An improved monolithic Newton-Raphson scheme for J_2 plastic flow with non-linear hardening and softening

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Problem statement

- $\dot{\boldsymbol{\varepsilon}}(\nabla v) = \dot{\boldsymbol{\varepsilon}}_e + \dot{\boldsymbol{\varepsilon}}_p = \mathbb{C}^{-1}\dot{\boldsymbol{\sigma}} + \dot{\varepsilon}_p\,\hat{\boldsymbol{n}}$
  $\rightarrow \dot{\boldsymbol{\sigma}} = \mathbb{C}(\dot{\boldsymbol{\varepsilon}}(\nabla v) - \dot{\varepsilon}_p\,\hat{\boldsymbol{n}})$
- $\nabla \cdot \boldsymbol{\sigma} = 0$
- $\mathcal{F}(\boldsymbol{\sigma},\, \bar{\varepsilon}_p,\, \dot{\bar{\varepsilon}}_p;\, \ldots) \leq 0$

Subject to velocity loading conditions on at least part of the external boundary

$\boldsymbol{\sigma}$	stress tensor
$\dot{\boldsymbol{\varepsilon}}, \dot{\boldsymbol{\varepsilon}}_e, \dot{\boldsymbol{\varepsilon}}_p$	strain rate tensor, elastic-, plastic-
$\mathbb{C}$	elastic stiffness tensor
$\dot{\varepsilon}_p$	scalar magnitude of plastic strain rate
$\hat{\boldsymbol{n}}$	unit tensor in dir. of plastic strain: $\sqrt{\hat{\boldsymbol{n}} : \hat{\boldsymbol{n}}} = 1$
$\mathcal{F}$	'yield function'
$\bar{\varepsilon}_p, \dot{\bar{\varepsilon}}_p$	optionally non-local equiv. pl. strain and -rate, following $\bar{\varepsilon} = \varepsilon + c^2\nabla^2\varepsilon$ (explicit) $\varepsilon = \bar{\varepsilon} - c^2\nabla^2\bar{\varepsilon}$ (implicit) **[1]**

Example of a non-linear plastic flow rule

Rate- and State-dependent bulk friction with explicit non-local involvement of strain rate and state in the evolution equation:

$$\mathcal{F} = J_2\,\mathrm{dev}\,\boldsymbol{\sigma} - C\cos\phi(\dot{\varepsilon}_p, \theta) + \sin\phi(\dot{\varepsilon}_p, \theta)\,\tfrac{1}{3}\mathrm{tr}\,\boldsymbol{\sigma}$$

$$\phi(\dot{\varepsilon}_p, \theta) = \tan^{-1}\left[\mu_* + a\log\frac{\dot{\varepsilon}_p}{\dot{\varepsilon}_*} + b\log\frac{\theta}{\theta_*}\right]$$

$$\dot{\theta} = \alpha_1\left[2 - \frac{\overline{\theta^{-1-b/a}}}{\theta^{-1-b/a}}\right] - \alpha_2\frac{\overline{\dot{\varepsilon}_p^2}}{\dot{\varepsilon}_p}\theta$$

Current best practices

Multi-level Newton with consistent tangent linearization **[2]**.

- Reliable quadratic convergence.
- Computationally expensive iterations of the global problem due to the requirement that the non-linear plastic flow rule is solved accurately at each iterate.
- Problematic if the plastic flow rule is non-local
- Prohibits cheaply, accurately finite-differenced Jacobians.

Proposed alternative

Algorithm of **[3]** improved for J_2-plasticity: instead of requiring the simultaneous solution of 9 unknowns in 3D $(v, \dot{\boldsymbol{\varepsilon}}_p)$, here we require the simultaneous solution of 4 unknowns $(v, \dot{\varepsilon}_p)$. The residual formulation reads:

$\vec{\mathcal{R}}\,(\boldsymbol{v},\, \dot{\varepsilon}_p) = \{$

$$P \leftarrow -\int K\,\mathrm{tr}\,\dot{\boldsymbol{\varepsilon}}(\nabla v)\,\mathrm{d}t$$

$$\tau_y = \tau_y(P, \dot{\bar{\varepsilon}}_p, \int \dot{\bar{\varepsilon}}_p\,\mathrm{d}t; \ldots) \qquad 1$$

$$\boldsymbol{\tau} \leftarrow \text{solve} \quad \dot{\boldsymbol{\tau}} = 2\,G\left[\mathrm{dev}\,\dot{\boldsymbol{\varepsilon}} - \dot{\varepsilon}_p\frac{\boldsymbol{\tau}}{\boxed{\tau_y}}\right] \qquad 2$$

$$\mathcal{R}_{\boldsymbol{v}} = \mathrm{div}\,(\boldsymbol{\tau} - P\mathbf{I})$$

$$\boldsymbol{\tau}^* \leftarrow 2\,G\,\mathrm{dev}\int \dot{\boldsymbol{\varepsilon}}\,\mathrm{d}t\;; \quad \tau^* = \sqrt{\boldsymbol{\tau}^* : \boldsymbol{\tau}^*} \qquad 3$$

