# OpenDM Two Parameter UMAT: C++ Manual

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# 1 Theory

## 1.1 Problem

### 1.1.1 Solid mechanics: infinitesimal deformation

Strong Form neglecting inertial effects and body forces:

$$\nabla \cdot \boldsymbol{\sigma} = 0 \quad \forall \boldsymbol{x} \in \Omega \tag{1}$$

BCs:

$$\begin{aligned} \boldsymbol{u} &= \bar{\boldsymbol{u}} \quad \forall \boldsymbol{x} \in \Gamma_d \\ \boldsymbol{\sigma} \cdot \boldsymbol{n} &= \bar{\boldsymbol{t}} \quad \forall \boldsymbol{x} \in \Gamma_n \end{aligned} \tag{2}$$

Strain:

$$\boldsymbol{\varepsilon} = \frac{1}{2}(\nabla \boldsymbol{u} + \nabla^T \boldsymbol{u})$$

### 1.1.2 Weak form

Weak Form:

$$\int_\Omega \nabla \boldsymbol{w} : \boldsymbol{\sigma} d\Omega = \int_{\Gamma_n} \boldsymbol{w} \cdot \bar{\boldsymbol{t}} d\Gamma$$

### 1.1.3 Material nonlinearity:

Material nonlinearity requires a special solver. Newton-Raphson is the classical choice. However, as discussed in Section~8. The displacement solution becomes incremental

$$\boldsymbol{u}_n = \sum_{j=0}^{n} \Delta \boldsymbol{u}$$

With updates at each NR solve at each load step:

$$\boldsymbol{u}_{n+1} = \boldsymbol{u}_n + \Delta \boldsymbol{u}_{n+1}$$

Make weak form a residual:

$$R = \int_{\Gamma_n} \boldsymbol{w} \cdot \bar{\boldsymbol{t}} d\Gamma - \int_\Omega \nabla \boldsymbol{w} : \boldsymbol{\sigma} d\Omega$$

Linearize with Taylor Series:

$$R(\boldsymbol{u}_{n+1}) = R(\boldsymbol{u}_n) + \frac{\partial R}{\partial \boldsymbol{u}}(\boldsymbol{u}_n)\delta \boldsymbol{u}_{n+1} + HOT$$

Progressing from a converged solution, $R(\boldsymbol{u}_n) = 0$, dropping higher order terms

$$\frac{\partial R}{\partial \boldsymbol{u}}(\boldsymbol{u}_n)\delta \boldsymbol{u}_{n+1} \approx R(\boldsymbol{u}_{n+1})$$

The quantity $\boldsymbol{u}_{n+1}$ is found iteratively in the Newton-Raphson scheme. So we solve a given load step $n$ for a number of NR increments $i$ as:

$$\frac{\partial R}{\partial \boldsymbol{u}}(\boldsymbol{u}_n^i)\delta \boldsymbol{u}_{n+1}^{i+1} = R(\boldsymbol{u}_n^i)$$

With our residual, this becomes:

$$\int_\Omega \nabla \boldsymbol{w} : \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{u}} \delta \boldsymbol{u}_{n+t}^{i+1} d\Omega = \int_{\Gamma_n} \boldsymbol{w} \cdot \bar{\boldsymbol{t}} - \int_\Omega \nabla \boldsymbol{w} : \boldsymbol{\sigma}(\boldsymbol{u}) d\Omega$$

Where stress depends on $\boldsymbol{u}_n^i$ in each term. Once the system of equations is solved for a give $i$, the displacement is updated. The residual is then recomputed, and can be used as a convergence check.
The term $\frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{u}}$ is the material tangent stiffness matrix.

#### 1.1.4 **TODO** Relevant coordinate systems and transformations

- Problem coordinates
- Material coordinates
- Transforming between the two
- Notation for each case

## 1.2 OpenDM Two Parameter Model

### 1.2.1 Physical motivation

- Damage formulation for woven CMCs (Cite Maire papers)
- Damage parameters represent cracking
  - d1: Aligned with principal direction of mat coords
  - d2: Perpendicular to principal direction of mat coords

1. **TODO** Add figure
2. **TODO** Add citation

### 1.2.2 Constitutive behavior

1. Helmholtz free energy

   $$\psi = \frac{1}{2\rho}(\boldsymbol{\varepsilon}^* : \tilde{\boldsymbol{C}} : \boldsymbol{\varepsilon}^*)$$

   Where $\boldsymbol{\varepsilon}^*$ is mechanical strain: $\boldsymbol{\varepsilon}^* = \boldsymbol{\varepsilon} - \boldsymbol{\varepsilon}^{th}$

2. Stress

   Stress is the derivative of the Helmholtz free energy with respect to strain:

   $$\boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}} = \tilde{\boldsymbol{C}} : \boldsymbol{\varepsilon}^*$$

3. Material stiffness matrix

   The material stiffness tensor is affected by the two damage parameters and their progression. This relationship depends on the strain and is calculated as follows:

   $$\tilde{\boldsymbol{C}} = (\tilde{\boldsymbol{S}})^{-1}$$

where $\tilde{\boldsymbol{S}}$ is the material compliance tensor for a given strain and history.

