Notes on the UMAT4COMSOL wrapper. UMAT4COMSOL: An Abaqus user material (UMAT) subroutine wrapper for COMSOL

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This document is intended to clarify the usage of the UMAT4COMSOL wrapper and the detail of the computational examples presented in:

S. Lucarini, E. Martinez-Paneda. UMAT4COMSOL: An Abaqus user material (UMAT) subroutine wrapper for COMSOL. Advances in Engineering Software. 2024.

Please cite the above paper if you are using this software.

Note that you need to tick the Allow external processes option in Comsol menu File-Preferences-Security. Also sometimes, it may be needed the use of only Gauss point stresses in Comsol for visualization (check that the default Result node does not plot solid.mises, solid.misesGp instead).

Small strain elastoplastic model

The benchmark of the Section 4.1 is located in the folder elastoplastic. Therein, it can be found the elastoplastic umat, the abaqus input and the comsol input.

The umat input properties are the following:

1: Elastic Young's modulus
2: Poisson ratio
3: Von Mises yield stress
4: Hardenng slope

The umat contains 7 state variables, which are the following:

1 - 6: components of the elastic strain tensor (xx,yy,zz,xy,xz,yz)
7: equivalent plastic stain

The usage in abaqus is straight forward by the adding the umat.f file to the job command:

abaqus job=elastoplastic.inp user=umat.f

The usage in Comsol needs first compilation via (.dll in windows, .so in Linux and Mac):

gfortran -c umat.f
gcc -c UMAT4COMSOL.c
gcc -shared -o UMAT4COMSOL.dll umat.o UMAT4COMSOL.o -lgfortran -lquadmath

An external material is added (in the Materials menu of the Model Builder) where the path to the compiled library (.dll) is typed, Import button clicked and the interface type General stress-strain relation is chosen. A state vector is added

(called "elast" in this case) where the number of state variables is chosen, and set to the number of umat state variables plus 13 (total of 20 in this case).

In the Materials Parameters tab the External Materials Parameters → General Stress-Strain Relation is selected, so that a vector of material model parameters appears. Then, selecting the General stress-strain relation in the Model Builder tree, the model parameter vector is introduced, which follows the umat properties vector format.

Finally, in the Solid Mechanics menu (of the Model Builder) an External Stress-Strain Relation is added, where the domains containing the material model are assigned to the external material, and select Geometrically linear formulation option.

Finite strain neo-Hookean hyperelastic model

The benchmark of the Section 4.2 is located in the folder neohookean. Therein, it can be found the neohookean umat, the abaqus input and the comsol input.

The umat input properties are the following:

1: Elastic Young's modulus
2: Poisson ratio

The umat contains no state variables

The usage in abaqus is straight forward by the adding the umat.f file to the job command:

abaqus job=neohookean.inp user=umat.f

The usage in Comsol needs first compilation via (.dll in windows, .so in Linux and Mac):

gfortran -c umat.f
gcc -c UMAT4COMSOLfinite.c
gcc -shared -o UMAT4COMSOLfinite.dll umat.o UMAT4COMSOLfinite.o -lgfortran -lquadmath

An external material is added (in the Materials menu of the Model Builder) where the path to the compiled library (.dll) is typed, Import button clicked and the interface type General stress-deformation relation is chosen. A state vector is added (called "elast" in this case) where the number of state variables is chosen, and set to the number of umat state variables plus 22 (total of 22 in this case).

In the Materials Parameters tab the External Materials Parameters → General Stress-Deformation Relation is selected, so that a vector of material model parameters appears. Then, selecting the General stress-deformation relation in the Model Builder tree, the model parameter vector is introduced, which follows the umat properties vector format.

Finally, in the Solid Mechanics menu (of the Model Builder) an External Stress-Strain Relation is added, where the domains containing the material model are assigned to the external material, and dis-select Geometrically linear formulation option.

Finite strain crystal plasticity

The benchmark of the Section 4.3 is located in the folder crystalplasticity. Therein, it can be found the Huang's crystal plasticty umat, the abaqus input and the comsol input.

The umat input properties are the following:

