Stationary creep with the BGRa model: Implementation in OpenGeoSys

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Contents

1 Preliminary definitions

Effective stress:

$$\sigma_{\text{eff}} = \sqrt{\frac{3}{2}} \|\boldsymbol{\sigma}^{\text{D}}\| = \sqrt{3 J_2} \tag{1}$$

The BGRa Model is given by

$$\boldsymbol{\sigma} = \mathscr{C} : \boldsymbol{\epsilon}_{\text{el}} \tag{2}$$

$$\boldsymbol{\epsilon}_{\text{el}} = \boldsymbol{\epsilon} - \boldsymbol{\epsilon}_{\text{cr}} - \boldsymbol{\epsilon}_{\text{th}} \tag{3}$$

$$\boldsymbol{\epsilon}_{\text{th}} = \alpha_T (T - T_0) \mathbf{I} \tag{4}$$

$$\dot{\boldsymbol{\epsilon}}_{\text{cr}} = \frac{3}{2} A \left(\frac{\sigma_{\text{eff}}}{\sigma_0}\right)^n \exp\left(-\frac{Q}{RT}\right) \frac{\boldsymbol{\sigma}^{\text{D}}}{\sigma_{\text{eff}}} == \sqrt{\frac{3}{2}} A \left(\frac{\sigma_{\text{eff}}}{\sigma_0}\right)^n \exp\left(-\frac{Q}{RT}\right) \frac{\boldsymbol{\sigma}^{\text{D}}}{\|\boldsymbol{\sigma}^{\text{D}}\|} \tag{5}$$

$$= A \left(\frac{3}{2}\right)^{\frac{n+1}{2}} \left(\frac{1}{\sigma_0^n}\right) \exp\left(-\frac{Q}{RT}\right) \|\boldsymbol{\sigma}^{\text{D}}\|^{n-1} \boldsymbol{\sigma}^{\text{D}} \tag{6}$$

By setting

$$b = A \left(\frac{3}{2}\right)^{\frac{n+1}{2}} \left(\frac{1}{\sigma_0^n}\right) \exp\left(-\frac{Q}{RT}\right) \tag{7}$$

one gets

$$\dot{\boldsymbol{\epsilon}}_{\text{cr}} = b \|\boldsymbol{\sigma}^{\text{D}}\|^{n-1} \boldsymbol{\sigma}^{\text{D}} \tag{8}$$

2 Implementation

The implementation is performed within a fully implicit scheme using nested Newton-Raphson algorithm as the standard material model interface in OGS-6. For details on the general scheme, see:

- Thomas Nagel, Wolfgang Minkley, et al. (Apr. 2017). "Implicit numerical integration and consistent linearization of inelastic constitutive models of rock salt". In: *Computers & Structures* 182, pp. 87–103. ISSN: 00457949
- Thomas Nagel, Norbert Böttcher, et al. (2017). *Computational Geotechnics*. SpringerBriefs in Energy January. Cham: Springer International Publishing, pp. 1–12. ISBN: 978-3-319-56960-4

and references therein.

2.1 Rate form

The above equations can be condensed into a single rate equation for the stress:

$$\begin{aligned} \Delta\boldsymbol{\sigma} &= \mathscr{C} : \left(\Delta\boldsymbol{\epsilon} - \alpha_T \Delta T\, \mathbf{I} - b\, \Delta t \|\boldsymbol{\sigma}^{\text{D}}\|^{n-1} \boldsymbol{\sigma}^{\text{D}}\right) \\ &= \mathscr{C} : (\Delta\boldsymbol{\epsilon} - \alpha_T \Delta T\, \mathbf{I}) - 2 b G \Delta t \|\boldsymbol{\sigma}^{\text{D}}\|^{n-1} \boldsymbol{\sigma}^{\text{D}} \end{aligned} \tag{9}$$

