**CPFE model guidelines**

Pre-requisite files to be modified before running the model:

* prein
* material.fmt
* input.txt
* dirname
* orientation.ori

**Initial set-up**

Create a directory with the user’s surname, containing the folders “bin” and “CPFEM”.

“Bin” contains all the files that run the model.

“CPFEM” contains the subfolders “Materials”, “Orientations”, “Results”.

“Materials” folder contains the material.fmt file.

“Orientations” folder contains the .ori files.

“Results” folder contains the model output, as well as the files: prein, input.txt, dirname.

N.B.: If the directory root to the model output is modified, the changes should be included in the dirname file.

**Material.fmt file**

This file contains the hardening law parameters that are required to run the model. These parameters can be approximated before running the model, by inserting them into the excel file “Voce law”, where they are fitted to the experimentally measured stress-strain curve.

1) Define how many parameters will be given below for the model to take as input. This number should match the number of columns in (5) below -> hardening law parameters.

2) Enter the maximum number of slip systems. This number should be equal to the number of rows in (4) and (5) below, as well as the dimensions of the square matrix in (6).

3) Compliance is the inverse of stiffness (units are MPa-1). These values are the S11, S12 and S44, and can be found in the literature (standard values for BCC steel are shown in this example).

4) Enter the active slip systems. The first 3 columns are the slip directions, while the last 3 are the slip planes. Any combination is acceptable, as long as any two rows are not identical. Also, each slip system has to obey the Weiss zone law: hu+kv+lw=0. The values entered represent normalised vectors (unit vector divided over its length –the length of the unit vector is equal to 1). Each slip plane and slip direction uses the corresponding values below:

(In the example file provided, the slip system is the {110}<111>.)

5) Hardening law parameters (the number of columns was defined earlier in (1)).

A: step values for strain increment.

B: initial hardening rate, corresponds to the elastic region of the stress-strain curve.

C: final hardening rate, corresponds to the plastic region of the stress-strain curve.

D: alpha value, defines the shape of the stress-strain curve during the transition stage from elastic to plastic behaviour.

E: taus, is the saturation slip resistance defining the stress level at which the curve should saturate.

F: strain rate sensitivity, defines the behaviour of the final part of the plastic region and dictates whether the stress will rise further or not. This value is the maximum critical resolved shear stress for that slip system.

6) Latent hardening matrix. This is a square matrix with dimensions equal to the maximum number of slip systems. This matrix determines the extent to which slip on one system causes hardening in the others. A matrix of ones means that all slip systems harden equally (i.e. a ratio of 1:1).

**Ori file**

The texture in the ori file should be orientated such that the intended deformation direction is aligned with the x-axis or RD. The layout is basically a list of euler angles in radians. The first column denotes the weights of each euler angle set (typically a column of ones), the remaining three columns denote phi1, PHI and phi2.

**prein file**

1-3: Number of divisions in x,y,z. Maximum number is 18, which gives 5832 elements. Each element is assigned an orientation value from the input starting texture.

4-6: Length of each element in x,y,z. Typical values: 1.

7: Shape of element. Typically 20 node tetrahedra (2) give more accurate results.

8: Select boundary behaviour.

(0): Boundary strain. Gives the option to include shear strain ε13.

(1): FC brick. Full constraints deformation. Use for rolling.

(2): Free x faces.

(3): Just x faces. Use for tension or compression.

9: Max number of slip systems. Match this to the number entered in the material.fmt file.

10: Select starting texture of the material.

(1): Bicrystal.

(2): Perturbed-ideal.

(3): Included grain.

(4): Input file orientation.ori contains Euler angles measured in radians (degree angles will not be accepted by the code and it will not run). The first column is assigned a weight of 1 (not important to the code), and the next 3 columns are the phi1, Phi, phi2 Euler angles. The number of orientations in the .ori file should match the number of elements entered in rows 1-3. More orientations could give higher accuracy but will increase running time.

