PRISMS-Plasticity

Crystal Plasticity

Simple tension example -FCC Copper

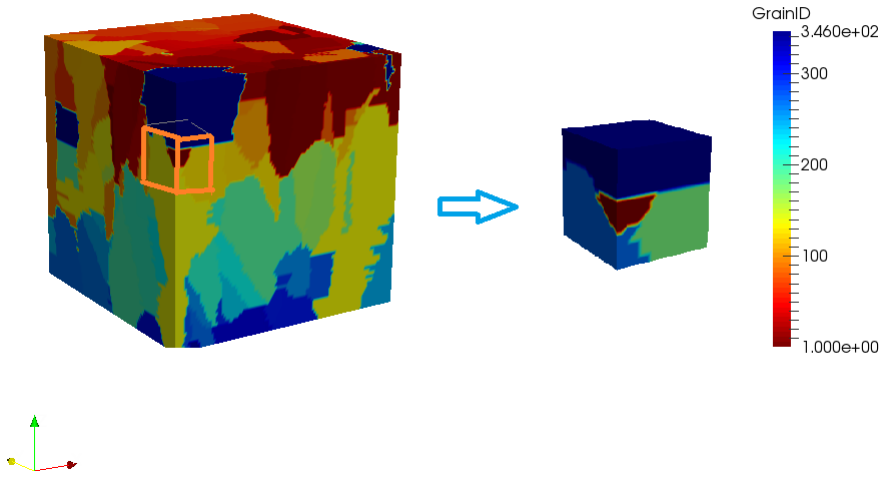

Figure 1: Input microstructure (3D Materials Atlas [2])

This is an illustrative example of a simple tension deformation problem. A real microstructure was tested with the material parameters of fcc Copper which were obtained from [1]

Input Parameters

```
/*FE parameters*/
#define feOrder 1 // Basis function interpolation order (1-linear)
#define quadOrder 2 // Quadrature point order n^3 (2->8 quadrature points)

/*Mesh parameters*/
//Set the length of the domain in all three dimensions
//Each axes spans from zero to the specified length
#define spanX 1.0
#define spanY 1.0
#define spanZ 1.0
// The number of elements in each direction is 2^(refineFactor) * subdivisions
// For optimal performance, use meshRefineFactor primarily to determine the
    element size
#define subdivisionsX 1
#define subdivisionsY 1
#define subdivisionsZ 1
```

```
#define meshRefineFactor 3 // 2^n*2^n*2^n elements(3->8*8*8 =512 elements)
#define writeMeshToEPS true //Only written for serial runs and if number of
    elements < 10000

/*Solution output parameters*/
#define writeOutput true // flag to write output vtu and pvtu files
#define outputDirectory "."
#define skipOutputSteps 0
#define output_Eqv_strain true
#define output_Eqv_stress true
#define output_Grain_ID true

/*Solver parameters*/
#define linearSolverType PETScWrappers::SolverCG // Type of linear solver
#define totalNumIncrements 100 // No. of increments
#define maxLinearSolverIterations 50000 // Maximum iterations for linear solver
#define relLinearSolverTolerance 1.0e-10 // Relative linear solver tolerance
#define maxNonLinearIterations 4 // Maximum no. of non-linear iterations
#define absNonLinearTolerance 1.0e-18 // Non-linear solver tolerance
#define relNonLinearTolerance 1.0e-3 // Relative non-linear solver tolerance
#define stopOnConvergenceFailure false // Flag to stop problem if convergence
    fails

/*Adaptive time-stepping parameters*/
#define enableAdaptiveTimeStepping false //Flag to enable adaptive time steps
#define adaptiveLoadStepFactor 0.5 // Load step factor
#define adaptiveLoadIncreaseFactor 1.25
#define succesiveIncForIncreasingTimeStep 10

//Elastic Parameters
double elasticStiffness[6][6]={{170.0e3, 124.0e3, 124.0e3, 0, 0, 0},
                               {124.0e3, 170.0e3, 124.0e3, 0, 0, 0},
                               {124.0e3, 124.0e3, 170.0e3, 0, 0, 0},
                               {0, 0, 0, 75.0e3, 0, 0},
                               {0, 0, 0, 0, 75.0e3, 0},
                               {0, 0, 0, 0, 0, 75.0e3}}; //     Elastic
                                   Stiffness Matrix -Voigt Notation (MPa)



//Crystal Plasticity parameters
#define numSlipSystems 12 // generally 12 for FCC
#define latentHardeningRatio 1.4 //q1

double initialSlipResistance[numSlipSystems]= {16.0, 16.0, 16.0, 16.0, 16.0,
    16.0, 16.0, 16.0, 16.0, 16.0, 16.0, 16.0}; //CRSS of the slip sytems
double initialHardeningModulus[numSlipSystems]= {180.0, 180.0, 180.0, 180.0,
    180.0, 180.0, 180.0, 180.0, 180.0, 180.0, 180.0, 180.0}; //Hardening moduli
    of slip systems
double powerLawExponent[numSlipSystems]= {2.25, 2.25, 2.25, 2.25, 2.25, 2.25,
    2.25, 2.25, 2.25, 2.25, 2.25, 2.25}; // Power law coefficient
```

```
double saturationStress[numSlipSystems]= {148.0, 148.0, 148.0, 148.0, 148.0,
    148.0, 148.0, 148.0, 148.0, 148.0, 148.0, 148.0}; // Saturation stress

//Slip systems files
#define slipDirectionsFile "slipDirections.txt" // Slip Directions File
#define slipNormalsFile "slipNormals.txt" // Slip Normals File


// Crystal Plasticity Constitutive model tolerances (for advanced users)
#define modelStressTolerance 1.0e-6 // Stress tolerance for the yield surface
    (MPa)
#define modelMaxSlipSearchIterations 20 // Maximum no. of active slip search
    iterations
#define modelMaxSolverIterations 10 // Maximum no. of iterations to achieve
    non-linear convergence
#define modelMaxPlasticSlipL2Norm 0.8 // L2-Norm of plastic slip strain-used for
    load-step adaptivity


//Read Input Microstructure
unsigned int numPts[3]={20, 20, 22}; // No. of voxels in x,y and z directions
#define grainIDFile "grainID.txt" // Grain ID File
#define headerLinesGrainIDFile 5 // No. of header Lines
#define grainOrientationsFile "orientations.txt" // Slip Normals File
```

