Conversion of ABAQUS user Material Subroutines

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Abstract

When using finite element pogram ABAQUS to compute material characteristics, one builds a user material subroutine if unique constitutive feature needs to be included. In ABAQUS/Standard, UMAT subroutine should be built, and in ABAQUS/Explicit, VUMAT should be used. Although two subroutines carry out the same type of task, two different programs should be made depending on the working environment, and it is not easy to program the subroutines following the manual without enough understanding of solid mechanics. In this paper, difference between UMAT and VUMAT subroutines is epitomized, and a conversion scheme from UMAT to VUMAT is discussed. An example shows that the two programs give the same stress computation result.

Keywords : *ABAQUS user material subroutine, UMAT, VUMAT, constitutive equation, finite element analysis*

1. Introduction

To predict and compare mechanical behavior of materials and structures, finite element method is being used widely. Although the user can develop a whole finite element program, as time cost and accuracy can not be compensated, commercial programs tend to be used.

One drawback of commercial programs was that they could not provide all materials and elements that the users desire. However that shortage is being overcome by adding a capability of user programmable subroutines. For example, commercial code ABAQUS has options for user subroutines such as user defined material and element. To employ ABAQUS user subroutines, users should build subroutines with FORTRAN language according to the guidelines in the reference manual (ABAQUS, 2006).

When using ABAQUS/Standard version, one who is interested in material behavior should program UMAT subroutine. Meanwhile if using ABAQUS/Explicit version, which is developed more recently for dynamic analysis, one should generate VUMAT subroutine. Explicit method is useful for analysis including fast dynamic events, and the author could reduce the computation time by three or four times by using explicit calculation although it surely depends on the specific type of the problem. The programming environment of VUMAT is different from UMAT in many aspects, so one should completely conceive about the difference and fully understand basics of solid mechanics to get satisfactory results.

In this paper, difference between UMAT and VUMAT is presented and a conversion method between UMAT and VUMAT is suggested. A simple stress analysis example was used to compare the results of UMAT and VUMAT calculations.

2. Governing equations

2.1 Stress rate

Constitutive equation describes the relation between deformation of material and stress. Because stress generally depends on history, it is necessary to build a constitutive equation in an incremental form.

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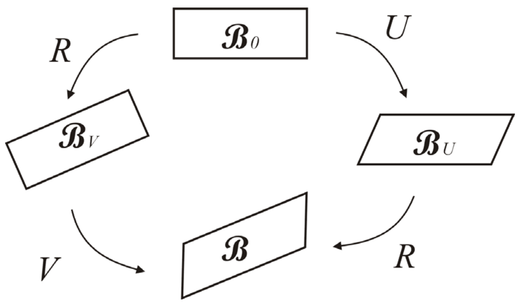

Fig. 1 Polar decomposition of deformation gradient, F

Polar decomposition of deformation gradient $\mathbf{F}$ is depicted in Fig. 1. Deformation gradient tensor can be written as the multiplication of rotation and stretch tensors (Flanagan and Taylor, 1987).

$$\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}} = \mathbf{RU} = \mathbf{VR} \tag{1}$$

$\mathbf{x}$ is the current position of a particle which was at position $\mathbf{X}$ in the undeformed configuration. Velocity gradient tensor $\mathbf{L}$ is written by

$$\mathbf{L} = \frac{\partial \mathbf{v}}{\partial \mathbf{x}} = \frac{\partial \mathbf{v}}{\partial \mathbf{X}}\frac{\partial \mathbf{X}}{\partial \mathbf{x}} = \dot{\mathbf{F}}\mathbf{F}^{-1} = \mathbf{D} + \mathbf{W} \tag{2}$$

where $\mathbf{v}$ is the particle velocity. The symmetric part of $\mathbf{L}$ is rate of deformation $\mathbf{D}$, and the antisymmetric part $\mathbf{W}$ is called spin tensor. The velocity gradient tensor can be alternatively expressed as follows using the polar decomposition.

$$\mathbf{L} = \dot{\mathbf{R}}\mathbf{R}^T + \mathbf{R}\dot{\mathbf{U}}\mathbf{U}^{-1}\mathbf{R}^T \tag{3}$$

