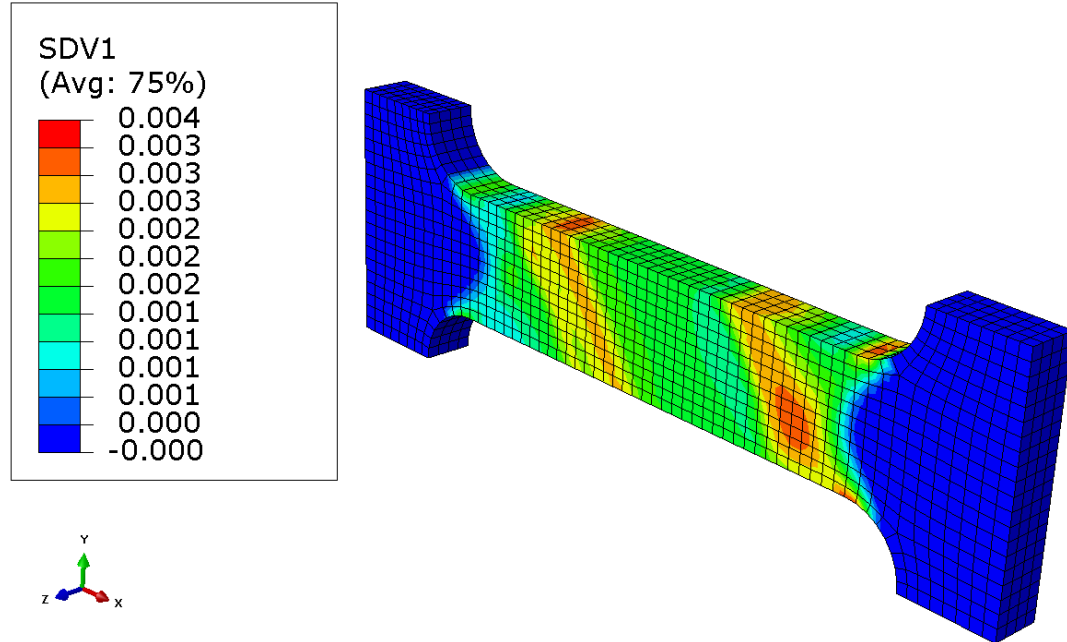




School of Engineering  
Brown University

## EN234: Computational methods in Structural and Solid Mechanics

### Homework 9: Explicit Dynamics: modeling PLC bands Due Fri Nov 17, 2017



In this problem you will code an ABAQUS VUMAT subroutine to implement a rate and state dependent plasticity model (called the ‘McCormick model’) that is intended to model the effects of dynamic strain ageing in a solute strengthened metal.

To keep things simple, we will assume that the strains are small (it turns out that the small strain code doesn’t need to be modified for a large deformation analysis; the reasons for this will be discussed in class later).

The McCormick model is a rate dependent viscoplasticity model. As discussed in class, we will decompose the strain rate into elastic and plastic parts

$$\dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^e + \dot{\epsilon}_{ij}^p$$

The elastic and plastic strain rates are

$$\dot{\epsilon}_{ij}^e = \frac{1+\nu}{E} \left( \dot{\sigma}_{ij} - \frac{\nu}{1+\nu} \dot{\sigma}_{kk} \delta_{ij} \right) \quad \dot{\epsilon}_{ij}^p = \dot{\epsilon}_e \frac{3 S_{ij}}{2 \sigma_e}$$

$$S_{ij} = \sigma_{ij} - \sigma_{kk} \delta_{ij} / 3 \quad \sigma_e = \sqrt{\frac{3}{2} S_{ij} S_{ij}} \quad \dot{\epsilon}_e = \sqrt{\frac{2}{3} \dot{\epsilon}_{ij}^p \dot{\epsilon}_{ij}^p}$$

where  $\dot{\varepsilon}^P(\sigma, t_a)$  is the plastic strain rate magnitude, which depends on the effective stress, and a state variable  $t_a$  that represents the age of dislocations, as follows

$$\dot{\varepsilon}_e = \dot{\varepsilon}_0 \exp \left\{ \frac{\sigma - \sigma_0(\varepsilon_e)}{S} - HC \right\}$$

