \tag{11}$$

i.e. that no (additional) external tractions are acting and body forces are zero.

2.3 Test case

The test cases illustrated in Fig. 1 using the above formulations have been added to `Tests/Data/Mechanics/Linear/Initial_States`.

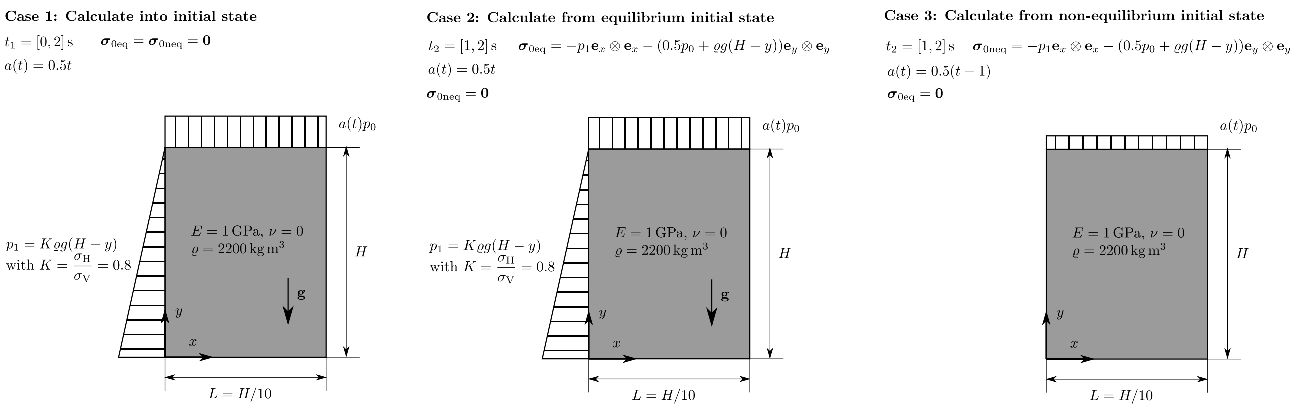

Figure 1: Test cases for the small deformation process.

3 [WIP] HM process

The linearised discretized weak forms of the two governing equations read:

$$\begin{aligned}\int_\Omega \boldsymbol{B}_u^\mathrm{T}\boldsymbol{C}\boldsymbol{B}_u\,\mathrm{d}\Omega\,\Delta\hat{\boldsymbol{u}} - \int_\Omega \boldsymbol{B}_u^\mathrm{T}\alpha_\mathrm{B}\boldsymbol{I}\boldsymbol{N}_p\,\mathrm{d}\Omega\,\Delta\hat{\boldsymbol{p}} = \\ = \int_{\partial\Omega_t}\boldsymbol{N}_u^\mathrm{T}\bar{\boldsymbol{t}}\,\mathrm{d}\Gamma + \int_\Omega \boldsymbol{N}_u^\mathrm{T}\varrho\boldsymbol{b}\,\mathrm{d}\Omega - \int_\Omega \boldsymbol{B}_u^\mathrm{T}(\boldsymbol{\sigma}' - \boldsymbol{\sigma}_{0\mathrm{neq}})\,\mathrm{d}\Omega + \int_\Omega \boldsymbol{B}_u^\mathrm{T}\alpha_\mathrm{B}(p - p_{0\mathrm{neq}})\boldsymbol{I}\,\mathrm{d}\Omega\end{aligned} \tag{12}$$

$$\begin{aligned}&\int_\Omega \boldsymbol{N}_p^\mathrm{T}\frac{\alpha_\mathrm{B}}{\Delta t}\boldsymbol{I}^\mathrm{T}\boldsymbol{B}_\mathrm{u}\,\mathrm{d}\Omega\,\Delta\hat{\boldsymbol{u}} + \left[\int_\Omega \boldsymbol{N}_p^\mathrm{T}\frac{S}{\Delta t}\boldsymbol{N}_p\,\mathrm{d}\Omega + \int_\Omega \nabla\boldsymbol{N}_p^\mathrm{T}\frac{\boldsymbol{K}}{\mu_\mathrm{LR}}\nabla\boldsymbol{N}_p\,\mathrm{d}\Omega\right]\Delta\hat{\boldsymbol{p}} = \\ &= \int_{\partial\Omega_w}\boldsymbol{N}_p^\mathrm{T}\dot{m}_n\,\mathrm{d}\Gamma - \int_\Omega \boldsymbol{N}_p^\mathrm{T}S\boldsymbol{N}_p\,\mathrm{d}\Omega\,(\hat{\boldsymbol{p}})'_\mathrm{S} - \int_\Omega \boldsymbol{N}_p^\mathrm{T}\alpha_\mathrm{B}\boldsymbol{I}^\mathrm{T}\boldsymbol{B}_\mathrm{u}\,\mathrm{d}\Omega\,(\hat{\boldsymbol{u}})'_\mathrm{S} - \int_\Omega \nabla\boldsymbol{N}_p^\mathrm{T}\frac{\boldsymbol{K}}{\mu_\mathrm{LR}}\nabla\boldsymbol{N}_p\,\mathrm{d}\Omega\,(\hat{\boldsymbol{p}} - \hat{\boldsymbol{p}}_{0\mathrm{neq}}) + \\ &+ \int_\Omega \nabla\boldsymbol{N}_p^\mathrm{T}\varrho_\mathrm{LR}\frac{\boldsymbol{K}}{\mu_\mathrm{LR}}\boldsymbol{b}\,\mathrm{d}\Omega\end{aligned} \tag{13}$$

Remark on the body-force term: Similar rationale as described under small deformation process in current implementation.

4 [WIP] RM process

to be done ...

Remark on the body-force term: Here, this term is crucial (uplift upon saturation increase).