The material compliance tensor for OpenDM two parameter model is calculated as follows:

$$\tilde{\boldsymbol{S}} = \boldsymbol{S}^0 + d^1\boldsymbol{H}^1 + d^2\boldsymbol{H}^2$$

$\boldsymbol{S}^0$ is the undamaged material compliance tensor.

$\boldsymbol{H}^i$ tensors are constants that modify the material compliance for each damage component. They are calculated as:

$$\boldsymbol{H}^1 = \begin{bmatrix} h_1^1 S_{11}^0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & h_3^1 S_{55}^0 & 0 \\ 0 & 0 & 0 & 0 & 0 & h_2^1 S_{66}^0 \end{bmatrix}$$

and

$$\boldsymbol{H}^2 = \begin{bmatrix} 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & h_1^2 S_{22}^0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & h_3^2 S_{44}^0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & h_2^2 S_{66}^0 \end{bmatrix}$$

The quantities $h_i^m$ are mode specific parameters that increase or decrease the effect of damage has on each mode.

$\boldsymbol{H}^1$ brings stiffness changes as a result of Mode I, II, and III microcracking in the CMC matrix as $d^1$ increases from zero. This corresponds to microcracks that are growing perpendicular to the principle material direction.

$\boldsymbol{H}^2$ Brings in the same microcracking effects, but for cracks that are parallel to the principle material direction.

4. Material tangent stiffness matrix

   The material tangent stiffness tensor is the derivative of the stress wrt strain:

$$\boldsymbol{C}_{tan} = \frac{\partial \boldsymbol{\sigma}}{\partial \boldsymbol{\varepsilon}} = \frac{\partial \tilde{\boldsymbol{C}}}{\partial \boldsymbol{\varepsilon}} + \tilde{\boldsymbol{C}}$$

   Material nonlinearity is reflected by the fact that the partial derivative of the material stiffness tensor with respect to strain is not zero. In the OpenDM model, this nonlinearity is caused by the two damage parameters $d^1$ and $d^2$

5. Damage values and evolution

   The damage variables evolve based on individual psuedo potentials:

$$F^i = f(y^i) - d^i$$

   Driving forces $y^i$ are calculated for each damage mode:

$$\begin{aligned} y^1 &= \frac{1}{2}(\varepsilon_{11}C_{1111}^0\varepsilon_{11} + b_2\varepsilon_{13}C_{1313}^0\varepsilon_{13} + b_1\varepsilon_{12}C_{1212}^0\varepsilon_{12}) \\ y^2 &= \frac{1}{2}(\varepsilon_{22}C_{2222}^0\varepsilon_{22} + b_2\varepsilon_{23}C_{2323}^0\varepsilon_{23} + b_1\varepsilon_{12}C_{1212}^0\varepsilon_{12}) \end{aligned} \tag{3}$$

   where $b_i$ are damage specific shear coupling parameters that increase the amount shear strains drive damage growth.

For convenience, another step is added here:

$$g^i = \frac{\langle\sqrt{y^i_{max}} - \sqrt{y^i_0}\rangle_+}{\sqrt{y^i_c}}$$

where we have added a history effect in $y^i_{max}$, which takes the largest $y^i$ value over time for each mode at the time of calculation for a given material point. $\langle\cdot\rangle_+$ is the positive Macaulay bracket.

$y^i_0$ is a model parameter that sets a threshold value of the driving force to start damage.

$y^i_c$ is a model parameter that changes the celerity of the damage progression.

The final step is

$$f(y^i) = d^i_c[1 - \exp^{-(g^i)^{(p^i)}}]$$

$d^i_c$ sets the maximum value of the damage parameter.

$p^i$ changes the shape of the curve of damage progression.