Here  $\dot{\varepsilon}_0$  is a characteristic strain rate (a material property),  $S$  and  $H$  are material constants controlling the instantaneous and steady-state strain rate sensitivity of the solid, while  $\sigma_0(\varepsilon_e)$  is the flow stress in a solute-free material. The flow stress evolves with plastic strain due to strain hardening. The strain hardening can be approximated using a power-law

$$\sigma_0(\varepsilon_e) = \sigma_{Y0} \left( 1 + \varepsilon_e / \varepsilon_0 \right)^m$$

where  $\{\sigma_{Y0}, \varepsilon_0, m\}$  are material parameters, and  $\varepsilon^P$  is the accumulated plastic strain. The variable  $C$  in the equation for strain rate represents the solute concentration around dislocations, which depends on the average age  $t_a$  of dislocations according to

$$C = 1 - \exp \left( - \left[ \frac{t_a}{t_d} \right]^\alpha \right)$$

where  $t_d, \alpha$  are material properties, and  $t_a$  is the average time that a mobile dislocation is pinned by obstacles. The age of dislocations  $t_a$  evolves with time and strain rate as follows

$$\frac{dt_a}{dt} = 1 - \frac{t_a}{\Omega} \frac{d\varepsilon_e}{dt}$$

The goal of this homework is to implement this material model as an ABAQUS VUMAT subroutine.

The VUMAT must accomplish the following calculation:

Given: (1) the stress components  $\sigma_{ij}^n$ ; (2) the age  $t_a$  (3) the accumulated plastic strain  $\varepsilon_e$  at the start of a time-step, and (4) the strain increment  $\Delta\varepsilon_{ij}$ ,

Calculate: the stresses  $\sigma_{ij}^{n+1}$ , along with updated values for  $t_a$  and  $\varepsilon_e$  at the end of a step.

We can use the procedure discussed in class (Lect 15) to do this. Even in an explicit dynamic simulation, it is a good idea to use a fully implicit stress update (with plastic strain rate based on the stress at the end of the time-step), to make sure that the critical time-step for stability of the explicit dynamic algorithm is not reduced. Here are the steps in the calculation:

- (1) Calculate the deviatoric strain increment  $\Delta e_{ij} = \Delta\varepsilon_{ij} - \Delta\varepsilon_{kk} \delta_{ij} / 3$
- (2) Calculate the deviatoric stress at the start of the step  $S_{ij}^n = \sigma_{ij}^n - \sigma_{kk}^n \delta_{ij} / 3$
- (3) Calculate the elastic predictor for the deviatoric stress  $S_{ij}^* = S_{ij}^n + \frac{E}{1+\nu} \Delta e_{ij}$  and hence calculate the predictor for effective stress  $\sigma_e^* = \sqrt{3 S_{ij}^* S_{ij}^* / 2}$
- (4) Solve the following equations for the plastic strain increment and the increment in  $t_a$  (use Newton-Raphson iteration – you can eliminate  $\Delta t_a$  by hand)

$$0 = \frac{\sigma_e^*}{S} - \frac{3E}{2(1+\nu)S} \Delta\varepsilon_e - \left\{ \frac{\sigma_0(\varepsilon_e + \Delta\varepsilon_e)}{S} + HC + \log \left( \frac{\Delta\varepsilon_e}{\Delta t \dot{\varepsilon}_0} \right) \right\}$$

$$C = 1 - \exp\left(-\left[\frac{t_a + \Delta t_a}{t_d}\right]^\alpha\right)$$

$$t_a + \Delta t_a = \frac{\Omega \Delta t}{\Delta \varepsilon_e} + \left(t_a - \frac{\Omega \Delta t_a}{\Delta \varepsilon_e}\right) \exp\left(-\frac{\Delta \varepsilon_e}{\Omega}\right)$$

$$\sigma_0 = \sigma_{Y0} \left(1 + (\varepsilon_e + \Delta \varepsilon_e) / \varepsilon_0^p\right)^m$$

Write your code carefully to make sure  $t_a + \Delta t_a$  is computed accurately even if the plastic strain increment is very small – it is a good idea to trap for small values and use the Taylor expansion if  $\Delta \varepsilon_e / \Omega$  becomes very small.

