

| $\delta x_1$ | $\delta y_1$ | $\delta z_1$ | $\delta I_1^x$ | $\delta I_1^y$ | $\delta x_2$ | $\delta y_2$ | $\delta z_2$ | $\delta I_2^x$ | $\delta I_2^y$ | $\delta x_3$ | $\delta y_3$ | $\delta z_3$ | $\delta I_3^x$ | $\delta I_3^y$ |             |
|--------------|--------------|--------------|----------------|----------------|--------------|--------------|--------------|----------------|----------------|--------------|--------------|--------------|----------------|----------------|-------------|
| 2            |              |              | 4              |                | 2            |              |              | 4              |                | 2            |              |              | 4              |                | $\dot{x}_1$ |
|              |              |              |                |                |              |              |              |                |                |              |              |              |                |                | $\dot{y}_1$ |
|              |              |              | 1 5            |                | 3            |              |              | 5              |                | 3            |              |              | 1 5            |                | $\dot{z}_1$ |
|              |              |              |                |                |              |              |              |                |                |              |              |              |                |                | $J_1^x$     |
|              |              |              |                |                | 2            |              |              | 4              |                | 2            |              |              | 4              |                | $J_1^y$     |
|              |              |              |                |                |              |              |              |                |                |              |              |              |                |                | $\dot{x}_2$ |
|              |              |              |                |                |              |              |              | 1 5            |                | 3            |              |              | 1 5            |                | $\dot{y}_2$ |
|              |              |              |                |                |              |              |              |                |                |              |              |              |                |                | $\dot{z}_2$ |
|              |              |              |                |                |              |              |              |                |                | 2            |              |              | 4              |                | $J_2^x$     |
|              |              |              |                |                |              |              |              |                |                |              |              |              |                |                | $J_2^y$     |
|              |              |              |                |                |              |              |              |                |                |              |              |              | 1 5            |                | $\dot{x}_3$ |
|              |              |              |                |                |              |              |              |                |                |              |              |              |                |                | $\dot{y}_3$ |
|              |              |              |                |                |              |              |              |                |                |              |              |              | 1 5            |                | $\dot{z}_3$ |
|              |              |              |                |                |              |              |              |                |                |              |              |              |                |                | $J_3^x$     |
|              |              |              |                |                |              |              |              |                |                |              |              |              |                |                | $J_3^y$     |

Weak Statement ( with diffusion and interface migration)

$$\int \left[ \frac{\underline{J} \cdot \delta \underline{I}}{M} + \frac{(v_n + \nabla \cdot \underline{J})(\delta r_n + \nabla \cdot (\underline{I}))}{m} \right] dA = -\delta G \quad \longrightarrow \quad \int \left[ \frac{\underline{J} \cdot \delta \underline{I}}{M} + \frac{v_n \delta r_n}{m} + \frac{v_n \nabla \cdot (\underline{I})}{m} + \frac{\nabla \cdot \underline{J} \delta r_n}{m} + \frac{\nabla \cdot \underline{J} \nabla \cdot (\underline{I})}{m} \right] dA = -\delta G$$



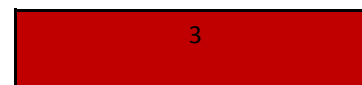
same as the part given in the class  
interface migration only, m



new terms, related to flux and virtual mass diffusion



new terms, flux and virtual displacement coupled



new terms, virtual mass diffusion and norm

2D case is already discussed in class, and the H matrix is given.

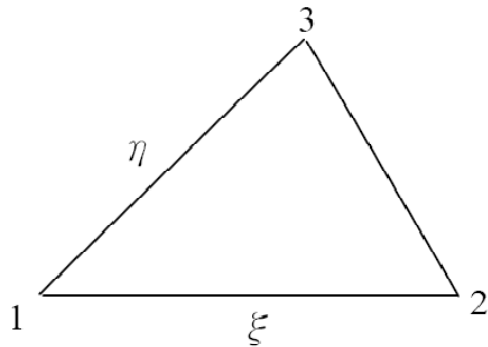
3D case for interface migration has been studied in previous projects, eg.

Here we extend the formulation to 3D case with both diffusion and interface migration

**Finite element method:**

Constant stress triangular element

**1. Local coordinates for CST element:**



So

$$N_1(\xi, \eta) = 1 - \xi - \eta; N_2(\xi, \eta) = \xi;$$

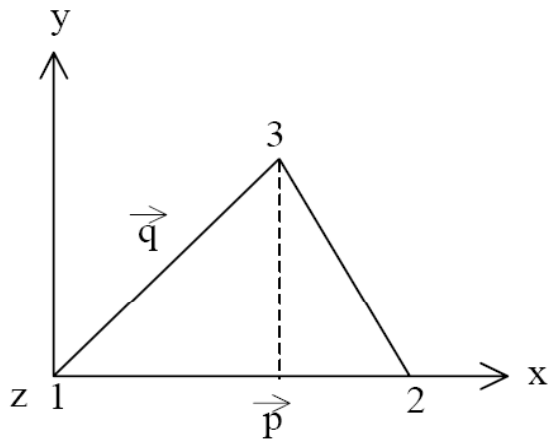
$$N_3(\xi, \eta) = \eta$$

$N_1$  at node 1 =  $N_1(0, 0) = 1 - 0 - 0 = 1$

$N_2$  at node 2 =  $N_2(1, \eta) = 1$

$N_3$  at node 3 =  $N_3(\xi, 1) = 1$

**2. Global coordinates for the triangular element:**



Node 1 ( 0, 0 )

Node 2 ( p, 0 )

Node 3 (  $\bar{q} \cdot \bar{p}_n, |\bar{q} - (\bar{q} \cdot \bar{q}_n)\bar{q}_n|$  )

The nodes have 3 variables in X-Y-Z system, but have only 2 variables in x-y-z system.

