PRISMS-Plasticity user manual-V02

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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 can be performed thorough Deal.II or by reading an external mesh.

Deal.II mesh generator

The mesh generation 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
```

Important Note:
It is always more efficient to use the *set Refine factor* to refine the mesh rather than using the *subdivisions in the x,y, and z directions*.

External Mesh Generation

The external mesh with the format of Gmsh can be read.

Flag to indicate whether to use external mesh.

```
set Use external mesh = true
```

Name of external mesh file.

```
set Name of file containing external mesh = n200-id4_hex.msh
```

The external mesh parameter: The ratio of defiend region size to the Domain size.

```
set External mesh parameter = 0.05
```

Note: When an external mesh is read, the x,y,z poistions are not precisely defined and it has some roundoff errors. This matters in the case of BCs assignment. Accordingly, here, a margin is defined in which if a point is located in this margin, it will be considered as BCs. The size of this region in each direction is=(External mesh parameter)*(Domain size in that direction).

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
```

Flag to write quadrature output

```
set Write Quadrature Output = true
```

Number of Quadrature Output Steps to skip

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

Note: Even if all output generation fields are disabled, a stressstrain.txt file is generated for each step which includes the Green strain tensor, Cauchy stress tensor, average twin activity volume (TwinRealVF), twin volume fraction (TwinMade), and average slip activity (SlipTotal). If one wants to compare the average slip and twin activities, i.e., TwinRealVF vs SlipTotal, they should consider that average twin activity volume is the twin pseudo-slip systems shear activity divided by Characteristic twin shear constant.
In the case of Quadrature Output file, it outputs the following variables for all quadrature points: GrainID, Phase ID, det(J), twin (1 if it is reoriented due to twinning and 0 if not), x,y,z (coordinates of quadrature point),rotnew(1), rotnew(2), rotnew(3) (updated Rodrigues vector of orientation), 9 components of Fe (elastic deformation gradient tensor), 9 components of Fp, 9 components of Cauchy stress tensor, slip activity for 48 slip systems (if there is less systems, it will be appeared as 0), and 12 twin activity volume (if there is less systems, it will be appeared as 0). Again, the twin activity volume is the twin pseudo-slip systems shear activity divided by Characteristic twin shear constant.

Boundary condition information

BCs can be applied by defining the applied displacements or velocity gradient tensor. The corresponding input lines for each of these methods is presented here.

Displacement method

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
```

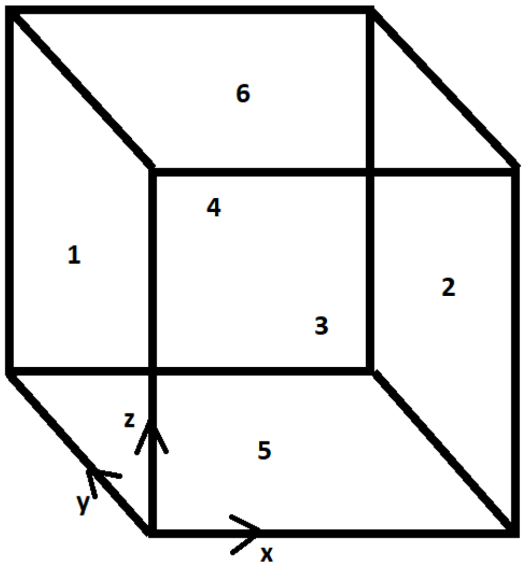

Figure 1: Description of faces required for defining BCs

Velocity gradient tensor

Flag to indicate whether to use velocity gradient tensor to apply BCs

```
set Use velocity gradient BC = true
```

Velocity gradient tensor including the multiplication factor

Row 1

```
set Velocity gradient row 1 = -0.005, 0, 0
```

Row 2

```
set Velocity gradient row 2 = 0, -0.005, 0
```

Row 3

```
set Velocity gradient row 3 = 0, 0, 0.01
```

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
```

Constitutive model solver parameters

Stress tolerance for the yield surface (MPa)

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

Maximum no. of active slip search iterations

```
set Max Slip Search 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
```

Multiphase Parameters

Flag to indicate if Multiphase is enabled

```
set Enable Multiphase = true
```

Number of phases in the sample

```
set Number of Phases = 2
```

The phase id is inserted in the **Grain ID file** after grain id, rot 1, rot 2, and rot 3 in 5th column.

Additional Voxel info

Number of Additional Voxel info Besides three orientation components and Phase if multiphase is enabled

```
set Additional Voxel info = 2
```

The aditional voxel info is inserted in the **Grain ID file** after the columns grain ID, rot 1, rot 2, rot 3, and phase id (in the case of multiphase).

User Defined Material Model Parameters

This section is related to the define **user defined material models** including the number of material constants and state variables, material constants, and initial value of state variables. Here, it is assumed we have two phases with user defined material models.