- (5) Calculate the updated stress from

$$\sigma_{ij} = S_{ij}^* \left(1 - \frac{3E\Delta \varepsilon_e}{2(1+\nu)\sigma_e^*}\right) + \frac{E}{3(1-2\nu)} (\Delta \varepsilon_{kk}) \delta_{ij}$$

You can develop your code in EN234FEA:

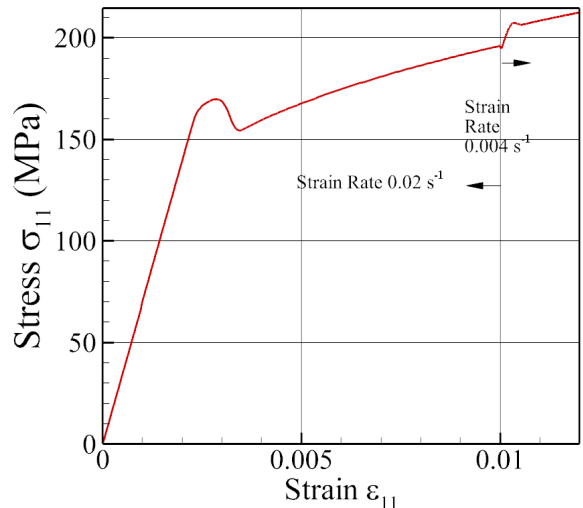
- (1) Download the file called Abaqus\_vumat\_McCormick.for from the website.
- (2) Add the .for file to your EN234FEA project in Eclipse or Visual Studio
- (3) Rename the subroutine called vumat() in the file called abaqus\_vumat.f90 to something else

The changes to the code will be fairly small:

- You will need an additional state variable to store  $t_a$
- You will need to use the McCormick hardening law to calculate the plastic strain increment

You can test your code with the sample input file called Abaqus\_vumat\_McCormick.in. This runs a simulation with a single element, which subjects the material to a strain rate jump test (the strain rate is dropped from 0.02 to 0.004 after 0.5 seconds). Note that:

- (4) The file assumes you will use 3 material state variables (the total accumulated plastic strain, the value of  $t_a$  and the increment in plastic strain. The latter is helpful to provide an initial guess for the plastic strain increment in the Newton iterations.
- (5) Check the file for the order in which the material parameters are specified (you can change this if you like, of course).
- (6) To debug your code change the number of steps to just 2 or 3 before running the full 20000 steps.
- (7) Simulations with the McCormick model need very small time-steps – the strain increment in any one step has to be smaller than  $\Omega$ , which is typically very small - otherwise you get spurious oscillations or even instability. The parameters in the file provided work, but if you change them the simulation might bomb.
- (8) The code saves a tecplot readable file called McCormick\_stressvstrain.dat, which contains columns of the total elapsed time, strain components, and stress components. The printing is done in the file called user\_print.f90 if you want to see the source code. Once you have your code working, you can plot S11 as a function of E11 in tecplot to see the stress-v-



strain curve for the material. You should see two of the features of the model: (1) There is a drop in flow stress when the material first starts to yield – this is because the age of the pinned dislocations  $t_d$  starts with a large value, and then drops when the dislocations are unpinned during the onset of plastic flow. (2) When the strain rate decreases, the material initially softens (this is hard to see as it is small), and then the flow stress increases. This is called ‘negative strain rate sensitivity’ – the flow stress decreases with increasing strain rate – and causes the material to behave in a strange way.

Once you have your VUMAT working in EN234FEA, please run it in ABAQUS/Explicit. Start by duplicating the same 1-element test that you used to test your subroutine in EN234FEA, and make sure you get the similar answers from ABAQUS. Use the following lines in the .inp file to set up the user material

```
*Material, name=Material-1
*DEPVAR
3
*Density
0.005,
*User Material, constants=11
70000., 0.3, 70., 0.001, 0.3, 1e-08, 2.23, 27.9
0.02, 0.00015, 0.336
*INITIAL CONDITION, type=Solution
SET-1,0.0,10.0,0.0
```

(the SET-1 specifies the name of an element set; you may need to change this)

Once your code runs with one element you can try something more sophisticated. The figure on the first page of this HW shows accumulated plastic strain contours in a tensile specimen that is being strained at about  $0.005 \text{ s}^{-1}$  strain rate (note that ABAQUS is able to plot contours of user-defined state variables). The simulation was run with element size and material properties specified in the EN234FEA example file for this problem, but using the default Abaqus/explicit time step. Instead of using mass scaling, a fictitious density was used.

When you run ABAQUS with an explicit dynamic simulation you need to select the precision of the computation – the default precision for explicit dynamics is single precision, but the VUMAT is coded with double precision variables. To do this start abaqus with

```
abaqus job=(input) user=(subroutine) double
```

Because of the strain rate softening in the McCormick model, the material does not deform uniformly, but forms bands of strain that propagate up and down the specimen. The strain bands are called ‘Portevin-Le Chatelier (PLC)’ bands.

As a solution to this homework, please

- (1) Hand in a pdf document that describes the simulations you ran to test your code and shows some representative results.
- (2) Push your code to your GitHub repository.