SSNV116 – POLYCRISTAL steel UMAT law - benchmark with Abaqus

Summary:

Within SINDRI research project [4] a benchmark between Abaqus and code_aster has been developped based on a Crystal Plasticity Finite Element (CPFE) behaviour law using the formalism of UMAT [1,2].

The geometry is a cube 1x1x1 originated from DREAM3D software which produces synthetic EBSD grains orientations. The sample is submitted to a fixed displacement to one end and clamped on another end.

With this test it is shown that code_aster results compares well to Abaqus.

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1 Reference problem

1.1 Geometry

The test cases simulate a polycrystal law on a representative elementary volume (VER) which is a cube sample of 10x10x10. The cube (figure 1) sample has been generated thanks to **Dream3D** software . The Dream3D output files have been converted into code_aster format thanks to the python script called **LengMorph** developed by UKC team and Bristol University.

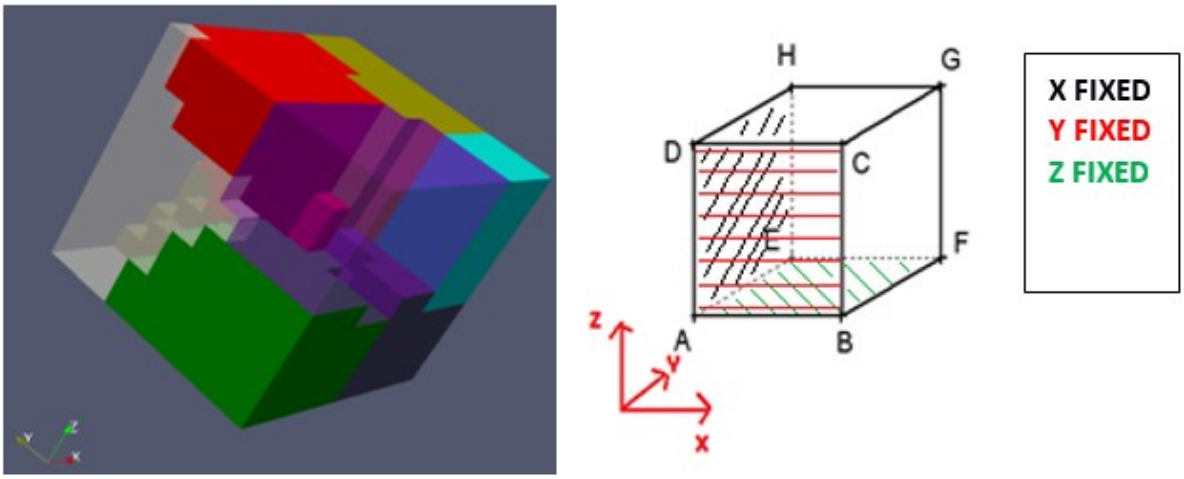


Figure 1. Cube sample generated by DREAM3D – 8 grains orientations

1.2 Material properties

The sample is composed of 8 to 64 grains with different size and different orientations. The properties of each grain are defined in the “MatPreoperies.inc” file which gather all the necessary parameters to run the crystal plasticity finite element model. There are 175 material parameters of which the most important one are described in the next paragraph.

Description of the relevant material properties: the elastic behaviour is common for all the grains and ruled by the generalized Hooke’s law in cubic symmetry (P1, P2, P3)

$$\sigma = C : \varepsilon \quad \text{with} \quad C = \begin{matrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{matrix} \quad \text{and}$$

$C_{11} = 183900 ; C_{12} = 123400 ; C_{44} = 91500$.

Each single crystal has one family of slip system defined by P25. The slip plane normal is the direction [110] is defined by the values (P33, P34, P35). The slip direction is [111] (P36, P37, P38). The parameters from P57 to P70 define the orientation of the grain. The parameters (P73, P97, P98, P99) characterized the different parameters of the flow rule respectively strain rate sensitivity factor n=50, the hardening modulus $h_0 = 0.1$,a fitting parameter $m = 0.14$, and the critical resolved shear stress $\tau_0 = 60\,MPa$ regarding the hardening law.

