PRISMS-plasticity user manual

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User input parameters file

FE parameters

Polynomial order of interpolation function. (1 $\implies$ linear basis functions)

```
set Order of finite elements = 1
```

Quadrature point order ($2 \implies 2^n$ quadrature points where n is the physical dimension)

```
set Order of quadrature = 2
```

Domain parameters

Assuming that the simulation domain is a cuboid of arbitrary dimensions.

Number of physical dimensions for the simulation

```
set Number of dimensions = 3
```

The size of the domain in the x direction.

```
set Domain size X = 1.0
```

The size of the domain in the y direction.

```
set Domain size Y = 1.0
```

The size of the domain in the z direction.

```
set Domain size Z = 1.0
```

Mesh parameters

Meshing is performed in a way that we start with a single unit cell, and slice it in x, y and z directions as many times as the refinement factor indicates. The mesh is then written out if the flag is set to true.

The number of mesh subdivisions in the x direction.

```
set Subdivisions X = 1
```

The number of mesh subdivisions in the y direction.

```
set Subdivisions Y = 1
```

The number of mesh subdivisions in the z direction.

```
set Subdivisions Z = 1
```

The number of initial refinements of the coarse mesh.

```
set Refine factor = 3
```

Only written for serial runs and if number of elements $<$ 10000

```
set Write Mesh To EPS = true
```

Solver output parameters

Flag to write output vtu and pvtu files

```
set Write Output = true
```

Output Directory name. For the current version, this directory has to be already present before running the simulation. A directory can be created using the `mkdir` unix command.

```
set Output Directory = results
```

Number of Output Steps to skip

```
set Skip Output Steps = 0
```

Output Equivalent strain

```
set Output Equivalent strain = true
```

Output Equivalent stress

```
set Output Equivalent stress = true
```

Output Grain ID

```
set Output Grain ID = true
```

Output Twin fractions(**true** Only when crystal structure is HCP)

```
set Output Twin fractions = true
```

Boundary condition information

File name containing BC information

```
set Boundary condition filename = BCinfo.txt
```

A sample boundary condition specification could look like:

```
# Header lines = 2
# FaceID DoF FinalDisplacement
5 1 0
5 2 0
5 3 0
6 3 0.01
```

FaceID refers to the face identifier and follows the numbering as indicated in Fig. 1. **DoF** refers to the direction of application of displacement, where 1, 2 and 3 refer to the x, y and z directions respectively. In the case of cyclic loading the displacement applied, refers to the displacement amplitude.

Number of header lines in BC file

```
set BC file number of header lines = 2
```

Number of boundary conditions

```
set Number of boundary conditions = 4
```

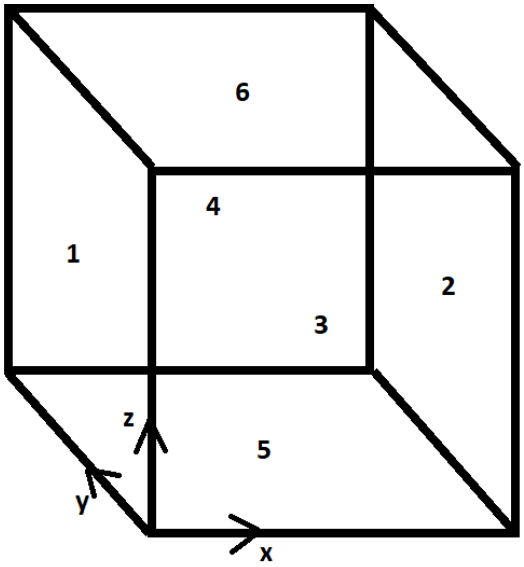

Figure 1: Description of faces required for defining BCs

Cyclic loading information

Flag to indicate if cyclic loading is enabled

```
set Enable cyclic loading = true
```

Face that is cyclically deformed

```
set Cyclic loading face = 6
```

Direction along which the face is cyclically deformed

```
set Cyclic loading direction = 3
```

Time for finishing quarter of a cyclic loading cycle. One cycle is time taken for starting from 0 displacement and ending at 0 displacement, with a positive loading rate.

```
set Quarter cycle time = 0.05
```

Solver parameters

ΔT for every increment

```
set Time increments = 0.01
```

Total simulation time

```
set Total time = 1
```

Maximum iterations for linear solver

```
set Maximum linear solver iterations = 50000
```

Relative linear solver tolerance

```
set Relative linear solver tolerance = 1.0e-10
```

Maximum no. of non-linear iterations

```
set Maximum non linear iterations = 4
```

Non-linear solver tolerance

```
set Absolute nonLinear solver tolerance = 1.0e-18
```

Relative non-linear solver tolerance

```
set Relative nonLinear solver tolerance = 1.0e-3
```

Elasticity parameters

Crystal structure of problem

```
set Crystal Structure = hcp
```

Input elastic stiffness matrix in Voigt notation as separate rows. The units are MPa.