### 3. Transformation from local coordinates to global coordinates:

Details of the transformation have been discussed in previous project x,

$$x = N_1(\xi, \eta)x_1 + N_2(\xi, \eta)x_2 + N_3(\xi, \eta)x_3 = (1 - \xi - \eta)x_1 + \xi x_2 + \eta x_3$$
$$y = N_1(\xi, \eta)y_1 + N_2(\xi, \eta)y_2 + N_3(\xi, \eta)y_3 = (1 - \xi - \eta)y_1 + \xi y_2 + \eta y_3$$

$$\frac{\partial x}{\partial \xi} = -x_1 + x_2, \quad \frac{\partial x}{\partial \eta} = -x_1 + x_3, \quad \frac{\partial y}{\partial \xi} = -y_1 + y_2, \quad \frac{\partial y}{\partial \eta} = -y_1 + y_3$$

For example:

$$\int_{\Omega} N_i(x, y)N_j(x, y)dydx = \int_0^{1-\xi} \int_0^{1-\xi} N_i(\xi, \eta)N_j(\xi, \eta)\det Jd\eta d\xi$$

where

$$J = \begin{bmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\ \frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} \end{bmatrix} \Rightarrow J = \begin{bmatrix} x_2 - x_1 & x_3 - x_1 \\ y_2 - y_1 & y_3 - y_1 \end{bmatrix},$$

$$\det J = (x_2 - x_1)(y_3 - y_1) - (x_3 - x_1)(y_2 - y_1) = 2A, \text{ where } A \text{ is the triangular area}$$

This is a standard process for transformation of integrands in multiple integration

Now we're ready to calculate the each term of the H matrix. It is basically the same as the homework, except for some tricks in FEM code.

In the following page, I will derive an example for each different type new term in 3D formulation.

Set  $N_1, N_2, N_3$  as the shape functions, then,

$$\delta \underline{r}_n = N_1 \delta \underline{r}_{n1} + N_2 \delta \underline{r}_{n2} + N_3 \delta \underline{r}_{n3} = N_1 (\underline{n} \cdot \delta \underline{r}_1) + N_2 (\underline{n} \cdot \delta \underline{r}_2) + N_3 (\underline{n} \cdot \delta \underline{r}_3)$$

$$\text{so, } \underline{v}_n = N_1 (\underline{n} \cdot \dot{\underline{r}}_1) + N_2 (\underline{n} \cdot \dot{\underline{r}}_2) + N_3 (\underline{n} \cdot \dot{\underline{r}}_3)$$

$\underline{n} = (a, b, c)$  is the unit normal direction of the element surface

For simplification, we use the same shape function for flux J. Notes: the flux J on an element surface only has two directions

So  $\delta \underline{I} = (N_1 \delta I_1^1 + N_2 \delta I_2^1 + N_3 \delta I_3^1, N_1 \delta I_1^2 + N_2 \delta I_2^2 + N_3 \delta I_3^2)$   $\underline{J}_m^n$  means the the flux of mth node in direction

$$\underline{J} = (N_1 J_1^1 + N_2 J_2^1 + N_3 J_3^1, N_1 J_1^2 + N_2 J_2^2 + N_3 J_3^2)$$

And  $\nabla \cdot \delta \underline{I} = (N_1 \delta I_1^1 + N_2 \delta I_2^1 + N_3 \delta I_3^1, N_1 \delta I_1^2 + N_2 \delta I_2^2 + N_3 \delta I_3^2)$

$$\nabla \cdot \underline{J} = N_{1,1} J_1^1 + N_{2,1} J_2^1 + N_{3,1} J_3^1 + N_{1,2} J_1^2 + N_{2,2} J_2^2 + N_{3,2} J_3^2$$

$$N_{m,n} = \frac{\partial N_m}{\partial n}, n = \xi, \eta$$

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$$\int \left[ \frac{\underline{J} \cdot \delta \underline{I}}{M} + \frac{\nabla \cdot \underline{J} \nabla \cdot (\underline{I})}{m} \right] dA = -\delta G$$

e.g.  $H_{4,9}$  relates to  $J_1^1$  and  $\delta I_2^1$  so  $H_{4,9} = \int \left[ \frac{N_1 N_2}{M} + \frac{N_{1,1} N_{2,1}}{m} \right] dA$

4

$$\int \left[ \frac{\underline{v}_n \nabla \cdot (\underline{I})}{m} \right] dA = -\delta G$$

e.g.

$$H_{3,10} \text{ relates to } \dot{z}_1 \text{ and } \delta I_2^2 \text{ so } H_{3,10} = \int \frac{N_1 c N_{2,2}}{m} dA$$

3

$$\int \left[ \frac{\nabla \cdot \underline{J} \delta r_n}{m} \right] dA = -\delta G$$

e.g.

$$H_{9,12} \text{ relates to } J_2^1 \text{ and } \delta y_3 \text{ so } H_{9,12} = \int \left[ \frac{N_{2,1} N_3 b}{m} \right] dA$$

Detailed integration of H is straightforward and not shown here. The whole H matrix can be found in the Matlab code.

al velocity coupled







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