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The P145, P146 precise that the resolution is in fully implicit integration in the finite strain nonlinear geometry rather than the small deformation theory. The maximum number of iterations for one-time step is limited to 100 (P154). The absolute tolerance on slip is $e=10^{-5}$. The parameter 156 precises which hardening law is used, here the power hardening law is used. P157, P158 define the parameters $h_D=3100$, $h=49000$ used in the expression of the intragranular stress. The properties of the grain end with the ID number of the grain (P173).

The UMAT law accounts for the length scale of each element.

1.3 Boundary conditions and loads

All the sample studied have the same type of boundary conditions. This problem is cubic symmetric. There are three orthogonal symmetric plans: (OZX), (OXY), (OYZ) and the material properties are identical in the orthogonal directions of these three symmetric plans.

Regarding the figure 7 the faces <ABCD> is fixed on the Y axis, <AEDH> is fixed on X axis, <ABFE> is fixed on Z axis. Finitely the face <EFGH> undergo a ramp displacement toward Y axis until Y_{max} .

1.4 Description of the tests

In this testcase the displacement is a ramp that reach Y µm in a given time. The Von Mises stress field will be computed.

pre-process

The simulation runs for 1 second. The command file describes the different steps followed by code-Aster. The UMAT law is executed with the native code_aster function **make_shared** . UMAT file necessitates 8 files:

- param_array.inc: fortran parameters instructions (could be defined directly in the main fortran routine);
- orien.inc : orientation of grains;
- xvalues.bin, yvalues.bin, zvalues.bin, el_centroid.bin: location of each element and calculation of its length scale;
- boundfeat.bin: read boundary feature.

UMAT routine

The UMAT routine accounts for various physical phenomena that are tested in elementary simulations (Models A to D). The time-step has a significant influence on the mechanical response and the convergence of the model due to the relation between the loading velocity and the time step. In case of larger time steps the simulation can end up with singular matrix errors generated by the UMAT routine itself (LUDCMP subroutine) as shown in Figure 2.

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```
--
PAUSE Singular matrix.
To resume execution, type go.  Other input will terminate the job.
```

