

A single folder with the following name MM1\*B\*\*\*-CMEL-2021-part\*.zip should be uploaded for each part on Moodle.

### **Part-1: Generation of 2-D digital microstructures**

The submission folder must contain the source codes, the gif file showing the microstructure evolution and a PDF report containing the results for each question

1. Write a code to generate a digital microstructure. The code should take as an input the following (a) size of the computational grid, (b) number of grains, (c) 2-D velocity vector, (d) frequency with which you write the output files. Include in the report the output image for equiaxed grains and elongated grains
2. Calculate what fraction of the pixels are grain interior pixels, grain boundary pixels and triple point pixels. Report this for a computational grid of 1024\*1024 with 100, 500 and 1000 grains respectively
3. Write a Matlab code using Voronoi to generate a digital microstructure with a given number of grains as input

### **Part-2: Generation and simulation of 3-D digital microstructures**

The submission folder must contain output ASCII file in ‘Los Alamos FFT’ format (for questions 1-2) and snapshots of visualised polycrystal should be included in the report

Download DREAM.3D version 6.5 from <http://dream3d.bluequartz.net/>

Download Paraview version 5.8 from <https://www.paraview.org/download/>

1. Use DREAM.3D software to generate a 3D microstructure with the following attributes (a) single phase, (b) elongated grains, (c) random texture. Use a computational grid of 64\*64\*64 and 500 grains
2. Use DREAM.3D software to generate a 3D microstructure with the following attributes (a) precipitation strengthened matrix with precipitates (volume fraction of 10%) only at the grain boundaries, (b) equiaxed grains, (c) random texture. Use a computational grid of 64\*64\*64 and 500 grains
3. Run a polycrystal simulation with different Zener ratio: isotropic, Copper and Stainless steel. Plot the histogram and the box plots of the local stress and strain concentration i.e.  $\frac{\sigma_{eq}(x)}{\langle \sigma_{eq} \rangle}$ . Write down your inferences. The grid size should be at least 32 in each direction and a minimum of 100 grains
4. Run a plate with a hole simulation. Write a code to generate a microstructure file for a plate of 512 x 512 with a hole in the centre with a radius of 5 voxels. Plot the stress profile from the tip of the void to the one end of the plate. How does it compare the stress profiles in front of a crack tip that you have seen in fracture mechanics?

5. Run a series of simulations with 2 phase microstructures with a varying fraction of second phases. Plot the variation of effective elastic modulus i.e.  $\frac{\langle \sigma_{33} \rangle}{\langle \varepsilon_{33} \rangle}$  with the fraction of second phase? Write down your observations

### **Part-3: Principal Component Analysis**

1. Pick an image of a microstructure of your choice. Let it be  $m * n$  pixels. Treat it as a dataset with  $m$  sampling points and  $n$  features. Perform PCA on the data set. Plot the Pareto plot. Reconstruct the image using 1, 5 ,10 and 15 principal components. Identify the number of components required to capture 95% of the variance in the original data. Use that many components to reconstruct the image. Write down your observations