With a backward Euler implementation the residual for the local stress integration algorithm reads:

$$\mathbf{r}_\sigma = \boldsymbol{\sigma}^{t+\Delta t} - \boldsymbol{\sigma}^{t} - \mathscr{C} : (\Delta\boldsymbol{\epsilon} - \alpha_T \Delta T\, \mathbf{I}) + 2 b G \Delta t \|\boldsymbol{\sigma}^{\text{D}}\|^{n-1} \boldsymbol{\sigma}^{\text{D}} \tag{10}$$

such that $\boldsymbol{\sigma}^{t+\Delta t}$ can be determined iteratively. The local Jacobian only requires the derivative

$$\mathscr{J}_{\sigma\sigma} = \frac{\partial \mathbf{r}_\sigma}{\partial \boldsymbol{\sigma}} = \mathscr{I} - 2 b G \|\boldsymbol{\sigma}^{\text{D}}\|^{n-1} \left(\mathscr{P}^{\text{D}} + (n-1) \|\boldsymbol{\sigma}^{\text{D}}\|^{-2} \boldsymbol{\sigma}^{\text{D}} \otimes \boldsymbol{\sigma}^{\text{D}}\right) \tag{11}$$

After convergence, the consistent tangent operator can then be extracted with the help of

$$\frac{\partial \mathbf{r}_\sigma}{\partial \boldsymbol{\epsilon}} = -\mathcal{C} \tag{12}$$

using

$$\left(\left. \frac{\partial \mathbf{r}}{\partial \boldsymbol{\sigma}} \right|_{t+\Delta t} \right) \frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\boldsymbol{\epsilon}^{t+\Delta t}} = -\frac{\partial \mathbf{r}}{\partial \boldsymbol{\epsilon}} \tag{13}$$

which in the present case can be written directly as

$$\frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\boldsymbol{\epsilon}^{t+\Delta t}} = \mathcal{J}_{\sigma\sigma}^{-1} : \mathcal{C} \tag{14}$$

2.2 Absolute form

The often more accurate absolute form would read (with the initial stress $\boldsymbol{\sigma}_0$ and initial temperature T_0):

$$\boldsymbol{\sigma} = \mathcal{C} : (\boldsymbol{\epsilon} - \alpha_T (T - T_0)\mathbf{I} - \boldsymbol{\epsilon}_{\mathrm{cr}}) + \boldsymbol{\sigma}_0 \tag{15}$$

$$\dot{\boldsymbol{\epsilon}}_{\mathrm{cr}} = b \|\boldsymbol{\sigma}^{\mathrm{D}}\|^{n-1} \boldsymbol{\sigma}^{\mathrm{D}} \tag{16}$$

With a backward Euler implementation the residual for the local stress integration algorithm reads:

$$\mathbf{r}_\sigma = \boldsymbol{\sigma}^{t+\Delta t} - \boldsymbol{\sigma}_0 - \mathcal{C} : \left(\boldsymbol{\epsilon}^{t+\Delta t} - \alpha_T (T^{t+\Delta t} - T_0)\mathbf{I} - \boldsymbol{\epsilon}_{\mathrm{cr}}^{t+\Delta t} \right) \tag{17}$$

$$\mathbf{r}_{\mathrm{cr}} = \frac{\boldsymbol{\epsilon}_{\mathrm{cr}}^{t+\Delta t} - \boldsymbol{\epsilon}_{\mathrm{cr}}^{t}}{\Delta t} - b \|(\boldsymbol{\sigma}^{t+\Delta t})^{\mathrm{D}}\|^{n-1} (\boldsymbol{\sigma}^{t+\Delta t})^{\mathrm{D}} \tag{18}$$