```
4371  !-------------------------------------------------------------
4372
4373
4374        SUBROUTINE LUDCMP (A, N, NP, INDX, D)
4375
4376  !-----  LU decomposition
4377
4378  !-----  Use single precision on cray
4379  !
4380        IMPLICIT REAL*8 (A-H,O-Z)
4381        PARAMETER (NMAX=200, TINY=1.0E-20)
4382        DIMENSION A(NP,NP), INDX(N), VV(NMAX)
4383
4384  c          WRITE(*,*) "DEBUGGING POINT LUDCMP:INIT"
4385
4386        D=1.
4387        DO I=1,N
4388           AAMAX=0.
4389
4390           DO J=1,N
4391              IF (ABS(A(I,J)).gt. AAMAX) AAMAX=ABS(A(I,J))
4392           END DO
4393
4394           IF (abs(AAMAX) .lt. 1.d-10) PAUSE 'Singular matrix.'
4395           VV(I)=1./AAMAX
4396        END DO
```

Figure 2: Termination message (up), UMAT script 'singular matrix' (down)

To avoid such error, it is proposed to use an optimal constant time-step of 0.0001. This coefficient is a heuristic estimation given the formula (1).

$$\frac{V_{loading} * time_{step}}{h_{sample\ length}} = \frac{D_{displacement} * time_{step}}{T_{total} * h_{sample\ length}} = 0{,}0001 \quad (1)$$

process

The resolution is performed with STAT_NON_LINE. Note that Abaqus uses “NLGEOM” options (Simo-Miehe large deformations) whilst code_aster uses small deformation.

Post-process

Once University of Bristol and EDF R&D UKC have run the same testcase, it is possible to compare at the same location the differences in stresses and displacement.

The results calculated with POST_ELEM/TEST_TABLE are the average of the Von Mises stress on Gauss Points of a selected element.

2 Reference solution

2.1 Calculation method of the reference solution

The reference solution is an external software calculation Abaqus FE software. The behaviour law theory has been expanded in the litterature [1,2].

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3 Model A

3.1 Characteristics

The model A is a linear mesh. code_aster results shown in figure 3. Non-linear deformation « NLGEOM » activated in Abaqus.

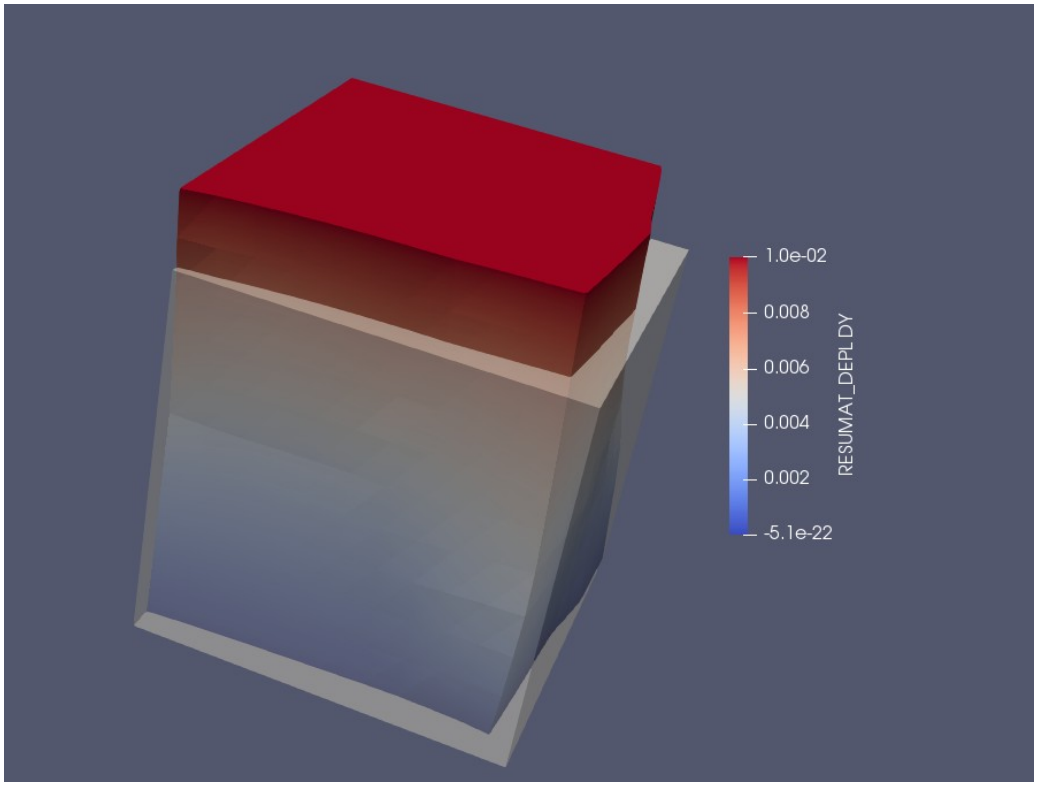


Figure 3 : Displacements observed

