Module 3: ParaDiS Project - Frank-Read source and density growth in aluminum

Project Brief

In this project, you will use discrete dislocation dynamics simulation to examine the increase in dislocation density in an Al sample, starting from a single Frank-Read source. You will examine the effect of (1) cross-slip, (2) the applied stress, and (3) the dislocation mobility parameters on the increase in dislocation density in a periodic simulation. This will allow you to examine how to provide information for higher length scale models, such as the density evolution equation you considered in Module 1.

Deliverables

You will produce a short report documenting your findings. Your report should contain a separate section for each of the tasks listed below, and provide the explicit deliverables requested for each task indicated by **[Report]** below. For the input scripts below, simply cut-and-paste your input script into your report. Your report should be formatted as a single pdf document comprising your report. You may wish to write your report in latex and convert using `pdflatex`, or in markdown and convert using `pandoc report.text --to latex --out report.pdf`; alternatively, you can put together a clearly formatted jupyter notebook. (`module load pandoc` and `module load texlive` to have the most up-to-date versions of each).

You should submit your report by creating a subdirectory called
`/class/mse404pla/sp26/<your_net_id>/Project3`
and copying your PDF into that directory by **11:59pm on 4 May 2025. *Late submissions will not be accepted*; let me know in advance if you will have difficulty with completion..**

Instructions

You will use `ParaDiS` throughout for your simulations. These codes are freely available (after signup) from the ParaDiS website; there are copies of these on the EWS linux workstations, including the compiled versions of the `ParaDiS` executables. There is also documentation for both available on EWS in the `/class/mse404pla/ParaDiS/doc` directory. The directories of interest are:

- Documentation for `ParaDiS` and `DDLab`: `/class/mse404pla/ParaDiS/doc`
- ParaDiS: `/class/mse404pla/ParaDiS/2.5.1`

The steps you will take below are:

1. Investigating the effect of cross-slip on the dislocation dynamics simulation.
2. Investigating the effect of stress on the increase in density.
3. Investigating the effect of dislocation mobility on the increase in density.
4. *Bonus:* comparing execution time, using the fast-multipole method.

In the directory `/class/mse404pla/ParaDiS/Project` you will find a starting control file and node file. Copy these to an appropriate subdirectory in your home directory. You will likely want to use a similar directory structure to what we used in the walkthrough.

NOTE: For this assignment, you will be running multiple dislocation dynamics simulations. If you use the *same output directory* for each run, `ParaDiS` will *append* the output of the current run to whatever is already there. This allows `ParaDiS` to "restart" a previous run, continuing from where it left off. This is **not the behavior you will be interested in** so either (a) make different output directories for each run, or (b) copy out what files you need to an appropriate place after running.

First, look through the control file. You will need to make a few edits to this to begin.

```
### This is the control file for the FCC Al Frank-Read source
# Output generated by this example will be placed under the directory
# specified by the <dirname> value and includes:
#    restart files
#    various properties files
dirname = "Output/"

#  Domain geometry
numXdoms = 1
numYdoms = 1
numZdoms = 1

#  Cell geometry
numXcells = 3
numYcells = 3
numZcells = 3

# Boundary type
xBoundType = 0
yBoundType = 0
zBoundType = 0

#  Dynamic load balancing
decompType = 1
DLBfreq = 0

# Discretization and topological change controls
maxSeg = 400
minSeg = 20
remeshRule = 3
enforceGlidePlanes =   1
splitMultiNodeFreq =   1

# Simulation time and timestepping controls
maxstep =   200000
timestepIntegrator =   "trapezoid"
```

```
nextDT = 1.0e-10;
rTol =  2.5
rmax = 5
rc =  5.0

# Fast Multipole Method controls
Rijmfile = "inputs/Rijm.cube.out"
RijmPBCfile = "inputs/RijmPBC.cube.out"

# fmEnabled =   1
# fmEnabled =   1
# fmMPOrder =   2
# fmTaylorOrder =   5
# fmCorrectionTbl =   "inputs/fm-ctab.Al.m2.t5.dat"

# Loading conditions
loadType = 0
appliedStress = [ 0, 0, 100e6, 0, 0, 0 ]

# Material and mobility parameters
mobilityLaw =   "FCC_0b"
shearModulus =   27e9  # Voigt Average
pois =   0.333
burgMag =   2.86e-10

# Mobility law and cross-slip
MobScrew =   60.000000e+04
MobEdge =    60.000000e+04
enableCrossSlip =   1

#  I/O controls and parameters
#
savecn =   1
savecnfreq =  2000
saveprop =   1
savepropfreq =  100
savetimers =   0
```

The `dirname` will need to be changed to the directory you want to use. In addition, note the parameters that describe the loading (constant stress, corresponding to a "creep" simulation), mobilities, and the enabling of cross-slip. Also take note of the parameters that control the number of steps, and how often information (restart files and material properties) are stored. You may want to change these as your simulations progress.

Part 1. Geometry

- **[Report]** Next, look at the datafile. What is this geometry? Dimensions, number of dislocation segments, Burgers vector, slip plane?

Part 2. Cross-slip

- **[Report]** Set up a run with a normal stress on the z axis of 100 MPa. **Turn off cross-slip**. What do you expect to happen when you run, and what do you see? Does the simulation result make sense?

Part 3. Effect of stress

Turn cross-slip back on. Proceed through a number of simulations, going a z normal stress from 50 MPa to 150 MPa in steps of 25 MPa.

- **[Report]** For each, make a plot of dislocation density with plastic strain. Try to reach 1% strain. What do you notice for the dislocation density with increasing stress?
- **[Report]** For each stress, take a few snapshots (hit the F10 key to generate a postscript file in the X-window) to show example dislocation configurations. Discuss what types of dislocation configurations you see (junctions, loops, superjogs).
- **[Report]** Is there a non-zero stress where the dislocation density does not grow? Explain.

Part 4. Effect of mobility

- **[Report]** Choose a loading stress of 100 MPa. Modify your dislocation mobilities: increase and decrease by a factor of 2. What changes do you notice in the dislocation density?

Part 5. *Bonus:* FMM

- **[Report]** Generate the fast multipole method data files for your simulation, and run one simulation to compare run times.