Superscript T denotes transpose. Cauchy stress $\boldsymbol{\sigma}$ is used as a stress measure in ABAQUS and the Jacobian times Cauchy stress $J\boldsymbol{\sigma}$ is known as Kirchhoff stress. Both stresses are based on the deformed body. When using stress components based on a rectangular coordinate system $\mathbf{e}'_i$ (i=1,2,3) rotating with the body, the Cauchy stress can be expressed by

$$\boldsymbol{\sigma} = \sigma'_{ij}\boldsymbol{e}'_i \otimes \boldsymbol{e}'_j \tag{4}$$

where the summation convention is used for the repeated indexes. The time derivative of the stress will be

$$\begin{aligned}\dot{\boldsymbol{\sigma}} &= \dot{\sigma}'_{ij}\boldsymbol{e}'_i \otimes \boldsymbol{e}'_j + \sigma'_{ij}\dot{\boldsymbol{e}}'_i \otimes \boldsymbol{e}'_j + \sigma'_{ij}\boldsymbol{e}'_i \otimes \dot{\boldsymbol{e}}'_j \\ &= \overset{\nabla}{\boldsymbol{\sigma}} + \sigma'_{ij}\dot{\boldsymbol{e}}'_i \otimes \boldsymbol{e}'_j + \sigma'_{ij}\boldsymbol{e}'_i \otimes \dot{\boldsymbol{e}}'_j\end{aligned} \tag{5}$$

The second and third terms of the right hand side account for the change due to the motion of the coordinate system, and the first term corresponds to the response of the material. Tensor $\mathbf{W}$ is physically interpreted as the rotation rate of the principal axes of tensor $\mathbf{D}$. In ABAQUS/Standard, time derivative of the basis vector can be expressed with $\mathbf{W}$ as (ABAQUS, 2006)

$$\dot{\boldsymbol{e}}'_i = \mathbf{W}\,\boldsymbol{e}'_i \tag{6}$$

Using (6)

$$\begin{aligned}\dot{\boldsymbol{\sigma}} &= \overset{\nabla}{\boldsymbol{\sigma}} + \sigma'_{ij}\mathbf{W}\boldsymbol{e}'_i \otimes \boldsymbol{e}'_j + \sigma'_{ij}\boldsymbol{e}'_i \otimes \mathbf{W}\,\boldsymbol{e}'_j \\ &= \overset{\nabla}{\boldsymbol{\sigma}} + \mathbf{W}\boldsymbol{\sigma} + \boldsymbol{\sigma}\mathbf{W}^T\end{aligned} \tag{7}$$

where $\overset{\nabla}{\boldsymbol{\sigma}} = \dot{\sigma}'_{ij}\boldsymbol{e}'_i \otimes \boldsymbol{e}'_j$ is called Jaumann rate of Cauchy stress. In ABAQUS/Explicit, slightly different relation is used as follows.

$$\dot{\boldsymbol{e}}'_i = \dot{\mathbf{R}}\mathbf{R}^T\,\boldsymbol{e}'_i = \Omega\,\boldsymbol{e}'_i \tag{8}$$

then,

$$\begin{aligned}\dot{\boldsymbol{\sigma}} &= \overset{\nabla}{\boldsymbol{\sigma}} + \sigma'_{ij}\Omega\,\boldsymbol{e}'_i \otimes \boldsymbol{e}'_j + \sigma'_{ij}\boldsymbol{e}'_i \otimes \Omega\,\boldsymbol{e}'_j \\ &= \overset{\nabla}{\boldsymbol{\sigma}} + \Omega\,\boldsymbol{\sigma} + \boldsymbol{\sigma}\,\Omega^T\end{aligned} \tag{9}$$

$\overset{\nabla}{\boldsymbol{\sigma}}$ is called Green-Naghdi rate, and it is usually denoted by a different notation $\overset{\nabla}{\boldsymbol{\sigma}}$.

2.2 Constitutive equations

2.2.1 ABAQUS Standard environment

In ABAQUS/Standard, it is required to compute the Jaumann rate of Cauchy stress in the user subroutine. ABAQUS main program takes care of the effect of the rotating body, and the corrotational constitutive increment of stress is calculated in the user material subroutine. Values read from the main memory are the components of stress and strain increment, and state variables at the current time step. The variables that must be updated in the user subroutine are stress and the Jacobian matrix. All components of the tensor quantities are described in terms of a fixed reference frame.

If the material is elastic and history-independent, the constitutive equation is simply written by

$$\overset{\nabla}{\boldsymbol{\sigma}}\Delta t = \Delta\boldsymbol{\sigma} = \mathbf{C}\Delta\boldsymbol{\varepsilon} = \mathbf{C}\mathbf{D}\Delta t \tag{10}$$

where $\mathbf{C}$ is the current elastic modulus of the deformed body.

