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

Thomas Nagel, Dmitri Naumov, Wenqing Wang

August 28, 2019

Contents

Preliminary version. Testing in progress.
Comments to thomas.nagel@ifgt.tu-freiberg.de.

1 Preliminary remarks

What we require is a way of treating initial conditions which, in conjunction with the boundary conditions and other driving forces, do not satisfy equilibrium (in the sense of a general balance equation) at $t = t_0$.

If such an "incompatible" or "non-equilibrium" state is provided, the first equilibrium iteration will generally drive the process to equilibrium with potentially large solution increments, or even fail.

In certain conditions, in which it is practically not feasible to determine a self-consistent initial state, we want to drive changes in the process only by a change in the external driving forces and suppress the initial equilibration.

The initial values of all variables will nevertheless fully enter constitutive relations.

The following allows all sorts of computations, so handle with care. With great power comes a great need to know what you're doing.

2 Small deformation

2.1 Alternative (generalized/residual-based) treatment

Consider the standard formulation:

$$\int_{\Omega} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{C} \boldsymbol{B} \, \mathrm{d}\Omega \, \Delta \hat{\boldsymbol{u}} = \underbrace{\int_{\partial \Omega_{\mathrm{N}}} \boldsymbol{N}^{\mathrm{T}} \bar{\boldsymbol{t}} \, \mathrm{d}\Gamma + \int_{\Omega} \boldsymbol{N}^{\mathrm{T}} \varrho \boldsymbol{b} \, \mathrm{d}\Omega - \int_{\Omega} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{\sigma} \, \mathrm{d}\Omega}_{= \boldsymbol{r}} \tag{1}$$

The residual here corresponds to the out-of-balance forces. Let $\boldsymbol{\sigma}$ be initialized to some initial value, and the external tractions and body forces also have an initial value. Now we can distinguish two cases:

1. The initial stress is in equilibrium with the external forces. In that case, $\boldsymbol{r}_0 = \boldsymbol{0}$ and only a change in boundary conditions will cause a deformation.

2. The initial stress is *not* in equilibrium with the external forces. In that case, $\boldsymbol{r}_0 \neq \boldsymbol{0}$ and we would obtain an immediate deformation even without any change in boundary conditions.

If the latter behaviour in case 2 is undesired (often the case) because it is impossible to obtain a self-consistent initial state, we could introduce a keyword[1], which simply takes the residuals obtained by assembling the initial state, stores them in a nodal vector, and subtracts them from now on from the standard residual, turning it into a modified residual:

$$\boldsymbol{F}_0^{\mathrm{oob}} = \boldsymbol{r}_0 = \int_{\partial \Omega_{\mathrm{N}}} \boldsymbol{N}^{\mathrm{T}} \bar{\boldsymbol{t}}_0 \, \mathrm{d}\Gamma + \int_{\Omega} \boldsymbol{N}^{\mathrm{T}} \varrho_0 \boldsymbol{b}_0 \, \mathrm{d}\Omega - \int_{\Omega} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{\sigma}_0 \, \mathrm{d}\Omega \tag{2}$$

$$\int_{\Omega} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{C} \boldsymbol{B} \, \mathrm{d}\Omega \, \Delta \hat{\boldsymbol{u}} = \underbrace{\int_{\partial \Omega_{\mathrm{N}}} \boldsymbol{N}^{\mathrm{T}} \bar{\boldsymbol{t}} \, \mathrm{d}\Gamma + \int_{\Omega} \boldsymbol{N}^{\mathrm{T}} \varrho \boldsymbol{b} \, \mathrm{d}\Omega - \int_{\Omega} \boldsymbol{B}^{\mathrm{T}} \boldsymbol{\sigma} \, \mathrm{d}\Omega - \boldsymbol{F}_0^{\mathrm{oob}}}_{= \boldsymbol{r}_{\mathrm{mod}}} \tag{3}$$

This in turn provides us with the following options:

1. Case A: total stress form is retained by default. Also, if consistent initial states are provided, $\boldsymbol{r}_0 = \boldsymbol{0}$, and `equilibrate_initial_state` or `neutralize_initial_imbalance` would simply return a zero-vector. Whether or not the keyword is set makes no difference.