An example of the maximum orientation density as a function of the number of orientations for simulated textures is given in the graph below, for a weak and a strong texture. The maximum density reaches a plateau above approximately 1000 orientations. However, when more orientations are selected the position of the maximum density may not be located at the original position in Euler space. Note that the intensity of simulated textures is always slightly underestimated, especially for strong textures.

C:\Users\Dimitris\Documents\OriginLab\85\User Files\temp 24h.tif

(5): Random. Random starting texture is assumed.

11: Enter number of orientation sets. Typically only 1 set is used.

12: Assigning orientation sets: Enter fraction for set 1. The value entered is the fraction of the orientations to be used from the file. Typically the fraction is 1.

13: Empty line (necessary).

14: Name of .ori file (exclude “.ori” extension from the filename). The .ori file should be placed in the folder: /home/username/CPFEM/Orientations/.

15: Number of property sets. Define how many .ori files will be given as input (typically 1). This option only appears when the “File orientations (4)” is chosen in line 10.

16: Empty line (necessary).

17: Name of material file (exclude the “.fmt” extension from the filename). The .fmt file should be placed in the folder: /home/username/CPFEM/Materials/

18: Make initial slip resistance equal? (y/n) Typically yes.

19: Enter initial slip resistance. This value is close to the ratio of yield stress divided by the Taylor factor, but it can be altered accordingly by fitting the predicted stress-strain curve to the experimental one.

20: Set a fraction to elastic only? (y/n) Specify if the elastic stress-strain region will be modelled with a certain number of points out of the total points used. More points can be allocated for better determination of the elastic region.

21: Size of increments (ε11 and ε13). Positive values for tension, negative for compression and rolling.

22: Number of increments (max 2000). Adjust according to the increment size to get the desired final strain.

23: Contraction ratio. Typically 0.

24-26: Set tied node conditions for x,y,z. (y/n) Typically no.

27: Name of file that the model calls to allocate output.

N.B.: Any empty lines appearing in the prein file are important and should not be removed, as this is how the file is read during execution.

**If input files are not accepted by code**

If the .fmt or .ori files appear correct but are not accepted by the code, use the command dos2unix in the Bash command window after navigating into the directory where the particular file is located (cd x/x/ ).

e.g. dos2unix \*.fmt will convert all .fmt files within the current folder you are in.

**Model output**

Files to be kept after running are:

* gstressout: contains the predicted stress values. The corresponding strain values for the predicted stress-strain curve are calculated up to the final strain as increments of magnitude equal to the final strain divided by the number of increments.
* output\_name-2000.csv (Excel file): contains the predicted Euler values. A .ori file can thus be created and the predicted texture can be plotted with appropriate software. The file name is given by the name specified in row 27 of the prein file. The last iteration is selected for the final texture. If the texture at another point of the curve is required, the corresponding file can be selected.
* output\_name-2000.frs: this file is used as input for the post-processor Fasplot3.exe to visualise the results.

**Command line**

To run the model and leave it running even after you log out, type:

nohup bash /home/username/bin/batch-run-p1.sh &

To check if the model is running properly (gives the contents of the output file which is a list of the iterations), type:

cat nohup.out

To run the model step by step and check its options, type:

/home/username/bin/fs3pre

Alternatively, the command line can also be used to obtain the files containing the model output.

gstress.pl<output\_filname.txt gives the gstressout file.

csvmkr.pl creates the .csv files from the .frs files.

**Additional functions**

Extracting lattice strains from CPFEM results:

To extract lattice strains for a particular plane two functions need to be run:

1. feistrs\_do\_zr.pl: creates a .csv file for a number of crystallographic planes at each increment.

2. extract\_means\_hcp.pl: creates a .dat file for the lattice strains in x,y, and z directions for each plane family.

The .dat file can be opened in Excel and the data extracted.

The above named scripts are for Zr and therefore HCP. There will be equivalent scripts available for FCC etc.