1 – 3: D11,D12,D44 elastic constants of orthotropic crystal

1-9: D1111, D1122, D2222,D1133, D2233, D3333, D1212, D1313, D2323 elastic constants in case of ortotropic crystal
1-21: D1111, D1122,D2222, D1133, D2233, D3333, D1112, D2212, D3312, D1212, D1113, D2213, D3313, D1213, D1313, D1123, D2223, D3323, D1223, D1323,D2323, elastic constants in case of ortotropic crystal
25: number of sets of slip systems (maximum 3)
33 - 35: normal to a typical slip plane in the 1st set of slip systems
36 - 38: a typical slip direction in the 1st set of slip systems
41 - 43: normal to a typical slip plane in the 2nd set of slip systems
44 - 46: a typical slip direction in the 2nd set of slip systems
49 - 51: normal to a typical slip plane in the 3rd set of slip systems
52 - 54: a typical slip direction in the 3rd set of slip systems
57 - 66: rotation matrix of the orientation of the crystal R1,R12,R12,R21,R22,R23,R31,R32,R33
73 -74: n, adot, exponent and rate of the power law of 1st set of slip systems
81 -82: n, adot, exponent and rate of the power law of 2nd set of slip systems
89 -93: n, adot, exponent and rate of the power law of 3rd set of slip systems
97 -99: h0,taus,tau0 initial hardening modulus, saturation yield stress and initial yield stress of 1st set of slip systems
105 -106: q,q1 self-hardening and latent hardening coefficients of 1st set of slip systems
113 -115: h0,taus,tau0 initial hardening modulus, saturation yield stress and initial yield stress of 2nd set of slip systems
121 -122: q,q1 self-hardening and latent hardening coefficients of 2nd set of slip systems
129 -131: h0,taus,tau0 initial hardening modulus, saturation yield stress and initial yield stress of 3rd set of slip systems
137 -138: q,q1 self-hardening and latent hardening coefficients of 3rd set of slip systems
145: parameter theta controlling the implicit
146: parameter for non linear geometry, 0: small 1: finite
153: parameter controlling whether the iteration method is used, 0: no iteration, 1: iteration
154: maximum number of iteration
155: absolute error of shear strains in slip systems

The umat contains a variable number of state variables depending on the number of slip sistems NSLPTL (using here one slip system set with a number of slip systems of NSLPTL=12 and a total number of state variables of NSTATV=150)

1 - NSLPTL: current strengths
NSLPTL+1 - 2*NSLPTL: shear strains
2*NSLPTL+1 - 3*NSLPTL: resolved shear stresses
3*NSLPTL+1 – 6*NSLPTL: slip planes normal vectors
6*NSLPTL+1 - 9*NSLPTL: slip direction vectors
9*NSLPTL+1 - 10*NSLPTL: total cumulative shear strain on each individual slip system
10*NSLPTL+1: total cumulative shear
10*NSLPTL+2 - NSTATV-26: additional optional parameters
NSTATV-25: number of slip systems in the 1st set
NSTATV-24: number of slip systems in the 2nd set
NSTATV-23: number of slip systems in the 3rd set
NSTATV-22: total number of slip systems in all sets

The usage in abaqus is straight forward by the adding the umat.f file to the job command:

abaqus job=crystalplasticity.inp user=umat.f

The usage in Comsol needs first compilation via (.dll in windows, .so in Linux and Mac):

gfortran -c umat.f
gcc -c UMAT4COMSOLfinite.c
gcc -shared -o UMAT4COMSOLfinite.dll umat.o UMAT4COMSOLfinite.o -lgfortran -lquadmath

An external material is added (in the Materials menu of the Model Builder) where the path to the compiled library (.dll) is typed, Import button clicked and the interface type General stress-deformation relation is chosen. A state vector is added (called "elast" in this case) where the number of state variables is chosen, and set to the number of umat state variables plus 22 (total of 172 in this case).

In the Materials Parameters tab the External Materials Parameters → General Stress-Deformation Relation is selected, so that a vector of material model parameters appears. Then, selecting the General stress-deformation relation in the Model Builder tree, the model parameter vector is introduced, which follows the umat properties vector format.

Finally, in the Solid Mechanics menu (of the Model Builder) an External Stress-Strain Relation is added, where the domains containing the material model are assigned to the external material, and dis-select Geometrically linear formulation option.

Coupled hydrogen diffusion and deformation in a single crystal

The benchmark of the Section 4.4 is located in the folder coupled. Therein, it can be found the Huang's crystal plasticity umat and the comsol input.

The usage procedure is similar to the Finite strain crystal plasticity section. A correction to the properties vector of the External material must be set to:
{168400000000., 121400000000., 75400000000., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 1., 0., 0., 0., 0., 0., 0., 0., 1., 1., 1., 1., 1., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 1., 0., 0., 0., 1., 0., 0., 0., 1., 0., 0., 0., 0., 0., 0., 0., 10., .001, 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 541000000.5, 109000000.5, 60000000.8, 0., 0., 0., 0., 0., 1., 1., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., 0., .5, 1., 0., 0., 0., 0., 0., 0., 1., 10., 0.00001, 0., 0., 0., 0., 0.}

Of special interest is that in this case, the value of one of the state variable is used in an included comsol Transport of diluted Species problem. To do this, a Reaction node is added where and expression in the reaction Rate is type containing the state variable reference "extmat1.state.elast121" corresponding to the state variable number 121. Then a staggered solution approach is used where the resolved value of the state variable is used in the resolution of the transport problem.

NOTE: Hardening parameters in the Crystal Plasticity and Coupled Hydrogen examples are different form the manuscript, so the results will differ.