$\mathrm{if}(\tau^* > \tau_y)$

$$\dot{\varepsilon}_p^* = \max\Big(0, \dot{\varepsilon}_p(\boldsymbol{\tau},\, P,\, \dot{\boldsymbol{\varepsilon}};\, \ldots)\Big) \qquad 4$$

$\mathrm{else}\;\; \dot{\varepsilon}_p^* = 0$

$$\mathcal{R}_{\dot{\varepsilon}_p} = \dot{\varepsilon}_p^* - \dot{\varepsilon}_p - \alpha_n\left[\int \dot{\varepsilon}_p\,\mathrm{d}t - \varepsilon_p^P\right] \qquad 5$$

$\leftarrow (\mathcal{R}_{\boldsymbol{v}},\, \mathcal{R}_{\dot{\varepsilon}_p})$

$\}$

1. Computation of yield strength τ_y based on proposed $\boldsymbol{v}, \dot{\varepsilon}_p$
2. Dirty trick! Replaced $\tau = \sqrt{\boldsymbol{\tau} : \boldsymbol{\tau}}$ with τ_y. This leads to a small, self-correcting deviation from the true solution. However, it is crucial to the proposed system reduction.
3. Elastic deviatoric stress prediction; J_2 of stress predictor.
4. Updated estimate of plastic strain rate magnitude, derived from the consistency condition $\dot{\mathcal{F}} = 0$.
5. The crux of the one-level residual. The unknown $\dot{\varepsilon}_p$ occurs in such a position that its effect on the residual is predominantly smooth. The last term is a damping term that favors polynomial extrapolation ($\dot{\varepsilon}_p^P$) at large time steps. The time step h is adapted separately to minimize the mismatch between the predictor and corrector **[3]**.

while $\neg$*finished* **do**

$$n = n + 1; \quad \alpha_n = 1/h_n + 1/(h_n + h_{n-1})$$

$$\varepsilon_p^P,\, \varepsilon_p\big|_n \leftarrow \text{extrapolate}\left\langle \varepsilon_p\big|_{n-3}, \ldots, \varepsilon_p\big|_{n-1}\right\rangle \qquad \text{a}$$

$$\dot{\varepsilon}_p^P \leftarrow \text{differentiate}\left\langle \varepsilon_p\big|_{n-3}, \ldots, \varepsilon_p\big|_{n}\right\rangle \qquad \text{a}$$

$$\left(\boldsymbol{u}_n,\, \varepsilon_p\big|_n\right) \leftarrow \text{minimize}\;\; \vec{\mathcal{R}}\,(\boldsymbol{u},\, \varepsilon_p) \qquad \text{b}$$

$$\xi_n = 1/(h_n + h_{n-1} + h_{n-2})/\alpha_n \qquad \text{c}$$

$$ERR = \xi_n\frac{\|\varepsilon_p - \varepsilon_p^P\|}{RTOL\|\varepsilon_p\| + ATOL} \qquad \text{c}$$

$$h^* = h_n\min(\beta_u,\, \max(\beta_l,\, \beta_s ERR^{-1/3})) \qquad \text{c}$$

if $ERR < 1$

$$\vec{\varepsilon_p} = \left(\vec{\varepsilon_p},\, \varepsilon_p\big|_n\right);\;\; \vec{h} = (\vec{h},\, h^*) \qquad \textbf{(continue)}$$

else

$$h_n = h^*; \quad n = n - 1 \qquad \textbf{(redo step)}$$

a. Sequences in angular brackets denote Newton polynomials.
b. $\|\vec{\mathcal{R}}\|$ is minimized by a Newton-Raphson procedure. The Jacobian is formed by finite-differencing the residual with respect to its independent variables $\boldsymbol{v}$ and $\dot{\varepsilon}_p$.
c. Adaptive time-stepping procedure based on minimization of the extrapolation error **[3]**.

Known properties of the algorithm

- Quadratic convergence.
- Second-order accurate in time.
- Variable time step, reasonably optimal adaptivity.
- Residual can be straightforwardly finite-differenced to form the Jacobian: cheap and accurate.
- Readily extensible to a wide range of hardening and softening laws, including those that are non-local.

Observed properties of the algorithm

- Quadratic convergence.
- Time step implicitly controlled by the propagation of the elastic-plastic boundary: adaptive time-stepping nearly always too zealous; advantage of second-order accuracy in time questionable.
- A zoo of numerical tuning parameters makes you waste time when the model is changed.

References

[1] Peerlings, R. H. J. et al. (1996). "Gradient Enhanced Damage for Quasi-Brittle Materials." International Journal for Numerical Methods in Engineering 39.19, 3391–3403.
[2] Duretz et al. (2018). "The benefits of using a consistent tangent operator for viscoelastoplastic computations in geodynamics." Geochemistry, Geophysics, Geosystems 19, 4904–4924.
[3] Eckert et al. (2004). "A BDF2 integration method with step size control for elasto-plasticity." Computational Mechanics 34.5, 377–386.