Nonlinear Finite Element Methods

Assignment for summer term 2019

1 Task

Considered is the phase transformation of a spherical inclusion of radius r_i within an ideally elastic-plastic matrix material (Young's modulus E, Poisson ratio ν, yield stress σ_y). The phase transformation is purely dilatational, i. e., it leads to a remanent volume increase with volumetric strain $\bar{\varepsilon}_\mathrm{v}$ without change of shape. The problem exhibits

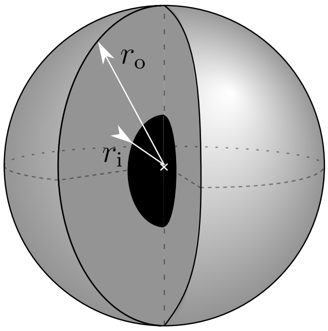

Figure 1: Inclusion in metallic matrix

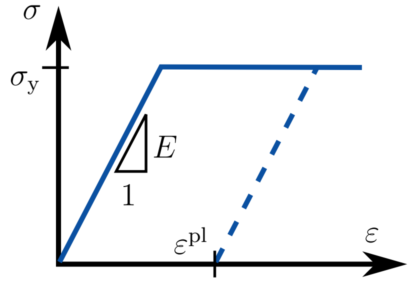

Figure 2: Elastic ideal-plastic material

a spherical symmetry with respect to the center of the inclusion. The matrix material is modeled as a concentric sphere of radius r_o. Consequently, the only non-trivial equilibrium condition in a spherical coordinate system r–ϕ–θ is

$$0 = \frac{\partial(r^2\sigma_{rr})}{\partial r} - r\,(\sigma_{\phi\phi} + \sigma_{\theta\theta}) \tag{1}$$

with non-vanishing stress components σ_{rr}, $\sigma_{\phi\phi}$ and $\sigma_{\theta\theta}$. The weak form of Eq. (1) reads

$$0 = \delta W = \int_{r_\mathrm{i}}^{r_\mathrm{o}} \underline{\delta\varepsilon}^\mathrm{T} \cdot \underline{\sigma}\, r^2\,\mathrm{d}r - \left[r^2\sigma_{rr}\delta u_r\right]_{r=r_\mathrm{i}}^{r_\mathrm{o}} \tag{2}$$

with stresses and strains written in Voigt notation as

$$\underline{\sigma} = \begin{bmatrix}\sigma_{rr}\\ \sigma_{\phi\phi}\\ \sigma_{\theta\theta}\end{bmatrix}, \quad \underline{\delta\varepsilon} = \begin{bmatrix}\delta\varepsilon_{rr} = \frac{\partial\delta u_r}{\partial r}\\ \delta\varepsilon_{\phi\phi} = \frac{\delta u_r}{r}\\ \delta\varepsilon_{\theta\theta} = \frac{\delta u_r}{r}\end{bmatrix}, \quad \text{and analogously } \underline{\varepsilon} = \begin{bmatrix}\varepsilon_{rr} = \frac{\partial u_r}{\partial r}\\ \varepsilon_{\phi\phi} = \frac{u_r}{r}\\ \varepsilon_{\theta\theta} = \frac{u_r}{r}\end{bmatrix}. \tag{3}$$

Therein, the displacement in radial direction $u_r(r)$ is the only non-vanishing displacement component. The boundary conditions for the problem in Figure 1 are $\sigma_{rr}(r = r_\mathrm{o}) = 0$ and $u_r(r = r_\mathrm{i}) = \frac{1}{3}\tau\bar{\varepsilon}_\mathrm{v} r_\mathrm{i}$, respectively. Therein, $\tau \in [0, 1]$ refers to the monotonically increasing time-like parameter, with which the load $\bar{\varepsilon}_\mathrm{v}$ is applied at $r = r_\mathrm{i}$.

Create a program (MatLab/Octave/Python) which solves this static FEM problem. The program has to be verified by comparisons with known analytical solutions and a convergence study shall be performed (see below).

2 Details

The following list gives a brief overview of the features which have to be implemented:

- The program shall be structured into main program, element routine and material routine, the latter two as separate `function` each
- local mesh refinement closer to the inclusion: $h^e(r = r_\mathrm{i}) = \frac{1}{5}h^e(r = r_\mathrm{o})$ (h^e: element size), see code sniplet in appendix
- linear shape functions for $u_r(r)$:

$$[\mathbf{N}](\xi) = \left[\frac{1}{2}(1-\xi), \frac{1}{2}(1+\xi)\right]^\mathrm{T} \text{ in } \Omega_\square = \{\xi \in [-1, 1]\} \tag{4}$$

- quadrature with a single Gauss point per element
- varying number of elements and time increment $\Delta\tau$
- Newton method with convergence criteria $\left\|\underline{\hat{\mathbf{G}}}\right\|_\infty < 0.005 \left\|\underline{\hat{\mathbf{F}}}_\mathrm{int}\right\|_\infty$, $\|\blacktriangle\underline{\hat{\mathbf{u}}}_k\|_\infty < 0.005\,\|\underline{\hat{\mathbf{u}}}\|_\infty$ (with $\|\underline{\hat{\circ}}\|_\infty$ denoting the infinity norm, i. e. the maximum component by amount of the column vector $\underline{\hat{\circ}}$)
- elastic ideal-plastic matrix material (Mises plasticity)

$$\sigma_{ij} = 2\mu(\varepsilon_{ij} - \varepsilon_{ij}^\mathrm{pl}) + \lambda\delta_{ij}(\varepsilon_{kk} - \varepsilon_{kk}^\mathrm{pl}) \quad \text{with } \mu = \frac{E}{2(1+\nu)}, \quad \lambda = \frac{\nu E}{(1-2\nu)(1+\nu)}$$

$$\Phi = \sigma^\mathrm{eq} - \sigma_\mathrm{y} \leq 0 \qquad \text{with } \sigma^\mathrm{eq} = \sqrt{\frac{3}{2}\sigma_{kl}^\mathrm{d}\sigma_{kl}^\mathrm{d}},\ \sigma_\mathrm{y} = \mathrm{const}$$

