MH2060 Crystal Plasticity Modelling Assignment

1. Objective: Analyse the effect of crystallographic orientation on single crystal behaviour using the DAMASK framework.

Create Aluminium single crystals with the following specifications:

- Grid size 16x16x16 voxels spanning a microstructure volume of 50x50x50 μm^3.
- Assign different orientations:
  (a) [1, 1, 0] → [0.9238795325112867, 0.3826834323650898, 0.0, 0.0]
  (b) [1, 0, 0] → [1.0000, 0.0000, 0.0000, 0.0000]
  (c) [1, 1, 1] → [0.8880562234694231, 0.459734862673287, 0.0, 0.0]
  (d) 45 deg about [1, 1, 1] → [0.9238795325112867, 0.22094238269039457, 0.22094238269039457, 0.22094238269039457]
  (e) 54.74 deg about [1, 1, 1] → [0.8880562234694231, 0.2654280467202779, 0.2654280467202779, 0.2654280467202779]
  (f) 60 deg about [1, 1, 1] → [0.8660254037844387, 0.28867513459481287, 0.28867513459481287, 0.28867513459481287]

Apply uniaxial tensile load in x-direction and deform at strain rate 0.001 s^{-1} up to 10% strain, assuming 100 time steps. All material properties including hardening parameters, slip systems are provided in the Material.yaml file. For single crystals with different orientations, plot a bar chart of the von Mises stress at the maximum strain for different orientations and comment on the orientation(s) that lead to minimum stress.

2. Objective: Analyse the effect of grain size on stress development in polycrystals using the DAMASK framework.

Create 3D Aluminium polycrystals with the following specifications:

- Grid size 16x16x16 voxels spanning a microstructure volume of 10x10x10 μm^3.
- Number of grains: 2, 8, 32, 64 (Four cases).
- Random crystallographic orientations in the form of sets of quaternions

Apply uniaxial tensile load on the polycrystals in the x-direction and deform at strain rate 0.001 s^{-1} up to 10% strain, assuming 100 time steps. All material properties are provided in the Material.yaml file. For polycrystals with different number of grains on the same grid, i.e., different average grain sizes:

(a) Plot a bar chart of the average von Mises stress (over all grains) vs number of grains at the final strain. A postprocessing script will be provided.
(b) Show colormaps of the von Mises stress and equivalent strain at the final strain for all four cases and highlight regions of maximum stress and strain.