Table 1: FCC Copper Slip Systems

System Number	Slip Direction	Slip Plane
1	[1 1 0]	(1 1 1)
2	[-1 0 1]	(1 1 1)
3	[0 1 -1]	(1 1 1)
4	[1 0 1]	(-1 1 1)
5	[-1 -1 0]	(-1 1 1)
6	[0 1 -1]	(-1 1 1)
7	[-1 0 1]	(1 -1 1)
8	[0 -1 -1]	(1 -1 1)
9	[1 1 0]	(1 -1 1)
10	[-1 1 0]	(-1 -1 1)
11	[1 0 1]	(-1 -1 1)
12	[0 -1 -1]	(-1 -1 1)

References

[1] Anand, L., and M. Kothari. "A computational procedure for rate-independent crystal plasticity." Journal of the Mechanics and Physics of Solids 44.4 (1996): 525-558.
[2] 3D Materials Atlas AL6XN+Reconstruction

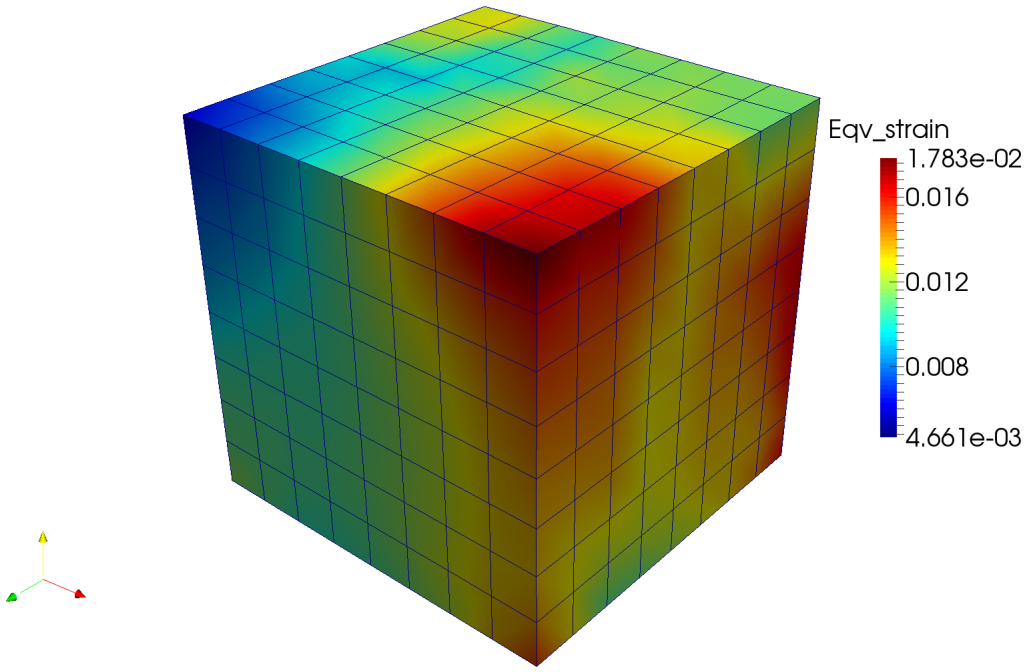

Figure 2: Equivalent strain