3.2 Fields tested et results

Identification	Référence	Tolérance (%)
VMIS SIEQ_ELGA ('el_gr_1')	131.8089396414	1.E-2

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4 Model B

4.1 Characteristics

The model B demonstrates the velocity dependence of the UMAT law. This test stands as pure numerical test (figure 4). It is the time step which controls the rate of the deformations (Table1).

Test scenarii plotted	Loading Rate (s)	Final time (s)	Total displacement prescribed (μm)	Time steps (s)
0.1s	1	0.1	0.1	0.001
1s	0.1	1	0.1	0.01
10s	0.01	10	0.1	0.1
100s	0.001	100	0.1	1
1000s	0.0001	1000	0.1	10
10000s	0.00001	10000	0.1	100

Table 1: Table of velocity-dependent rate

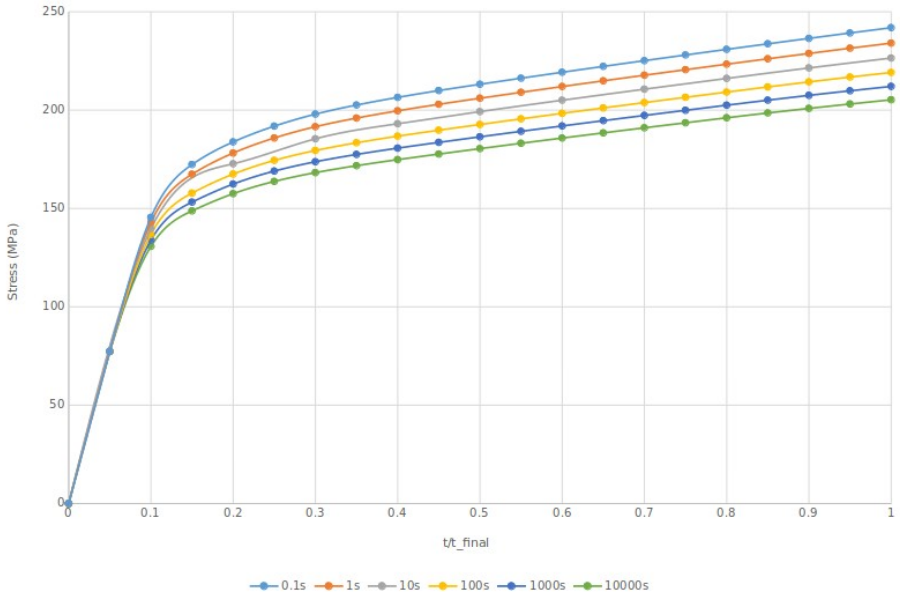


Figure 3: Visco-plasticity results

4.2 Fields tested et results

GROUP_MA= ‘GRAIN1’ at t=0.1s

Identification	Référence	Tolérance (%)
VMIS SIEQ_ELGA (0.1s)	184.089	2.5E-1
VMIS SIEQ_ELGA (1s)	184.089	2.5E-1
VMIS SIEQ_ELGA (10s)	184.089	2.5E-1
VMIS SIEQ_ELGA (100s)	184.089	1.5E-1
VMIS SIEQ_ELGA (1000s)	184.089	1.5 E-1
VMIS SIEQ_ELGA (10000s)	184.089	1.E-4

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5 Model C

5.1 Characteristics

In this test-case a cyclic loading in tension and compression has been applied until 0,5% of deformation during 10 cycles. The aim of this test is to observe the numerical robustness of the UMAT law in compression and tension.

The sample that undergoes the cyclic loading is the same like in MODEL B. The maximal deformation is 0,5% of deformation during 1 second. The simulation runs smoothly, and provide the expected results which are shown in Figure 4. It exhibits the numerical plot of the average displacement extracted at the plane face on which the displacement is imposed.

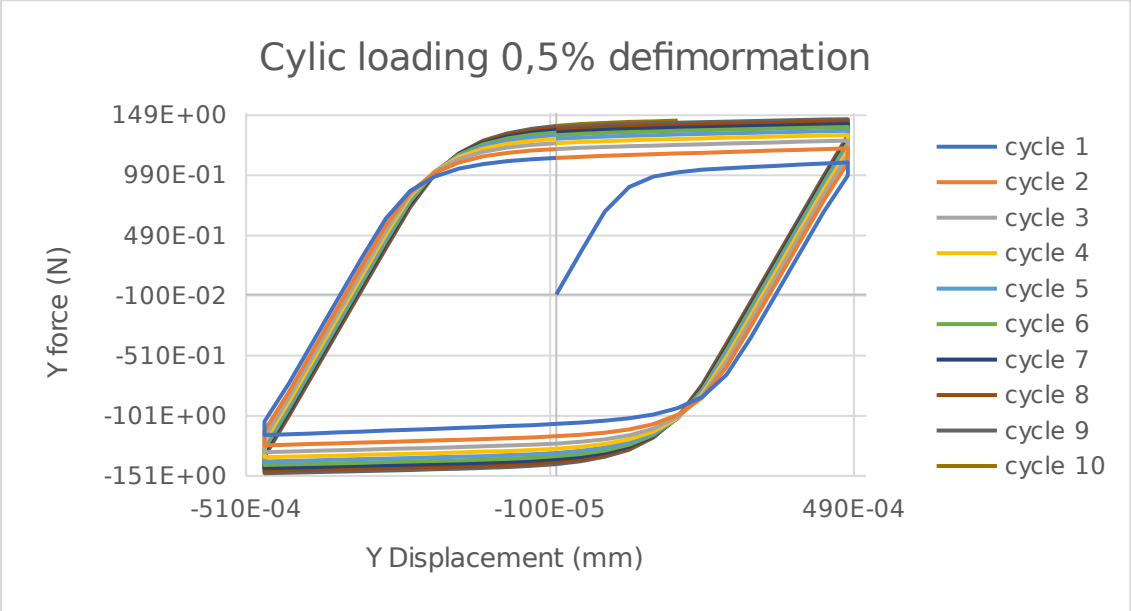


Figure 4: Cyclic loading results

5.2 Fields tested et results

GROUP_MA= ‘GRAIN1’

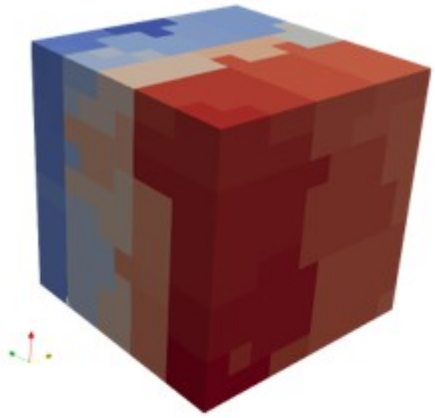
Identification	Référence	Tolérance (%)
VMIS SIEQ_ELGA (1s)	190.0009	1.E-4
VMIS SIEQ_ELGA (2s)	190.0009	2.E-1

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6 Model D

6.1 Characteristics