Row 1

```
set Elastic Stiffness row 1 = 170.0e3, 124.0e3, 124.0e3, 0, 0,
   0
```

Row 2

```
set Elastic Stiffness row 2 = 124.0e3, 170.0e3, 124.0e3, 0, 0,
   0
```

Row 3

```
set Elastic Stiffness row 3 = 124.0e3, 124.0e3, 170.0e3, 0, 0,
   0
```

Row 4

```
set Elastic Stiffness row 4 = 0, 0, 0, 75.0e3, 0, 0
```

Row 5

```
set Elastic Stiffness row 5 = 0, 0, 0, 0, 75.0e3, 0
```

Row 6

```
set Elastic Stiffness row 6 = 0, 0, 0, 0, 0, 75.0e3
```

Slip parameters

Number of Slip Systems

```
set Number of Slip Systems = 18
```

Latent Hardening Ratio

```
set Latent Hardening Ratio = 1.4
```

Initial slip resistances

```
set Initial Slip Resistance =
  0.25,0.25,0.25,10,10,10,10,10,10,10,10,10,15,15,15,15,15,15
```

Hardening moduli of slip systems

```
set Initial Hardening Modulus = 5.0, 5.0, 5.0, 100, 100.0,
  100.0, 100.0, 100.0, 100.0, 100.0, 100.0, 100.0, 200.0,
  200.0, 200.0, 200.0, 200.0, 200.0
```

Power law coefficient in slip rate equation

```
set Power Law Exponent = 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1,
  1, 1, 1, 1, 1, 1
```

Saturation stress

```
set Saturation Stress = 185.0, 185.0, 185.0, 160.0, 160.0,
  160.0, 160.0, 160.0, 160.0, 160.0, 160.0, 160.0, 200.0,
  200.0, 200.0, 200.0, 200.0, 200.0
```

Slip Directions File

```
set Slip Directions File = slipDirections.txt
```

Slip Normals File

```
set Slip Normals File = slipNormals.txt
```

Ratio between backstress and CRSS during load reversal

```
set Backstress Factor = 0.0
```

Twin parameters

Flag to indicate if system twins

```
set Twinning enabled = true
```

Number of Twin Systems

```
set Number of Twin Systems = 6
```

Initial CRSS of the twin sytems

```
set Initial Slip Resistance Twin = 2.0, 2.0, 2.0, 2.0, 2.0,
  2.0
```

Hardening moduli of twin systems

```
set Initial Hardening Modulus Twin = 10.00, 10.00, 10.00,
  10.00, 10.00, 10.00
```

Power law exponents of twin systems

```
set Power Law Exponent Twin = 0.25, 0.25, 0.25, 0.25, 0.25,
  0.25
```

Saturation stress of twin systems

```
set Saturation Stress Twin = 185.00, 185.00, 185.00, 185.00,
  185.00, 185.00
```

Characteristic twin shear

```
set Characteristic Twin Shear = 0.126
```

Twin growth saturation factor

```
set Twin Saturation Factor = 0.25
```

Threshold fraction of characteristic twin shear (< 1)

```
set Twin Threshold Fraction = 0.25
```

Twin Directions File

```
set Twin Directions File = twinDirections.txt
```

Twin Normals File

```
set Twin Normals File = twinNormals.txt
```

Constitutive model parameters

Stress tolerance for the yield surface (MPa)

```
set Stress Tolerance = 1.0e-9
```

L^2-Norm of plastic strain-used for load-step adaptivity

```
set Max Plastic Slip L2 Norm = 2.5
```

Maximum no. of active slip search iterations

```
set Max Slip Search Iterations = 1
```

Maximum no. of iterations to achieve non-linear convergence

```
set Max Solver Iterations = 1
```

Input microstructure

Number of voxels in x direction

```
set Voxels in X direction = 20
```

Number of voxels in y direction

```
set Voxels in Y direction = 20
```

Number of voxels in z direction

```
set Voxels in Z direction = 20
```

Grain IDs file name

```
set Grain ID file name = grainID.txt
```

Number of header Lines in grain orientations file(these are to be skipped)

```
set Header Lines GrainID File = 20
```

Grain orientations file name

```
set Orientations file name = orientations.txt
```

Building the library

Obtain the code from github repository:

```
git clone https://github.com/prisms-center/plasticity
```

Change directory into the newly cloned folder:

```
cd plasticity
```

Building the library:

```
cmake .
make -j 8
```

Build the crystal plasticity application:

```
cd applications/crystalPlasticity
cmake .
make release
```

Running an example simulation

```
cd fcc/compression
```

Running the compression example case:

```
mpirun -n 8 ../../main prm.in
```