2.2.2 ABAQUS Explicit environment

Important difference in ABAQUS/Explicit is that components of some tensor quantities are given with respect to the coordinate system rotating with the material. The symmetric part of Eq. (3) is the rate of deformation, and that can be rewritten by

$$\begin{aligned}\mathbf{D} &= \frac{1}{2}\mathbf{R}\left(\dot{\mathbf{U}}\mathbf{U}^{-1} + \mathbf{U}^{-1}\dot{\mathbf{U}}\right)\mathbf{R}^T \\ &= \mathbf{R}\mathbf{d}\mathbf{R}^T\end{aligned} \tag{11}$$

where $\mathbf{d} = \frac{1}{2}\left(\dot{\mathbf{U}}\mathbf{U}^{-1} + \mathbf{U}^{-1}\dot{\mathbf{U}}\right)$ means the rate of deformation of the body Bu before the rigid body rotation depicted in Fig. 1. Eq. (11) is known as Piola transformation between $\mathbf{D}$ and $\mathbf{d}$ (Lubliner, 1990). If a stress tensor acting on the unrotated body Bu is denoted by $\mathbf{T}$ which corresponds to $\boldsymbol{\sigma}$ on the rotated body B, then from the traction law on B,

$$\mathbf{t} = \boldsymbol{\sigma}\mathbf{n} \tag{12}$$

and for the body Bu

$$\mathbf{R}^T\mathbf{t} = \mathbf{T}\mathbf{R}^T\mathbf{n} \tag{13}$$

will hold. Hence we get a similar relation of $\boldsymbol{\sigma} = \mathbf{R}\mathbf{T}\mathbf{R}^T$ for stress (Bonet and Wood, 1997). Tensors $\mathbf{d}$ and $\mathbf{T}$ are the rate of deformation and stress for the unrotated body, and a relation between them is constitutive property which is independent of the observer or coordinate system. This property is called the frame indifference.

The tensor components given from ABAQUS/Explicit main program are those of $\boldsymbol{\sigma}$ and $\Delta\boldsymbol{\varepsilon}$ (i.e., $\mathbf{D}\Delta t$) with respect to the corrotational coordinate system, and they are denoted by $\Delta\varepsilon'_{ij}$ or $[\Delta\varepsilon]'$ with superscript dash. The components with respect to a fixed laboratory frame will be representd without the dash. When the basis vectors rotating with the body are $\mathbf{e}'_i$ (i=1,2,3), we have the following relation.

$$\mathbf{e}'_i = \mathbf{R}\mathbf{e}_i \tag{14}$$

and

$$R_{ij} = \mathbf{e}_i \cdot \mathbf{R}\mathbf{e}_j = \mathbf{e}_i \cdot \mathbf{e}'_j = \mathbf{R}^T\mathbf{e}'_i \cdot \mathbf{e}'_j = R'^T_{ji} = R'_{ij} \tag{15}$$

That is, the components of $\mathbf{R}$ remain the same regardless of the coordinate frames. Meanwhile,

$$\begin{aligned}d_{ij}' &= \mathbf{e}'_i \cdot \mathbf{d}\,\mathbf{e}'_j = \mathbf{e}'_i \cdot \left(d_{kl}\mathbf{e}_k \otimes \mathbf{e}_l\right)\mathbf{e}'_j \\ &= d_{kl}\left(\mathbf{e}'_i \cdot \mathbf{e}_k\right)\left(\mathbf{e}_l \cdot \mathbf{e}'_j\right) \\ &= d_{kl}R_{ki}R_{lj}\end{aligned} \tag{16}$$

or

$$[\mathbf{d}]' = [\mathbf{R}]^T[\mathbf{d}][\mathbf{R}] \tag{17}$$

From (11),

$$[\mathbf{D}]' = [\mathbf{R}]'[\mathbf{d}]'[\mathbf{R}]'^T = [\mathbf{R}][\mathbf{d}]'[\mathbf{R}]^T \tag{18}$$

therefore, we have

$$[\mathbf{D}]' = [\mathbf{d}] \tag{19}$$

As written above, $[\mathbf{D}]'$ or D_{ij}' is available as strainInc array from ABAQUS/Explicit main program. ABAQUS/Explicit provides the current stress components by stressOld array. By the same procedure as before we can get

$$[\boldsymbol{\sigma}]' = [\mathbf{T}] \tag{20}$$

Hence stressOld array is exactly the component of $\mathbf{T}$ in the fixed coordinate system.

