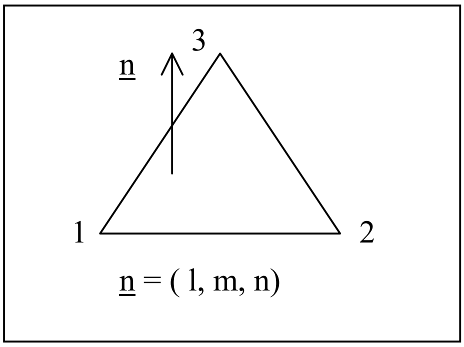
Weak Statement:

$\int \frac{V_n}{L} \delta r_n dA = -\delta G$, which is derived from energy point of view, where V_n denotes normal speed of interface, δr_n denotes the normal displacement of interface, and L denotes the atomic mobility (see equation 4 in Ref. 1).

Constant Strain Triangular element (H matrix):

Consider a triangular element as the following figure, where $\underline{n}$ is the normal surface of the surface of the element.



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

$$\delta r_n = N_1 \delta r_{n1} + N_2 \delta r_{n2} + N_3 \delta r_{n3} = N_1(\underline{n} \cdot \delta r_1) + N_2(\underline{n} \cdot \delta r_2) + N_3(\underline{n} \cdot \delta r_3)$$

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

$$\Rightarrow \delta r_n = N_1 l \dot{x}_1 + N_2 m \dot{y}_1 + N_3 n \dot{z}_1 + N_1 l \dot{x}_2 + N_2 m \dot{y}_2 + N_3 n \dot{z}_2 + N_1 l \dot{x}_3 + N_2 m \dot{y}_3 + N_3 n \dot{z}_3$$

let

$$N_1 l = \hat{N}_1, N_1 m = \hat{N}_2, N_1 n = \hat{N}_3, N_2 l = \hat{N}_4, N_2 m = \hat{N}_5, N_2 n = \hat{N}_6, N_3 l = \hat{N}_7, N_3 m = \hat{N}_8, N_3 n = \hat{N}_9$$

$$\delta r_n = \begin{bmatrix} \delta x_1 & \delta y_1 & \delta z_1 & \delta x_2 & \delta y_2 & \delta z_2 & \delta x_3 & \delta y_3 & \delta z_3 \end{bmatrix} \begin{bmatrix} \hat{N}_1 \\ \hat{N}_2 \\ \hat{N}_3 \\ \hat{N}_4 \\ \hat{N}_5 \\ \hat{N}_6 \\ \hat{N}_7 \\ \hat{N}_8 \\ \hat{N}_9 \end{bmatrix}$$

$$v_n = \begin{bmatrix} \hat{N}_1 & \hat{N}_2 & \hat{N}_3 & \hat{N}_4 & \hat{N}_5 & \hat{N}_6 & \hat{N}_7 & \hat{N}_8 & \hat{N}_9 \end{bmatrix} \begin{bmatrix} \dot{x}_1 \\ \dot{y}_1 \\ \dot{z}_1 \\ \dot{x}_2 \\ \dot{y}_2 \\ \dot{z}_2 \\ \dot{x}_3 \\ \dot{y}_3 \\ \dot{z}_3 \end{bmatrix}$$

then, the weak statement becomes,

$$\int \frac{v_n}{L} \delta r_n dA = \frac{1}{L} \int \delta r_n v_n dA = \frac{1}{L} \int [\delta x]^T \left[\hat{N}\right] \left[\hat{N}\right]^T \left[\dot{x}\right] dA = [\delta x]^T \frac{1}{L} \int \left[\hat{N}\right] \left[\hat{N}\right]^T dA \left[\dot{x}\right]$$

Let $[H] = \frac{1}{L} \int \left[\hat{N}\right] \left[\hat{N}\right]^T dA$

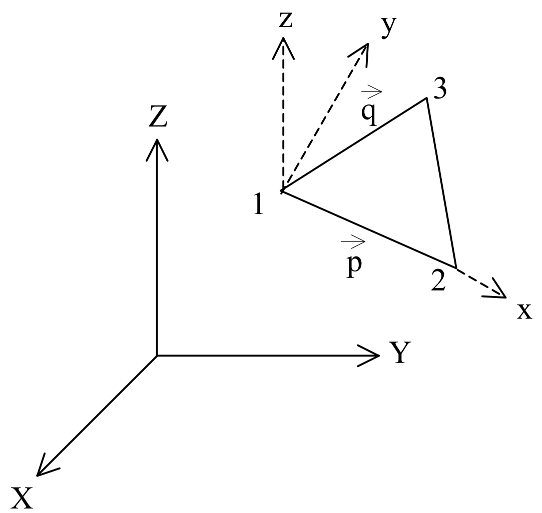
Or in tensorial form

$$\int \frac{v_n}{L} \delta r_n dA = \int \frac{1}{L} N_\alpha \dot{x}_\alpha N_\beta \delta x_\beta dA = \delta x_\beta \frac{1}{L} \int N_\alpha N_\beta dA \, \dot{x}_\alpha$$

