

Objective: To transform the frame of reference to normal and tangential coordinates in the diffuse interface region of a 2D circular precipitate.

Why we need to transform?

$$\frac{\partial \sigma}{\partial r} = 0$$

$$\rho \frac{\partial^2 u_i}{\partial t^2} + b \frac{\partial u_i}{\partial t} = \frac{\partial \sigma_{ij}}{\partial x_j}$$

The second equation is solved by:

$$\rho \frac{\partial^2 u}{\partial t^2} = \frac{u_i^{t+1} - 2u_i^t + u_i^{t-1}}{dt * dt}$$

$$b \frac{\partial u_i}{\partial t} = \frac{u_i^{t+1} - u_i^{t-1}}{2dt}$$

$$\frac{\partial \sigma_{xx}}{\partial x} = \frac{\sigma_{xx}^{i+1,j} - \sigma_{xx}^{i-1,j}}{2dx}$$

$$\frac{\partial \sigma_{yy}}{\partial y} = \frac{\sigma_{yy}^{i,j+1} - \sigma_{yy}^{i,j-1}}{2dy}$$

$$\frac{\partial \sigma_{xy}}{\partial x} = \frac{\sigma_{xy}^{i+1,j} - \sigma_{xy}^{i-1,j}}{2dx}$$

$$\frac{\partial \sigma_{xy}}{\partial y} = \frac{\sigma_{xy}^{i,j+1} - \sigma_{xy}^{i,j-1}}{2dy}$$

solved using In the previous report of plane interface inverse plottation model we have observed that in order to have a continuous stress and strain profile in the system we require the coordinates be in normal and tangential axes, calculation of C_{ijkl} in the diffuse interface by inverse interpolation.

Formulation:

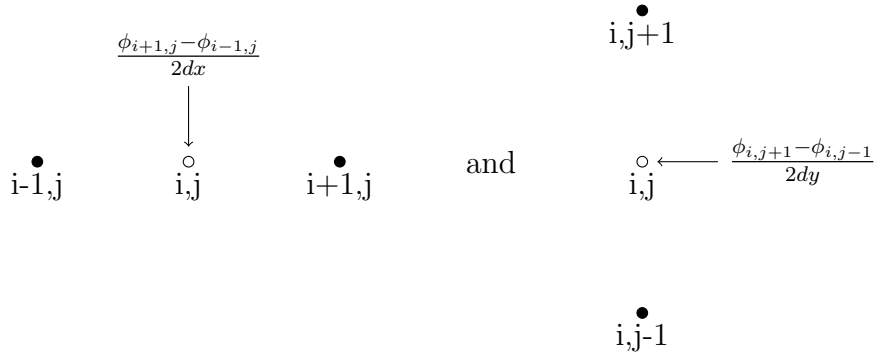
finding normal vector:
normal vector

$$n = -\frac{\nabla\phi}{|\nabla\phi|} \quad (1)$$

$$\nabla\phi_x = -\frac{\phi(x+1) - \phi(x-1)}{2dx} \quad (2)$$

$$\nabla\phi_y = -\frac{\phi(y+1) - \phi(y-1)}{2dy} \quad (3)$$

$$n_{x,y} = \frac{\nabla\phi_{x,y}}{\sqrt{\nabla\phi_x^2 + \nabla\phi_y^2}} \quad (4)$$



Discretization: Central difference is used.

I have stored the index of the points where atleast one of n_x, n_y vector is non-zero in a file named *domain-transform.txt*.

