User Defined Crystal Plasticity Material Model

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Introduction and Compiling

The PRISMS-Plasticity software has this capability to incorporate new crystal plasticity constitutive model. To do that, the only function one need to redefine is the calculatePlasticity.cc in /src/materialModels/crystalPlasticity/. Also, if one need to define some auxiliary functions to use in the new calculatePlasticity.cc, they can modify userFunctions.cc. Finally, the PRISMS-Plasticity need to be recompiled after this substitution.

The constants and variables of the user defined constitutive model should be defined inside the input file, which will be discussed later. The variable definitions used inside calculatePlasticity.cc is defined in the next section.

Definitions of the variable

Input Variables

```
F_tau
```

Deformation gradient tensor estimate for time τ, which is defined by 3*3 matrix.

```
Fe_conv[cellID][quadPtID]
```

Global converged elastic part of the deformation gradient tensor from time t corresponding to the element `cellID` and quadrature point `quadPtID` , which is defined by 3*3 matrix.

```
Fp_conv[cellID][quadPtID]
```

Global converged plastic part of the deformation gradient tensor from time t corresponding to the element `cellID` and quadrature point `quadPtID` , which is defined by 3*3 matrix.

```
s_alpha_conv[cellID][quadPtID]
```

Global converged slip system resistance for time τ corresponding to the element `cellID`, quadrature point `quadPtID` and slip/twin system `i`. Here twin is considered as pseudo-slip hence a single variable to denote slip system resistances.

```
rot_conv[cellID][quadPtID]
```

Global converged Rodrigues vector from time t corresponding to the element `cellID` and quadrature point `quadPtID`.

```
rotnew_conv[cellID][quadPtID]
```

Global converged updated Rodrigues vector from time t corresponding to the element `cellID` and quadrature point `quadPtID`.

```
stateVar_conv[cellID][quadPtID]
```

Global converged user defined state variables from time t corresponding to the element `cellID` and quadrature point `quadPtID`. This is a vector with the length of number of user defined state variables.

`UserMatConstants`

It is a vector of user defined constitutive model constants, which are set in input file.

Output Variables

`Fp_iter[cellID][quadPtID]`

Locally converged plastic part of the deformation gradient tensor at time τ corresponding to the element `cellID` and quadrature point `quadPtID` , which is defined by 3*3 matrix.

`Fe_iter[cellID][quadPtID]`

Locally converged elastic part of the deformation gradient tensor at time τ corresponding to the element `cellID` and quadrature point `quadPtID`, which is defined by 3*3 matrix.

`T`

Locally converged Cauchy stress tensor at time τ, which is defined by 3*3 matrix.

`P`

Locally converged first Piola-Kirchoff stress tesnsor at time τ, which is defined by 3*3 matrix.

`twinfraction_iter[cellID][quadPtID][i]`

Locally converged total twin fraction for time τ corresponding to the element `cellID`, quadrature point `quadPtID` and twin system `i`.

`slipfraction_iter[cellID][quadPtID][i]`

Locally converged accumulated slip for time τ corresponding to the element `cellID`, quadrature point `quadPtID` and slip system `i`.

`s_alpha_iter[cellID][quadPtID][i]`

Locally converged slip system resistance for time τ corresponding to the element `cellID`, quadrature point `quadPtID` and slip/twin system `i`. Here twin is considered as pseudo-slip hence a single variable to denote slip system resistances.

`rot_iter[cellID][quadPtID]`

Locally converged Rodrigues vector from time t corresponding to the element `cellID` and quadrature point `quadPtID`. This variable changes solely in case of twinning.

`rotnew_iter[cellID][quadPtID]`

Locally converged updated Rodrigues vector from time t corresponding to the element `cellID` and quadrature point `quadPtID`. This variable is updated using the function reorient().

`stateVar_iter[cellID][quadPtID]`

Locally converged user defined state variables from time t corresponding to the element `cellID` and quadrature point `quadPtID`. This variable is updated using the function reorient().

```
dP_dF
```

Elasto-plastic tangent modulus is a fourth order tensor, which is defined here as a 4 dimentional array of 3*3*3*3, estimates for assembly of global stiffness matrix.

Example: Rate dependent crystal plasticity model

A Rate dependent crystal plasticity model presented by Kalidindi 1992 as his PhD thesis "Polycrystal plasticity : constitutive modeling and deformation processing" is implemented here as an example. Two source files of calculatePlasticity.cc and userFunctions.cc in the folder/src/materialModels/crystalPlasticity/MaterialModels/RateDependentModel/ are the codes for this model. One should copy these two files and substitute them with those inside /src/materialModels/crystalPlasticity/ and compile the code again.

The changes in the input file required for this model is as follows. To understand the input file better, one can read the **/doc/User manual.pdf**. An example is also put for this model in the folder /applications/crystalPlasticity/fcc/FCC_UserDefinedMaterialModel/ which uses this user defined material model and simulate an FCC cube consists of 400 random orientations during compression test.

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 = 8
```

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

```
set Number of User Material State Variables 1 = 0
```

Material Constants in a Material model Phase 1

```
set User Material Constants 1 = 0.0001, 0.04, 0.000000001,
  0.0000001, 0.00000001,  11.0, 1000, 1000
```

Material State Variables in a Material model Phase 1

```
set User Material State Variables Initial Values 1 = 0
```

Model Parameters

```
delgam_ref = UserMatConstants(0)
```

This is the reference shearing increment assumed to be identical for all slip and twin systems.

```
strexp = UserMatConstants(1)
```

This is the strain-rate sensitivity exponent assumed to be identical for all slip systems.

```
sliptol = UserMatConstants(2)
```

This is the tolerance specified to check for convergence of the slip increments.

```
tol2 = UserMatConstants(3)
```

This is the tolerance specified to check for convergence of the stress measure conjugate to the Green-Lagrange elastic strain measure, T^*.

```
tol3 = UserMatConstants(4)
```

This is the tolerance specified to check for convergence of the slip system resistances.

```
tolstr = UserMatConstants(5)
```

This stress tolerance is used to ensure that the change in T^* remains bounded across subsequent Newton-Raphson iterations of the constitutive model.

```
nitr1 =  UserMatConstants(6)
```

This denotes the maximum number of iterations to check for convergence of T^*.

```
nitr2 =  UserMatConstants(7)
```

This denotes the maximum number of iterations to check for convergence of the slip system resistance.