Coordinate System Mapping:

Consider 3 nodes in a coordinate system X-Y-Z

node1 (X_1, Y_1, Z_1) , node2 (X_2, Y_2, Z_2) , node3 (X_3, Y_3, Z_3)



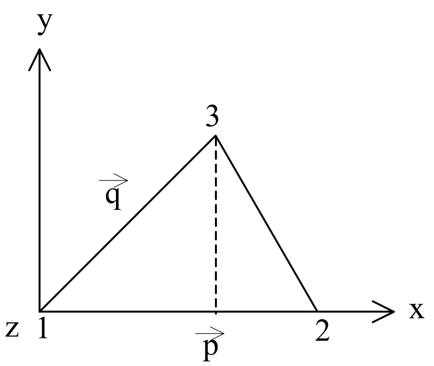
$$\vec{p} = (x_2 \quad y_2 \quad z_2) - (x_1 \quad y_1 \quad z_1)$$
$$\vec{q} = (x_3 \quad y_3 \quad z_3) - (x_1 \quad y_1 \quad z_1)$$

Consider another coordinate system x-y-z where x axis is along $\vec{p}$, z axis is normal to the plane consisting of $\vec{p}$ and $\vec{q}$, so z has the direction of $\vec{p} \times \vec{q}$

The unit vector parallel to x-axis is $\vec{e}_x = \vec{p} \big/ \left|\vec{p}\right|$

The unit vector parallel to z-axis is $\vec{e}_z = \vec{p}\times\vec{q} \big/ \left|\vec{p}\times\vec{q}\right|$

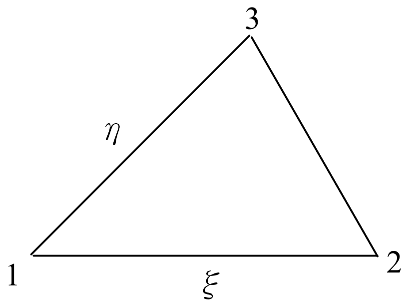
And y-axis is perpendicular to x, z axes.
So, the triangular 1, 2, 3 will be the following coordinates in xyz system.



Node 1 (0, 0)
Node 2 (p, 0)
Node 3 $(\vec{q} \bullet \vec{p}_n, \left|\vec{q} - (\vec{q} \bullet \vec{q}_n)\vec{q}_n\right|)$

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

CST element (constant stress triangular) formulation:
Introduce triangular coordinate



So
$N_1(\xi, \quad \eta) = 1 - \xi - \eta \,;\, N_2(\xi, \quad \eta) = \xi\,;$
$N_3(\xi, \quad \eta) = \eta$
N_1 at node 1 $= N_1(0, \quad 0) = 1 - 0 - 0 = 1$
N_2 at node 2 $= N_2(1, \quad \eta) = 1$
N_3 at node 3 $= N_3(\xi, \quad 1) = 1$

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

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

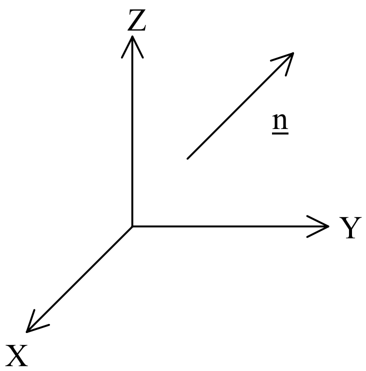
$$\frac{\partial x}{\partial \xi} = -x_1 + x_2, \frac{\partial x}{\partial \eta} = -x_1 + x_3, \frac{\partial y}{\partial \xi} = -y_1 + y_2, \frac{\partial y}{\partial \eta} = -y_1 + y_3$$

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

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

Consider the normal direction of element in X-Y-Z, which is parallel to z axis.

$$\underline{n} = \frac{p \times q}{|p \times q|} = (l, m, n)$$



For node 1

$$N_1 \delta r_1 = N_1(\xi, \eta)\underline{\vec{n}} \bullet \delta r_1 = N_1(\xi, \eta)(l\delta x_1 + m\delta y_1 + n\delta z_1)$$
$$N_2 \delta r_2 = N_2(\xi, \eta)(l\delta x_2 + m\delta y_2 + n\delta z_2)$$
$$N_3 \delta r_3 = N_3(\xi, \eta)(l\delta x_3 + m\delta y_3 + n\delta z_3)$$

$$\hat{N}_1 = N_1(\xi, \eta)l, \hat{N}_2 = N_1(\xi, \eta)m, \hat{N}_3 = N_1(\xi, \eta)n$$