Rotation matrix of transformation:

A 2D array $a[2][2]$ is used to store rotation transformation matrix and it is written at each index of domain in a file called *rotation-matrix.txt*

Notation used:

$$a[0][0] = a_{nx} = n_x$$

$$a[0][1] = a_{ny} = n_y$$

$$a[1][0] = a_{tx} = -n_y$$

$$a[1][1] = a_{ty} = n_x$$

C_{ijkl} transformation to C_{ntrs} :

1. Notation: In C_{ijkl} i, j, k, l takes x, y . The reduced form of C_{ijkl} due to symmetry operation is

$$\begin{bmatrix} C_{11} & C_{12} & C_{16} \\ C_{21} & C_{22} & C_{26} \\ C_{61} & C_{62} & C_{66} \end{bmatrix} = \begin{bmatrix} C_{xxxx} & C_{xxyy} & C_{xxxy} \\ C_{yyxx} & C_{yyyy} & C_{yyxy} \\ C_{xyxx} & C_{xyyy} & C_{xyxy} \end{bmatrix}$$

only six independent components of C_{ntrs} at each index of domain is stored in a file.

2. $C_{ntrs}^{\alpha,\beta}$ at each index of the domain is obtained from $C_{ijkl}^{\alpha,\beta}$ and stored in files respectively. $C_{ntrs}^{\alpha,\beta} = a_{ni}a_{tj}a_{rk}a_{sl}C_{ijkl}^{\alpha,\beta}$

Stress and strains in the domain calculations: Let $\sigma_{nn}, \sigma_{nt}, \sigma_{tt}, \epsilon_{nn}, \epsilon_{nt}, \epsilon_{tt}$ be the total stress and strain components in the domain region. Let $\epsilon_{nn}^{\alpha,\beta}, \epsilon_{nt}^{\alpha,\beta}$ be the strain of the corresponding components α, β in the diffuse interface region.

First strains in the diffuse interface regio has been transformed into normal coordinates as follows.

$$\epsilon_{nt} = a_{ni}a_{tj}\epsilon_{ij}$$

$$S_{nt}^{\alpha,\beta} = \begin{bmatrix} C_{nnnn}^{\alpha,\beta} & 2C_{nnnt}^{\alpha,\beta} \\ C_{ntnn}^{\alpha,\beta} & 2C_{ntnt}^{\alpha,\beta} \end{bmatrix}^{-1} \quad (5)$$

Let

$$\begin{bmatrix} \sigma_{nn} \\ \sigma_{nt} \end{bmatrix} = \left(S_{nt}^{\alpha}\phi + S_{nt}^{\beta}(1-\phi) \right)^{-1} \left(\begin{bmatrix} \epsilon_{nn} \\ \epsilon_{nt} \end{bmatrix} + S_{nt}^{\alpha} \begin{bmatrix} C_{nnnt}^{\alpha}\epsilon_{tt} \\ C_{ntnt}^{\alpha}\epsilon_{tt} \end{bmatrix} \phi + S_{nt}^{\beta} \begin{bmatrix} C_{nnnt}^{\beta}\epsilon_{tt} \\ C_{ntnt}^{\beta}\epsilon_{tt} \end{bmatrix} (1-\phi) \right) \quad (6)$$

$$\begin{bmatrix} \epsilon_{nn}^{\alpha,\beta} \\ \epsilon_{nt}^{\alpha,\beta} \end{bmatrix} = S_{nt}^{\alpha,\beta} \begin{bmatrix} \sigma_{nn} - C_{nnnt}^{\alpha,\beta}\epsilon_{tt} \\ \sigma_{nt} - C_{ntnt}^{\alpha,\beta}\epsilon_{tt} \end{bmatrix} \quad (7)$$

This is used to calculate σ_{tt} as follows:

$$\sigma_{tt} = \sigma_{tt}^{\alpha}\phi + \sigma_{tt}^{\beta}(1-\phi) \quad (8)$$

$$\sigma_{tt}^{\alpha,\beta} = C_{ttnn}^{\alpha,\beta}\epsilon_{nn}^{\alpha,\beta} + 2C_{tntn}^{\alpha,\beta}\epsilon_{nt}^{\alpha,\beta} + C_{tttt}^{\alpha,\beta}\epsilon_{tt}$$