[1] `equilibrate_initial_state` or `neutralize_initial_imbalance`

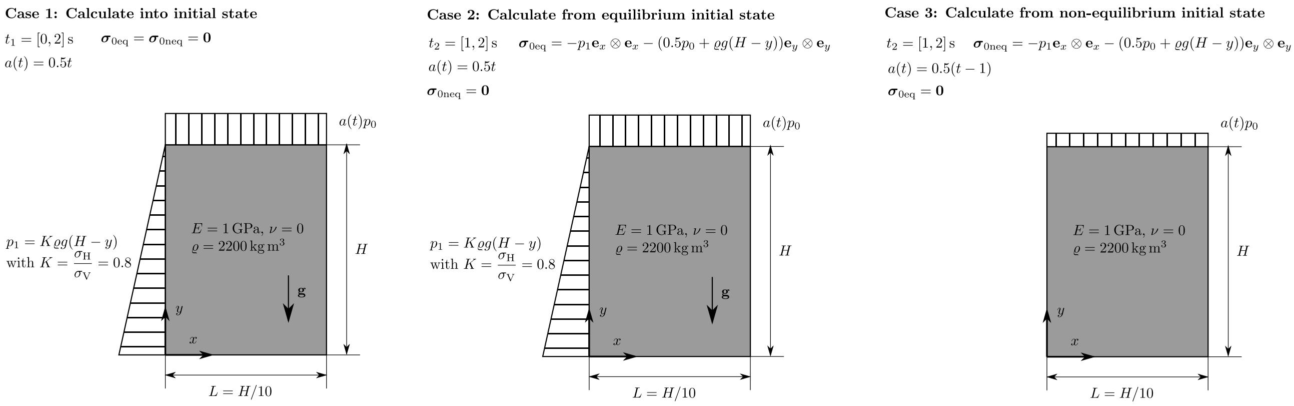

Figure 1: Test cases for the small deformation process.

2. Case B: Incremental form. If external loads not in equilibrium with initial stresses are provided, again only a change in these loads will now cause deformation because the initial non-equilibrium fraction is neutralized by $\boldsymbol{F}_0^\mathrm{oob}$. If all external loads are initially set to zero, then the simple incremental form is recovered, as in that case

$$\boldsymbol{F}_0^\mathrm{oob} = \boldsymbol{r}_0 = -\int\limits_\Omega \boldsymbol{B}^\mathrm{T}\boldsymbol{\sigma}_0\,\mathrm{d}\Omega \tag{4}$$

in which case only non-zero driving forces cause deformation. Intermediate cases such as $\boldsymbol{b} \neq \boldsymbol{0}$ and $\bar{\boldsymbol{t}} \neq \boldsymbol{0}$ are likewise possible.

There seem to be several advantages to this approach: The treatment is easily generalized to other processes without introducing a range of non-equilibrium initial states in addition to the actual physical initial states (less potential for confusion). Also, body-force effects due to density variations are covered naturally.

2.2 Test case

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

3 HM process

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

$$\begin{aligned}\int\limits_\Omega \boldsymbol{B}_u^\mathrm{T}\boldsymbol{C}\boldsymbol{B}_u\,\mathrm{d}\Omega\,\Delta\hat{\boldsymbol{u}} - \int\limits_\Omega \boldsymbol{B}_u^\mathrm{T}\alpha_\mathrm{B}\boldsymbol{I}\boldsymbol{N}_p\,\mathrm{d}\Omega\,\Delta\hat{\boldsymbol{p}} &= \\ = \int\limits_{\partial\Omega_t} \boldsymbol{N}_u^\mathrm{T}\bar{\boldsymbol{t}}\,\mathrm{d}\Gamma + \int\limits_\Omega \boldsymbol{N}_u^\mathrm{T}\varrho\boldsymbol{b}\,\mathrm{d}\Omega - \int\limits_\Omega \boldsymbol{B}_u^\mathrm{T}\boldsymbol{\sigma}'\,\mathrm{d}\Omega + \int\limits_\Omega \boldsymbol{B}_u^\mathrm{T}\alpha_\mathrm{B}p\boldsymbol{I}\,\mathrm{d}\Omega - {}^u\boldsymbol{F}_0^\mathrm{oob}\end{aligned} \tag{5}$$

with

$${}^u\boldsymbol{F}_0^\mathrm{oob} = \int\limits_{\partial\Omega_t} \boldsymbol{N}_u^\mathrm{T}\bar{\boldsymbol{t}}_0\,\mathrm{d}\Gamma + \int\limits_\Omega \boldsymbol{N}_u^\mathrm{T}\varrho_0\boldsymbol{b}_0\,\mathrm{d}\Omega - \int\limits_\Omega \boldsymbol{B}_u^\mathrm{T}\boldsymbol{\sigma}_0'\,\mathrm{d}\Omega + \int\limits_\Omega \boldsymbol{B}_u^\mathrm{T}\alpha_\mathrm{B}p_0\boldsymbol{I}\,\mathrm{d}\Omega \tag{6}$$