In this test-case 64 grains case is tested.



6.2 Fields tested et results

GROUP_MA= ‘GRAIN1’ at t=0.1s. Reference is 8 grains (Model A).

Identification	Référence	Tolérance (%)
VMIS SIEQ_ELGA (64grains)	131.8089396414	1.E-2

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7 Concluding remarks

The results obtained during this benchmark demonstrate:
- The capability in code_aster to read the initial UMAT routine developed by University of Bristol for ABAQUS with a good confidence on the results calculated;
- The UMAT routine read in code_aster appears to be robust with good computing performance;
- Further tests have been performed in code_aster, studying effect of the number of grains and cyclic behaviour. The results obtained meet expectations, both in terms of physical lenghtscale behavior;
- The generation of the models have been made using a recently developed automatised process generating Crystal Plasticity Finite Element (CPFE) models from experimental Electron Backscatter Diffraction (EBSD), also developed during the SINDRI project [2]. This demonstrates the effectiveness of this standardized procedure.

8 Litterature

[1] Microstructure-informed, predictive crystal plasticity finite element model of fatigue-dwells, Dylan Agius , Abdullah Al Mamuna.
[2] A User-Material subroutine incorporating single crystal plasticity in the Abaqus finite element program, Yonggang Huang
[3] Nanomechanics of Hall–Petch relationship in nanocrystalline materials C.S. Pande, K.P. Cooper, Materials Science and Technology Division, Naval Research Laboratory, Washington, DC 20375-5343, USA
[4] https://southwestnuclearhub.ac.uk/epsrc-funding-sindri-prosperity-partnership/
[5] Latent hardening in single crystals, II. Analytical characterization and predictions, John L. Bassani, Tien-Yue Wuf
[6] https://www.doitpoms.ac.uk/tlplib/work_harden/aims.php
[7] A quantitative study of stress fields ahead of a slip band blocked by a grain boundary in unalloyed magnesium, Mohsen Taheri Andani1,2*, Aaditya Lakshmanan3

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