6. Analytical tangent stiffness matrix

Starting from the equation for stress in Voigt notation,

$$\sigma_i = \tilde{C}_{ik}\varepsilon_k,$$

the analytical tangent stiffness matrix can be calculated.

$$\frac{\partial\sigma_i}{\partial\varepsilon_j} = \frac{\partial\tilde{C}_{ik}}{\partial\varepsilon_j}\varepsilon_k + \tilde{C}_{ij}$$

The difficult part of the above equation is $\frac{\partial\tilde{c}_{ik}}{\partial\varepsilon_j}$, which is calculated as

$$\frac{\partial\tilde{C}_{ik}}{\partial\varepsilon_j} = \frac{\partial\tilde{S}^{-1}_{ik}}{\partial\varepsilon_j}.$$

The derivative of the inverse of the effective compliance tensor can be computed if we start from the indentity for the inverse.

$$\begin{aligned}
\tilde{S}^{-1}_{ik}S_{kl} &= \delta_{il} \\
\frac{\partial}{\partial\epsilon_j}(\tilde{S}^{-1}_{ik}S_{kl}) &= 0_{ilj} \\
\frac{\partial\tilde{S}^{-1}_{ik}}{\partial\varepsilon_j}\tilde{S}_{kl} + \tilde{S}^{-1}_{ik}\frac{\partial\tilde{S}_{kl}}{\partial\varepsilon_j} &= 0_{ilj} \\
\frac{\partial\tilde{S}^{-1}_{ik}}{\partial\varepsilon_j}\tilde{S}_{kl} &= -\tilde{S}^{-1}_{ik}\frac{\partial\tilde{S}_{kl}}{\partial\varepsilon_j} \\
\frac{\partial\tilde{S}^{-1}_{ik}}{\partial\varepsilon_j} = -\tilde{S}^{-1}_{ik}\frac{\partial\tilde{S}_{km}}{\partial\varepsilon_j}\tilde{S}^{-1}_{ml} &= -\tilde{C}_{ik}\frac{\partial\tilde{S}_{km}}{\partial\varepsilon_j}\tilde{C}_{ml}
\end{aligned} \tag{4}$$

This includes the assumption that the compliance tensor is invertible, but that is a must have in mechanics. The next step is the derivative of the compliance tensor.

$$\frac{\partial\tilde{S}_{km}}{\partial\varepsilon_j} = \frac{\partial}{\partial\varepsilon_j}(S^0_{km} + \sum_{n=1}^{2} d^n H^n_{km}) = \sum_{n=1}^{2}\frac{\partial d^n}{\partial\varepsilon_j}H^n_{km}$$

The derivative for each damage mode can then be calculated

$$\frac{\partial d^n}{\partial \varepsilon_j} = \frac{\partial}{\partial \varepsilon_j}(d_c^n(1 - \exp^{-(g^n)(p^m)})) = \frac{\partial}{\partial \varepsilon_j}(-d_c^n \exp^{-(g^n)(p^n)})$$

The only non-constants in this formula is $g^n$. We can use the chain rule to simplify this.

$$\frac{\partial d^n}{\partial \varepsilon_j} = \frac{\partial d^n}{\partial g^n}\frac{\partial g^n}{\partial \varepsilon_j}$$

The derivative with respect to $g^n$ is then

$$\frac{\partial d^n}{\partial g^n} = d_c^n p^n (g^n)(p^n - 1) \exp^{-(g^n)^{p^n}}$$

Now, looking at $g^n$.

$$\frac{\partial g^n}{\partial \varepsilon_j} = \frac{\partial}{\partial \varepsilon_j}(\frac{\langle\sqrt{y_{max}^n} - \sqrt{y_0^n}\rangle_+}{\sqrt{y_c^n}})$$

In this case, there is again only one term that depends on $\boldsymbol{\varepsilon}$, $y_{max}^n$. Again the chain rule can be exercised.

$$\frac{\partial g^n}{\partial \varepsilon_j} = \frac{\partial g^n}{\partial y_{max}^n}\frac{\partial y_{max}^n}{\partial \varepsilon_j}$$

And the next derivative can be calculated.

$$\frac{\partial g^n}{\partial y_{max}^n} = \begin{cases} 0 & \langle\sqrt{y_{max}^n} - \sqrt{y_0^n}\rangle_+ > 0 \\ \frac{1}{2\sqrt{y_{max}^n}\sqrt{y_c^n}} & else \end{cases}$$

Finally, the end of the chain is near. The driving forces explicitly depend on $\boldsymbol{\varepsilon}$. Their derivatives are vectorial are calculated for a given load step $i$ as

$$\frac{\partial y_{max}^n}{\partial \varepsilon_j} = \begin{cases} 0 & y_i^n > y_{max}^n \\ \frac{\partial y_{max}^n}{\partial \varepsilon_j} & else \end{cases}$$

Then for each driving force, the final derivative in Voigt notation is

$$\begin{aligned} \frac{\partial y^1}{\partial \boldsymbol{\varepsilon}} &= [C_{11}^0 \varepsilon_1 0 0 0 b^2 C_{55}^0 \varepsilon_5 b^1 C_{66}^0 \varepsilon_6] \\ \frac{\partial y^2}{\partial \boldsymbol{\varepsilon}} &= [0 C_{22}^0 \varepsilon_2 0 b^2 C_{44}^0 \varepsilon_4 0 b^1 C_{66}^0 \varepsilon_6] \end{aligned} \tag{5}$$