$$
\begin{aligned}
&\int_{\Omega} \boldsymbol{N}_p^{\mathrm{T}} \frac{\alpha_{\mathrm{B}}}{\Delta t} \boldsymbol{I}^{\mathrm{T}} \boldsymbol{B}_{\mathrm{u}} \,\mathrm{d}\Omega \,\Delta \hat{\boldsymbol{u}} + \left[\int_{\Omega} \boldsymbol{N}_p^{\mathrm{T}} \frac{S}{\Delta t} \boldsymbol{N}_p \,\mathrm{d}\Omega + \int_{\Omega} \nabla \boldsymbol{N}_p^{\mathrm{T}} \frac{\boldsymbol{K}}{\mu_{\mathrm{LR}}} \nabla \boldsymbol{N}_p \,\mathrm{d}\Omega \right] \Delta \hat{\boldsymbol{p}} = \\
&= \int_{\partial \Omega_w} \boldsymbol{N}_p^{\mathrm{T}} \dot{m}_n \,\mathrm{d}\Gamma - \int_{\Omega} \boldsymbol{N}_p^{\mathrm{T}} S \boldsymbol{N}_p \,\mathrm{d}\Omega (\hat{\boldsymbol{p}})_{\mathrm{S}}' - \int_{\Omega} \boldsymbol{N}_p^{\mathrm{T}} \alpha_{\mathrm{B}} \boldsymbol{I}^{\mathrm{T}} \boldsymbol{B}_{\mathrm{u}} \,\mathrm{d}\Omega (\hat{\boldsymbol{u}})_{\mathrm{S}}' - \int_{\Omega} \nabla \boldsymbol{N}_p^{\mathrm{T}} \frac{\boldsymbol{K}}{\mu_{\mathrm{LR}}} \nabla \boldsymbol{N}_p \,\mathrm{d}\Omega \,\hat{\boldsymbol{p}} + \qquad (7) \\
&+ \int_{\Omega} \nabla \boldsymbol{N}_p^{\mathrm{T}} \varrho_{\mathrm{LR}} \frac{\boldsymbol{K}}{\mu_{\mathrm{LR}}} \boldsymbol{b} \,\mathrm{d}\Omega - {}^{p}\boldsymbol{F}_0^{\mathrm{oob}}
\end{aligned}
$$

with

$$
{}^{p}\boldsymbol{F}_0^{\mathrm{oob}} = \int_{\partial \Omega_w} \boldsymbol{N}_p^{\mathrm{T}} \dot{m}_{\mathrm{n}0} \,\mathrm{d}\Gamma - \int_{\Omega} \nabla \boldsymbol{N}_p^{\mathrm{T}} \frac{\boldsymbol{K}_0}{\mu_{\mathrm{LR}0}} \nabla \boldsymbol{N}_p \,\mathrm{d}\Omega \,\hat{\boldsymbol{p}}_0 + \int_{\Omega} \nabla \boldsymbol{N}_p^{\mathrm{T}} \varrho_{\mathrm{LR}0} \frac{\boldsymbol{K}_0}{\mu_{\mathrm{LR}0}} \boldsymbol{b}_0 \,\mathrm{d}\Omega \qquad (8)
$$

where initial rates are implicitly assumed to vanish. Otherwise, values for the rates at the initial state need to be additionally provided. For now, the working hypothesis is that the initial state is a steady state.

Remark on the keyword structure: For a coupled process, the initial state treatment should be accessible *individually* for each governing equation, i.e. each ${}^{i}\boldsymbol{F}_0^{\mathrm{oob}}$.

4 RM process

The mechanical residual is modified to

$$
\mathbf{r}_u = \int_{\Omega} \left(\mathbf{B}_u^{\mathrm{T}} \boldsymbol{\sigma} - \mathbf{N}_u^{\mathrm{T}} \varrho \mathbf{b} \right) \mathrm{d}\Omega - \int_{\partial \Omega_t} \mathbf{N}_u^{\mathrm{T}} \bar{\mathbf{t}} \,\mathrm{d}\Gamma \qquad (9)
$$

$$
= \int_{\Omega} \left(\mathbf{B}_u^{\mathrm{T}} \boldsymbol{\sigma}_{\mathrm{eff}} - \mathbf{N}_u^{\mathrm{T}} \varrho \mathbf{b} \right) \mathrm{d}\Omega + \int_{\Omega} \mathbf{B}_u^{\mathrm{T}} \alpha_{\mathrm{B}} (p_{\mathrm{GR}} - \chi(S_{\mathrm{L}}) p_{\mathrm{cap}}) \mathbf{I} \,\mathrm{d}\Omega - \int_{\partial \Omega_t} \mathbf{N}_u^{\mathrm{T}} \bar{\mathbf{t}} \,\mathrm{d}\Gamma - {}^{u}\boldsymbol{F}_0^{\mathrm{oob}} \qquad (10)
$$