A constitituve equation independent of rigid body rotation can be described for the body Bu in Fig. 1. For a simple elastic material, it can be assumed that

$$\dot{\mathbf{T}} = \mathbf{C}\mathbf{d} \tag{21}$$

where $\mathbf{C}$ is the elasticity tensor. Referring to (9) and (21), Green-Naghdi stress rate is

$$\overset{\Delta}{\sigma} = \overset{\Delta}{\sigma}_{ij}\,\mathbf{e}_i \otimes \mathbf{e}_j = \dot{\sigma}'_{ij}\mathbf{e}'_i \otimes \mathbf{e}'_j = \dot{\sigma}'_{ij}\mathbf{R}\mathbf{e}_i \otimes \mathbf{R}\mathbf{e}_j = \mathbf{R}\dot{\mathbf{T}}\mathbf{R}^T \tag{22}$$

and substituting (11) and (22), we get the following equation for the body B in Fig. 1.

$$\overset{\Delta}{\sigma} = \mathbf{R}\mathbf{R}\mathbf{C}\mathbf{R}^T\mathbf{R}^T\mathbf{D} \tag{23}$$

If (23) is written in the components with respect to the rotating frame, we have

$$[\dot{\sigma}]' = [\dot{\mathbf{T}}] = [\mathbf{C}][\mathbf{d}] = [\mathbf{C}][\mathbf{D}]' \tag{24}$$

That is, the elastic modulus times the values of strainInc array gives the stress increment. Finally, stressNew array is obtained by adding the stress increment to stressOld array.

2.3 Conversion between ABAQUS UMAT and VUMAT

Users usually learn ABAQUS/Standard first and it is supposed that they are more familiar with ABAQUS/Standard user material subroutine UMAT than VUMAT. If one is interested in impact problems or wants to skip calculating the Jacobian matrix, he needs to use ABAQUS/Explicit VUMAT. For those users, a conversion scheme from UMAT to VUMAT is synopsized below. First, main features of UMAT and VUMAT are listed as follows.

〈Features of ABAQUS UMAT〉

① All tensor components are based on a fixed coordinate system $\mathbf{e}_i$ (i=1,2,3).

② Three-dimensional strain increment and stress components are given by DSTRAN and STRESS arrays and their order is (11), (22), (33), (12), (13), (23).

③ Increment by Jaumann stress rate $\overset{\nabla}{\sigma}(=\dot{\sigma} - \mathbf{W}\sigma + \sigma\mathbf{W})$ is necessary to update stress.

〈Features of ABAQUS VUMAT〉

① Components of stress, strain increment, stretch tensor $\mathbf{V}$ (stretchOld array) are given based on the rotating frame $\mathbf{e}'_i$ (i=1,2,3) attached to the material.

② Components of deformation gradient tensor $\mathbf{F}$ is based on the fixed frame.

③ Three-dimensional components of stain increment and Cauchy stress are provided by strainInc and stressOld arrays in the order of (11), (22), (33), (12), (23), (31).

④ Increment by Green-Naghdi stress rate $\overset{\Delta}{\sigma}(=\dot{\sigma} - \Omega\sigma + \sigma\Omega)$ is necessary to update stress (stress New array).

⑤ All subroutines generated by the user should start with letter k.

⑥ Include "include 'vaba_param.inc'" in every user subroutine.

To transform UMAT to VUMAT, one should first rotate the relevant tensor components from the rotating frame to the global frame, and then switch the order of the shear components (13) and (23). With these preprocessing in VUMAT, one can incorporate UMAT into VUMAT subroutine.

Rotation transformation matrix $[\mathbf{R}]$ between the fixed frame $\mathbf{e}_i$ (i=1,2,3) and rotating frame $\mathbf{e}'_i$ (i=1,2,3) is not provided by ABAQUS/Explicit, so one need to get the rotation matrix by using $\mathbf{F} = \mathbf{RU} = \mathbf{VR}$ or $\mathbf{RUR}^T = \mathbf{V}$ relations. That is,

$$V'_{ij} = R_{ik}U'_{kl}R_{jl} = U_{ij} \tag{25}$$

and

$$F_{ij} = R_{ik}U_{kj} = R_{ik}V'_{kj} \tag{26}$$

Hence, from $[\mathbf{F}]$ and $[\mathbf{V}]'$ values given by ABAQUS, one can get $[\mathbf{R}]$ matrix. Normally, time increment is very small in explicit calculation, so difference between $[\mathbf{R}]$ at time step t and $t+\Delta t$ is not significant. After getting $[\mathbf{R}]$,

$$[\sigma]=[\mathbf{R}][\sigma]'[\mathbf{R}]^T \tag{27}$$

$$[\mathbf{D}]\Delta t=[\mathbf{R}][\mathbf{D}]'[\mathbf{R}]^T\Delta t \tag{28}$$

are used to get the components of the stress and strain increment with respect to the fixed frame. These components are used for the constitutive equation of UMAT.