- radial return mapping algorithm in material routine with algorithmically consistent material tangent stiffness matrix

The assignment shall be completed in groups of *two students*. One student is responsible for developing the main program including pre- and postprocessing. The other students develops the element routine and the material routine. The particular material parameters (E, ν, σ_0), loading $\bar{\varepsilon}_\mathrm{v}$ and geometric properties r_i and r_o to be implemented depend on your variant as given in Table 1. *Each group of students has to work on that variant that corresponds to the last digit of the sum of their matriculation numbers.*

3 Workflow

1. Theory
   - Discretize the weak form (2) in space (i. e. in r).
   - Identify the $\underline{\underline{\mathbf{B}}}$ matrix to be defined as $\underline{\varepsilon} = \underline{\underline{\mathbf{B}}} \cdot \underline{\hat{\mathbf{u}}}^e$ for the shape functions in Eq. (4).
   - Identify the vectors of internal and external nodal forces $\underline{\hat{\mathbf{F}}}^e_{\mathrm{int}}$ and $\underline{\hat{\mathbf{F}}}_{\mathrm{ext}}$.
2. Implementation in MatLab/Octave/Python:
   - Implement $\underline{\underline{\mathbf{B}}}$ and $[\mathbf{N}]$ into an element routine to compute $\underline{\hat{\mathbf{F}}}^e_{\mathrm{int}}$ (*Hint:* The Jacobian of the element is identical to the FEM of rods considered in the exercises.)
   - Develop the main program which assembles total nodal forces for each time increment and performs the Newton-Raphson scheme.
   - Note that the material routine requires internal state variables (the plastic strains) for which memory has to be allocated and which have to be passed through main program and element routine.
3. Verification:

   a) According to classical theory of elasticity, the exact solution of the considered boundary value problem Eqs. (1)–(3) for *linear-elastic material* in the limiting case $r_\mathrm{o}/r_\mathrm{i} \to \infty$ is

$$u_r^{\mathrm{elast}} = \frac{r_\mathrm{i}^3 \bar{\varepsilon}_\mathrm{v}}{3r^2}\,, \qquad \sigma_{rr}^{\mathrm{elast}} = -\frac{2E\bar{\varepsilon}_\mathrm{v}}{3(1+\nu)}\frac{r_\mathrm{i}^3}{r^3} \tag{5}$$

   and plasticity initiates at a dilatation of the inclusion of

$$\bar{\varepsilon}_\mathrm{v}^{\mathrm{init}} = (1+\nu)\frac{\sigma_0}{E}\,, \tag{6}$$

   In a first step, apply a load $\bar{\varepsilon}_\mathrm{v} < \bar{\varepsilon}_\mathrm{v}^{\mathrm{init}}$ in the elastic regime. Perform a convergence study with respect to the number of elements and verify your

Table 1: Assignment of parameters

variant	E [MPa]	ν	σ_0 [MPa]	r_i [µm]	r_o [µm]	$\bar{\varepsilon}_\mathrm{v}$
1	200 000	0.20	200	5	20	0.01
2	70 000	0.25	70	10	40	0.01
3	70 000	0.30	70	15	60	0.01
4	200 000	0.30	200	20	80	0.01
5	100 000	0.30	100	25	100	0.01
6	200 000	0.20	400	5	25	0.02
7	70 000	0.25	140	10	50	0.02
8	70 000	0.30	140	15	75	0.02
9	200 000	0.30	400	20	100	0.02
0	100 000	0.30	200	25	125	0.02

FEM solution by means of the exact solution (5). Verify that the Newton-Raphson method converges within a single iteration for the linear problem.

b) In the next step, perform a convergence study with respect to number of elements and time increments $\Delta\tau$ for the full load $\bar{\varepsilon}_{\mathrm{v}}$ in the plastic regime. Identify the necessary number of elements and the required $\Delta\tau$.

4. Results:
   - Extract the distributions of $u_r(r)$, $\sigma_{rr}(r)$ and $\sigma_{\phi\phi}(r)$ at final loading $\tau = 1$ from your FEM simulation.
   - Demonstrate the nonlinearity of the problem by extracting the time history of the radial stress at the inclusion $\sigma_{rr}(r \approx r_{\mathrm{i}}, \tau)$ for $\tau \in [0, 1]$.

4 Documentation

In addition to the program code, a short *technical documentation* is to be created (in hard-copy form) containing:

1. a brief overview over the implemented theory
2. an overview over the program structure (routines, files, ...), as text or graphically
3. a short user's manual answering the following questions:
   - How to start the program?
   - Where does the program get its input from?
   - What output does the program generate and where does it store it to?
4. verification and results as requested in section 3 ("Verification" means that expectations on the numerical results are formulated and that it is discussed whether the obtained numerical results meet these expectations and where potential deviations between expectation and actual results might arise from.)

5 Remarks

- The successful completion of the task is a prerequisite to be admitted to the final examination. Depending on the evaluation of the assignment, *up to five bonus points can be gained for the examination.*
- Questions on the assignment should be posed in classes or after the lecture.
- The deadline for the assignment is **Friday, 12th of July, 2019** when the program has to be sent to Geralf.Huetter@imfd.tu-freiberg.de and the documentation has to be in hard-copy form at mailbox of the institute (in front of WEI-130). Each group has to present their program individually in the subsequent week.

Appendix

Click **here** in AdobeReader to download code sniplet for generating a local mesh refinement.