with

$$
{}^{u}\boldsymbol{F}_0^{\mathrm{oob}} = \int_{\Omega} \left(\mathbf{B}_u^{\mathrm{T}} \boldsymbol{\sigma}_{\mathrm{eff}0} - \mathbf{N}_u^{\mathrm{T}} \varrho_0 \mathbf{b}_0 \right) \mathrm{d}\Omega + \int_{\Omega} \mathbf{B}_u^{\mathrm{T}} \alpha_{\mathrm{B}} (p_{\mathrm{GR}0} - \chi(S_{\mathrm{L}0}) p_{\mathrm{cap}0}) \mathbf{I} \,\mathrm{d}\Omega - \int_{\partial \Omega_t} \mathbf{N}_u^{\mathrm{T}} \bar{\mathbf{t}}_0 \,\mathrm{d}\Gamma \qquad (11)
$$

The hydraulic residual is modified such

$$
\mathbf{r}_p = \int_{\Omega} \mathbf{N}_p^{\mathrm{T}} \varrho_{\mathrm{LR}} a_S \Delta t^{-1} \left[S_{\mathrm{L}}(p_{\mathrm{GR}} - \mathbf{N}_p \hat{\mathbf{p}}_{\mathrm{L}}^{t+1}) - S_{\mathrm{L}}(p_{\mathrm{GR}} - \mathbf{N}_p \hat{\mathbf{p}}_{\mathrm{L}}^{t}) \right] \mathrm{d}\Omega + \int_{\Omega} \mathbf{N}_p^{\mathrm{T}} \varrho_{\mathrm{LR}} a_p \mathbf{N}_p \,\mathrm{d}\Omega (\hat{\mathbf{p}}_{\mathrm{L}})_{\mathrm{S}}' + \qquad (12)
$$

$$
\begin{aligned}
&+ \int_{\Omega} \mathbf{N}_p^{\mathrm{T}} S_{\mathrm{L}} \varrho_{\mathrm{LR}} \alpha_{\mathrm{B}} \mathbf{I}^{\mathrm{T}} \mathbf{B}_{\mathrm{u}} \,\mathrm{d}\Omega (\hat{\mathbf{u}})_{\mathrm{S}}' + \int_{\Omega} \nabla \mathbf{N}_p^{\mathrm{T}} \varrho_{\mathrm{LR}} \frac{k_{\mathrm{rel}}(S_{\mathrm{L}}) \mathbf{K}}{\mu_{\mathrm{LR}}} \nabla \mathbf{N}_p \,\mathrm{d}\Omega \,\hat{\mathbf{p}}_{\mathrm{L}} - \\
&- \int_{\Omega} \nabla \mathbf{N}_p^{\mathrm{T}} \varrho_{\mathrm{LR}}^2 \frac{k_{\mathrm{rel}}(S_{\mathrm{L}}) \mathbf{K}}{\mu_{\mathrm{LR}}} \mathbf{b} \,\mathrm{d}\Omega - \int_{\partial \Omega_w} \mathbf{N}_p^{\mathrm{T}} \dot{m}_{\mathrm{L}} \,\mathrm{d}\Gamma - {}^{p}\boldsymbol{F}_0^{\mathrm{oob}} \qquad (13)
\end{aligned}
$$

with

$$
{}^{p}\boldsymbol{F}_0^{\mathrm{oob}} = \int_{\Omega} \nabla \mathbf{N}_p^{\mathrm{T}} \varrho_{\mathrm{LR}0} \frac{k_{\mathrm{rel}}(S_{\mathrm{L}0}) \mathbf{K}_0}{\mu_{\mathrm{LR}0}} \nabla \mathbf{N}_p \,\mathrm{d}\Omega \,\hat{\mathbf{p}}_{\mathrm{L}0} - \int_{\Omega} \nabla \mathbf{N}_p^{\mathrm{T}} \varrho_{\mathrm{LR}0}^2 \frac{k_{\mathrm{rel}}(S_{\mathrm{L}0}) \mathbf{K}}{\mu_{\mathrm{LR}0}} \mathbf{b}_0 \,\mathrm{d}\Omega - \int_{\partial \Omega_w} \mathbf{N}_p^{\mathrm{T}} \dot{m}_{\mathrm{L}0} \,\mathrm{d}\Gamma \qquad (14)
$$