Because Green-Naghdi rate is desired in VUMAT and Jaumann rate in UMAT, small correction will be considered as follows (Gullerud *et al.*, 2003).

$$\begin{aligned}\overset{\Delta}{\sigma} &= \dot{\sigma}-\Omega\sigma+\sigma\Omega-\mathbf{W}\sigma+\sigma\mathbf{W}-(-\mathbf{W}\sigma+\sigma\mathbf{W}) \\ &= \overset{\nabla}{\sigma}-(\Omega-\mathbf{W})\sigma+\sigma(\Omega-\mathbf{W})\end{aligned} \tag{29}$$

Here, $-(\Omega-\mathbf{W})\Delta t$ is provided as relSpinInc array in ABAQUS/Explicit (ABAQUS, 2006). Therefore after getting $\overset{\nabla}{\sigma}$, the correction terms by $-(\Omega-\mathbf{W})\Delta t$ can be added to get $\overset{\nabla}{\sigma}$ for VUMAT. Finally, the components of the updated stress should be rotated back to the rotating frame.

3. Numerical example

Accurately of the conversion scheme between UMAT and VUMAT is exemplified by a test problem. Tensile loading is applied on a plate-shaped body rotating around the pinned vertex point in the plane as shown in Fig. 2. The tensile load increased proportionally from zero and then decreased with time. The material behavior is assumed as isotropic with linear elasticity as in (30), so the components of elasticity tensor $\mathbf{C}$ are independent of coordinate system.

$$\overset{\nabla}{\sigma}=\mathbf{C}\,\mathbf{D} \tag{30}$$

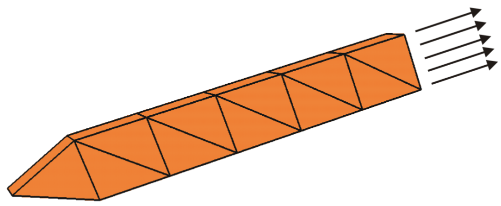

Fig. 2 Finite element model of rotating plate

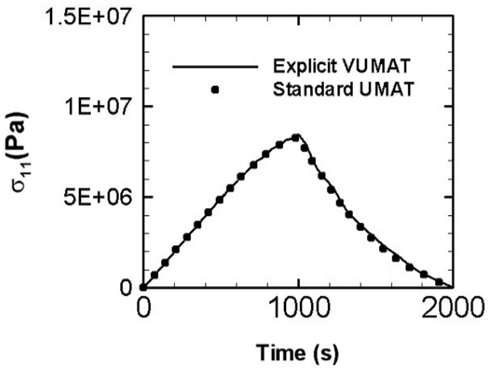

Fig. 3 Comparison of ABAQUS Standard and Explicit results

The material response was calculated by UMAT in ABAQUS/Standard. The conversion scheme is used with the UMAT subroutine included in the VUMAT subroutine for the explicit calculation. Fig. 3 shows the calculated stress state in the body. The two results are almost identical, which demonstrates the accuracy of the conversion scheme. ABAQUS Viewer plots σ_{11} which is a Cauchy stress component on a global frame, and the stress value increases linearly according to the external loading and bends little bit later as the rotation angle gets large, and then falls back to zero with the unloading. In the explicit calculation, the loading is applied slow enough to avoid any inertia effect.

4. Conclusion

A conversion scheme is provided for a user material subroutine written in ABAQUS/Standard environment to be applied for ABAQUS/Explicit. Some instructions about programming ABAQUS user material subroutines were given, and difference between UMAT and VUMAT was summarized. An example of stress calculation shows that the conversion method works accurately.

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References

ABAQUS (2006) ABAQUS 6.6.1 Reference manual, *HKS*, Providence.

Bonet, J., Wood, R.D. (1997) Nonlinear Continuum Mechanics for Finite Elment Analysis, *Cambridge University Press*, pp.57~116.

Flanagan, D.P., Taylor, L.M. (1987) An Accurate Numerical Algorithm for Stress Integration with Finite Rotations, *Computre Methods in Applied Mechanics and Engineering*, 62, pp.305~320.

Gullerud, A., Koppenhoefer, K., Roy, A.R., RoyChowdhury, S., Walters, M., Dodds Jr, R.H. (2003) WARP3D-Release 14.1 User Manual, *University of Illinois*, Chapter 1.

Lubliner, J. (1990) Plasticity Theory, *MacMillan*, pp.450~463.

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