To summarize in broad strokes, the material tangent stiffness tensor is calculated as follows:

$$\begin{aligned} \frac{\partial \sigma_i}{\partial \varepsilon_j} &= \frac{\partial \tilde{C}_{ik}}{\partial \varepsilon_j}\varepsilon_k^* + \tilde{C}_{ij} \\ &= -\tilde{C}_{il}\frac{\partial \tilde{S}_{lm}}{\partial \varepsilon_j}\tilde{C}_{mk}\varepsilon_k^* + \tilde{C}_{ij} \\ &= -\tilde{C}_{il}(\frac{\partial d^1}{\partial \varepsilon_j}H_{lm}^1 + \frac{\partial d^2}{\partial \varepsilon_j}H_{lm}^2)\tilde{C}_{mk}\varepsilon_k^* + \tilde{C}_{ij} \end{aligned}$$

With the quantities

$$\begin{aligned} \frac{\partial d^1}{\partial \varepsilon_j} &= \frac{\partial d^1}{\partial g^1}\frac{\partial g^1}{\partial y_{max}^1}\frac{\partial y_{max}^1}{\partial \varepsilon_j} \\ \frac{\partial d^2}{\partial \varepsilon_j} &= \frac{\partial d^2}{\partial g^2}\frac{\partial g^2}{\partial y_{max}^2}\frac{\partial y_{max}^2}{\partial \varepsilon_j} \end{aligned}$$

Of which, all of the required derivatives have been calculated.

7. Numerical tangent stiffness matrix

   The tangent stiffness matrix can be calculated numerically. This avoids all of the complicated math shown above, but can add some computational expense.

   If a Taylor series expansion of a stress component is taken at the current strain,

$$\sigma_i(\boldsymbol{\varepsilon} + \delta\varepsilon_j) = \sigma_i(\boldsymbol{\varepsilon}) + \frac{\partial \sigma_i}{\partial \varepsilon_j}(\boldsymbol{\varepsilon})(\delta\varepsilon_j) + O(\delta\varepsilon_j^2)$$

   Where we have abused notation to show that $\boldsymbol{\varepsilon} + \delta\varepsilon_j$ is the current strain perturbed in the $j^{th}$ component a magnitude $\delta\varepsilon$.

   This Taylor series can be rearranged to get an approximation of the material tangent stiffness matrix.

$$\boldsymbol{C}_{tan} = \frac{\partial \sigma_i}{\partial \varepsilon_j} \approx \frac{\sigma_i(\boldsymbol{\varepsilon} + \delta\varepsilon_j) - \sigma_i(\boldsymbol{\varepsilon})}{\delta\varepsilon_j}$$

   In practice, for each of the six perturbations of strain a new vector of stresses are calculated. Those new stresses are subtracted from the base set of stresses and a column of the tangent stiffness matrix is obtained.

   The numerical tangent stiffness matrix has the same problems with symmetry as the analytical one. It is also symmetrized to simplify analysis.

   One must also be careful about the value of the strain perturbation. A smaller value is more accurate, but can lead to numerical troubles.

8. General comments about the tangent stiffness matrix

   In numerical studies with the material, we have found the tangent stiffness matrix to become non-positive definite. In the material modeling world, this means the material is softening. In other words, an increase in strain causes a decrease in stress. This has major applications on the numerical solution. An arclength solver can be used to capture general behavior. One can also solve strictly displacement controlled problems to avoid issues.

   Also, both the numerical and analytical tangent stiffness tensors are not generally symmetric. This has significant impacts on the computational expense of the method. To remedy this, the tangent matrix is always symmetrized as follows:

$$\boldsymbol{C}_{tan}^{sym} = \frac{1}{2}(\boldsymbol{C}_{tan} + \boldsymbol{C}_{tan}^{T})$$

   This symmetrized tangent is no longer analytical, so we are effectively restricted to quasi-newton solver methods.

## 2 Model Parameters

| Parameter | Number | Effect |
|---|---|---|
| $h_i^m$ | 6 | scales damage mode $m$ effect on compliance from fracture mode $i$ |
| $b_i$ | 2 | scales contribution of shear strains to driving forces |
| $y_0^i$ | 2 | sets a threshold value of the driving force for mode $m$ |
| $y_c^i$ | 2 | changes the celerity of the damage progression |
| $d_c^i$ | 2 | sets the maximum value of the damage parameter |
| $p^i$ | 2 | changes the shape of the curve of damage progression |