Flag to indicate if User Material Model is enabled

```
set Enable User Material Model = true
```

Flag to indicate if User Material Model is enabled Phase 1

```
set Enable User Material Model 1 = true
```

Number of User Material Constants in a Material model Phase 1

```
set Number of User Material Constants 1 = 5
```

Number of User Material State Variables in a Material model Phase 1

```
set Number of User Material State Variables 1 = 2
```

Material Constants in a Material model Phase 1

```
set User Material Constants 1 = 0.25, 0.35, 20000,-1,-0.256
```

Material State Variables in a Material model Phase 1

```
set User Material State Variables Initial Values 1 = -0.1,
  10000
```

Flag to indicate if User Material Model is enabled Phase 2

```
set Enable User Material Model 2 = true
```

Number of User Material Constants in a Material model Phase 2

```
set Number of User Material Constants 2 = 10
```

Number of User Material State Variables in a Material model Phase 2

```
set Number of User Material State Variables 2 = 1
```

Material Constants in a Material model Phase 2

```
set User Material Constants 2 =
  1,-0.1,0.1,0,20,1,-0.1,0.1,0,20
```

Material State Variables in a Material model Phase 2

```
set User Material State Variables Initial Values 2 = -10000
```

Elasticity parameters

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
```

Kinematic hardening parameters

Flag to indicate if kinematic hardening is enabled

```
set Enable Kinematic Hardening = true
```

C1 Slip Kinematic Hardening parameters

```
set C1 Slip Kinematic Hardening = 10.0, 10.0, 10.0, 10.0,
  10.0, 10.0, 10.0, 10.0, 10.0, 10.0, 10.0, 10.0, 10.0, 10.0,
  10.0, 10.0, 10.0, 10.0
```

C2 Slip Kinematic Hardening parameters

```
set C2 Slip Kinematic Hardening = 1, 1, 1, 1, 1, 1, 1, 1, 1,
  1, 1, 1, 1, 1, 1, 1, 1, 1
```

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 = 0.129
```

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
```

If the kinematic hardening is enabled, one should define the kinematic hardening parameters C1 and C2 for the twinning systems.

C1 Twin Kinematic Hardening parameters

```
set C1 Twin Kinematic Hardening = 10.0, 10.0, 10.0, 10.0,
  10.0, 10.0
```

C2 Twin Kinematic Hardening parameters

```
set C2 Twin Kinematic Hardening = 1, 1, 1, 1, 1, 1
```

Defining the second phase in Multiphase problem

In the case of Multiphase problems, another set of material parameters should be defined after the first one, which is the primary phase (Phase 1). In this case, the phase number will be added to the input lines. For example, here, a very simple second phase is also defined. If user defined material model is used for this phase 2, it should be defined in the section User Defined Material Model Parameters as described above.

Elasticity parameters for phase 2

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

Row 1

```
set Elastic Stiffness 2 row 1 = 170.0e3, 124.0e3, 124.0e3, 0,
  0, 0
```

Row 2

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

Row 3

```
set Elastic Stiffness 2 row 3 = 124.0e3, 124.0e3, 170.0e3, 0,
  0, 0
```

Row 4

```
set Elastic Stiffness 2 row 4 = 0, 0, 0, 75.0e3, 0, 0
```

Row 5

```
set Elastic Stiffness 2 row 5 = 0, 0, 0, 0, 75.0e3, 0
```

Row 6

```
set Elastic Stiffness 2 row 6 = 0, 0, 0, 0, 0, 75.0e3
```

Slip parameters for phase 2

Number of Slip Systems for Phase 2

```
set Number of Slip Systems 2 = 12
```

Latent Hardening Ratio for Phase 2

```
set Latent Hardening Ratio 2 = 1
```

Initial slip resistances for Phase 2

```
set Initial Slip Resistance 2 =
  0.25,0.25,0.25,10,10,10,10,10,10,10,10,10
```

Hardening moduli of slip systems for Phase 2

```
set Initial Hardening Modulus 2 = 5.0, 5.0, 5.0, 100, 100.0,
  100.0, 100.0, 100.0, 100.0, 100.0, 100.0, 100.0
```

Power law coefficient in slip rate equation for Phase 2

```
set Power Law Exponent 2 = 0, 0, 0, 1, 1, 1, 1, 1, 1, 1, 1, 1
```

Saturation stress for Phase 2

```
set Saturation Stress 2 = 185.0, 185.0, 185.0, 160.0, 160.0,
  160.0, 160.0, 160.0, 160.0, 160.0, 160.0, 160.0
```

Slip Directions File for Phase 2

```
set Slip Directions File 2 = slipDirections.txt
```

Slip Normals File for Phase 2

```
set Slip Normals File 2 = slipNormals.txt
```

Building the library

Obtain the code from github repository:

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

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
mkdir results
```

Running the compression example case:

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

Reference

M. Yaghoobi, S. Ganesan, S. Sundar, A. Lakshmanan, S. Rudraraju, J.E. Allison, V. Sundararaghavan, “PRISMS-Plasticity: An open-source crystal plasticity finite element software” Computational Materials Science 169 (2019) 109078.