This formulation shows very directly the straight-forward extension to BGRb.
The local Jacobian has the four entries

$$\mathcal{J}_{\sigma\sigma} = \frac{\partial \mathbf{r}_\sigma}{\partial \boldsymbol{\sigma}} = \mathcal{I} \tag{19}$$

$$\mathcal{J}_{\sigma\epsilon_{\mathrm{cr}}} = \frac{\partial \mathbf{r}_\sigma}{\partial \boldsymbol{\epsilon}_{\mathrm{cr}}} = \mathcal{C} \tag{20}$$

$$\mathcal{J}_{\epsilon_{\mathrm{cr}}\sigma} = \frac{\partial \mathbf{r}_{\mathrm{cr}}}{\partial \boldsymbol{\sigma}} = -2bG \|\boldsymbol{\sigma}^{\mathrm{D}}\|^{n-1} \left(\mathcal{P}^{\mathrm{D}} + (n-1) \|\boldsymbol{\sigma}^{\mathrm{D}}\|^{-2} \boldsymbol{\sigma}^{\mathrm{D}} \otimes \boldsymbol{\sigma}^{\mathrm{D}} \right) \tag{21}$$

$$\mathcal{J}_{\epsilon_{\mathrm{cr}}\epsilon_{\mathrm{cr}}} = \frac{\partial \mathbf{r}_{\mathrm{cr}}}{\partial \boldsymbol{\epsilon}_{\mathrm{cr}}} = \frac{1}{\Delta t} \mathcal{I} \tag{22}$$

After convergence, the consistent tangent operator can then be extracted with the help of

$$\frac{\partial \mathbf{r}_\sigma}{\partial \boldsymbol{\epsilon}} = -\mathcal{C} \tag{23}$$

$$\frac{\partial \mathbf{r}_{\mathrm{cr}}}{\partial \boldsymbol{\epsilon}} = \mathcal{O} \tag{24}$$

using

$$\frac{\mathrm{d}\mathbf{z}}{\mathrm{d}\boldsymbol{\epsilon}^{t+\Delta t}} = -\left[\mathcal{J}|_{t+\Delta t} \right]^{-1} \frac{\partial \mathbf{r}}{\partial \boldsymbol{\epsilon}} \quad \text{with} \quad \mathbf{z} = [\boldsymbol{\sigma}, \, \boldsymbol{\epsilon}_{\mathrm{cr}}]^{\mathrm{T}} \tag{25}$$

2.3 Remarks on the TM coupling

The consistent tangent is required as per the linearisation of the term

$$\int_\Omega \mathbf{B}_u^{\mathrm{T}} \boldsymbol{\sigma}(\boldsymbol{\epsilon}, T) \, \mathrm{d}\Omega \tag{26}$$

along the displacement increment:

$$\mathrm{D}_{\Delta\mathbf{u}} \int_{\Omega} \mathbf{B}_u^{\mathrm{T}} \boldsymbol{\sigma}(\boldsymbol{\epsilon}, T)\, \mathrm{d}\Omega = \int_{\Omega} \mathbf{B}_u^{\mathrm{T}} \frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}\boldsymbol{\epsilon}} \mathbf{B}_u \,\mathrm{d}\Omega\, \Delta\hat{\mathbf{u}} = \mathbf{K}_{uu} \Delta\hat{\mathbf{u}} \tag{27}$$

Linearisation into the direction of the temperature increment yields the coupling matrix:

$$\mathrm{D}_{\Delta T} \int_{\Omega} \mathbf{B}_u^{\mathrm{T}} \boldsymbol{\sigma}(\boldsymbol{\epsilon}, T)\, \mathrm{d}\Omega = \int_{\Omega} \mathbf{B}_u^{\mathrm{T}} \frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}T} \mathbf{N}_T \,\mathrm{d}\Omega\, \Delta\hat{\mathbf{T}} = \mathbf{K}_{uT} \Delta\hat{\mathbf{T}} \tag{28}$$

For the BGRa model, we find

$$\frac{\mathrm{d}\boldsymbol{\sigma}}{\mathrm{d}T} = -\mathscr{C} : \left[\alpha_T \mathbf{I} + \frac{Q}{RT^2} \dot{\boldsymbol{\epsilon}}_{\mathrm{cr}} \Delta t \right] \tag{29}$$

References

Nagel, Thomas, Wolfgang Minkley, et al. (Apr. 2017). “Implicit numerical integration and consistent linearization of inelastic constitutive models of rock salt”. In: *Computers & Structures* 182, pp. 87–103. ISSN: 00457949.

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