Let $\hat{N}_4 = N_2(\xi, \eta)l, \hat{N}_5 = N_2(\xi, \eta)m, \hat{N}_6 = N_2(\xi, \eta)n$

$$\hat{N}_7 = N_3(\xi, \eta)l, \hat{N}_8 = N_3(\xi, \eta)m, \hat{N}_9 = N_3(\xi, \eta)n$$

$$H_{ij} = \int_0^1 \int_0^{1-\xi} \hat{N}_1 \hat{N}_2 \det J d\eta d\xi$$

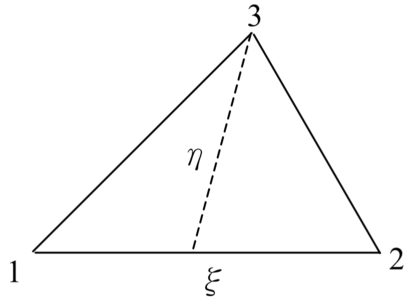
where $\det J = (x_2 - x_1)(y_2 - y_1) - (x_3 - x_1)(y_2 - y_1) = 2A$

A = triangle area

Then, the H matrix for CST

$$H=\frac{A}{12}\begin{bmatrix} 2l^2 & 2l\cdot m & 2l\cdot n & l^2 & l\cdot m & l\cdot n & l^2 & l\cdot m & l\cdot n \\ 2l\cdot m & 2m^2 & 2m\cdot n & l\cdot m & m^2 & m\cdot n & l\cdot m & m^2 & m\cdot n \\ 2l\cdot n & 2m\cdot n & 2n^2 & l\cdot n & m\cdot n & n^2 & l\cdot n & m\cdot n & n^2 \\ l^2 & l\cdot m & l\cdot n & 2l^2 & 2l\cdot m & 2l\cdot n & l^2 & l\cdot m & l\cdot n \\ l\cdot m & m^2 & m\cdot n & 2l\cdot m & 2m^2 & 2m\cdot n & l\cdot m & m^2 & m\cdot n \; m \\ l\cdot n & m\cdot n & n^2 & 2l\cdot n & 2m\cdot n & 2n^2 & l\cdot n & m\cdot n & n^2 \\ l^2 & l\cdot m & l\cdot n & l^2 & l\cdot m & l\cdot n & 2l^2 & 2l\cdot m & 2l\cdot n \\ l\cdot m & m^2 & m\cdot n & l\cdot m & m^2 & m\cdot n & 2l\cdot m & 2m^2 & 2m\cdot n \\ l\cdot n & m\cdot n & n^2 & l\cdot n & m\cdot n & n^2 & 2l\cdot n & 2m\cdot n & 2n^2 \end{bmatrix}$$

Similarly, we can do the formulation for the triangle element degenerated from bilinear quadrilateral element.



$$N_1(\xi,\eta)=\frac{1}{4}(1-\xi)(1-\eta)$$
$$N_2(\xi,\eta)=\frac{1}{4}(1+\xi)(1-\eta)$$
$$N_3(\xi,\eta)=\frac{1}{2}(1+\eta)$$

Then, let $\hat{N}_1 = N_1 l, \hat{N}_2 = N_1 m, \hat{N}_3 = N_1 n,$

$$\hat{N}_4 = N_2 l, \hat{N}_5 = N_2 m, \hat{N}_6 = N_2 n,$$
$$\hat{N}_7 = N_3 l, \hat{N}_8 = N_3 m, \hat{N}_9 = N_3 n$$

Then $H_{ij} = \int_{-1}^{0}\int_{-1}^{1+2\xi} \hat{N}_i \hat{N}_j \det J d\eta d\xi + \int_{0}^{1}\int_{-1}^{1-2\xi} \hat{N}_i \hat{N}_j \det J d\eta d\xi$

This should be able to provide a similar H matrix.

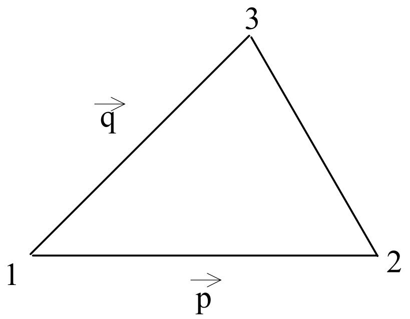
Formulation of F column:

Consider the RHS. of δG

We know $G=\gamma A+gV$, assume γ

$\delta G=\gamma\delta A+g\delta V$

First, try to approximate δA



$\vec{A} = \vec{p} \times \vec{q}$, $\vec{p} = \mathbf{x_2} - \mathbf{x_1}$, $\vec{q} = \mathbf{x_3} - \mathbf{x_1}$

$$\vec{A}' = \frac{1}{2}\left(\vec{p} + \delta\vec{p}\right)\times\left(\vec{q} + \delta\vec{q}\right) = \frac{1}{2}\left(\vec{p}\times\vec{q} + \delta\vec{p}\times\vec{q} + \vec{p}\times\delta\vec{q} + \delta\vec{p}\times\delta\vec{q}\right)$$

$$\delta\vec{A} = \vec{A}' - \vec{A} = \frac{1}{2}\left(\vec{p} + \delta\vec{p}\right)\times\left(\vec{q} + \delta\vec{q}\right) - \frac{1}{2}\vec{p}\times\vec{q} = \frac{1}{2}\left(\delta\vec{p}\times\vec{q} + \vec{p}\times\delta\vec{q} + \delta\vec{p}\times\delta\vec{q}\right)$$

Assuming $\delta p, \delta q$ are small, so, $\delta\vec{p}\times\delta\vec{q} \approx 0$

$$\Rightarrow \delta A \approx \frac{1}{2}\left(\delta\vec{p}\times\vec{q} + \vec{p}\times\delta\vec{q}\right)$$

let $\vec{p}_n = \dfrac{\vec{p}}{|\vec{p}|}, \vec{q}_n = \dfrac{\vec{q}}{|\vec{q}|}$

$$\delta\vec{p} = \left(\delta \underset{-2}{r} \bullet \vec{p}_n\right)\vec{p}_n - \left(\delta \underset{-1}{r} \bullet \vec{p}_n\right)\vec{p}_n = \left[\left(\delta \underset{-2}{r} - \delta \underset{-1}{r}\right)\bullet \vec{p}_n\right]\vec{p}_n$$

$$similarly, \delta\vec{q} = \left[\left(\delta \underset{-3}{r} - \delta \underset{-1}{r}\right)\bullet \vec{q}_n\right]\vec{q}_n$$

$$\delta\vec{A} \approx \frac{1}{2}\left(\delta\vec{p}\times\vec{q} + \vec{p}\times\delta\vec{q}\right) = \frac{1}{2}\left\{\left[\left(\delta \underset{-2}{r} - \delta \underset{-1}{r}\right)\bullet \vec{p}_n\right]\vec{p}_n \times \vec{q}_n|\vec{q}| + |\vec{p}|\vec{p}\times\left[\left(\delta \underset{-3}{r} - \delta \underset{-1}{r}\right)\bullet \vec{q}_n\right]\vec{q}_n\right\}$$

$$= \frac{1}{2}\left\{\left(\delta \underset{-2}{r} - \delta \underset{-1}{r}\right)\bullet \vec{p}_n|\vec{q}| + |\vec{p}|\left[\left(\delta \underset{-3}{r} - \delta \underset{-1}{r}\right)\bullet \vec{q}_n\right]\right\}\vec{p}_n \times \vec{q}_n$$

$$= \frac{1}{2}\left\{\begin{array}{l}|\vec{q}|\left[\left(\delta x_2 - \delta x_1\right)p_{nx} + \left(\delta y_2 - \delta y_1\right)p_{ny} + \left(\delta z_2 - \delta z_1\right)p_{nz}\right] \\ + |\vec{p}|\left[\left(\delta x_e - \delta x_1\right)q_{nx} + \left(\delta y_e - \delta y_1\right)q_{ny} + \left(\delta z_e - \delta z_1\right)q_{nz}\right]\end{array}\right\}\vec{p}_n \times \vec{q}_n$$

where
$$p_{nx} = \frac{\vec{p}_x}{|\vec{p}|} = \frac{x_2 - x_1}{|\vec{p}|}, p_{ny} = \frac{y_2 - y_1}{|\vec{p}|}, p_{nz} = \frac{z_2 - z_1}{|\vec{p}|}$$
$$q_{nx} = \frac{x_3 - x_1}{|\vec{q}|}, q_{ny} = \frac{y_3 - y_1}{|\vec{q}|}, q_{nz} = \frac{z_3 - z_1}{|\vec{q}|}$$

so,

$$\delta\vec{A} = \frac{1}{2}\left\{\begin{array}{l}\frac{|\vec{q}|}{|\vec{p}|}(x_2 - x_1)(\delta x_2 - \delta x_1) + \frac{|\vec{q}|}{|\vec{p}|}(y_2 - y_1)(\delta y_2 - \delta y_1) + \frac{|\vec{q}|}{|\vec{p}|}(z_2 - z_1)(\delta z_2 - \delta z_1) \\ + \frac{|\vec{p}|}{|\vec{q}|}(x_3 - x_1)(\delta x_3 - \delta x_1) + \frac{|\vec{p}|}{|\vec{q}|}(y_3 - y_1)(\delta y_3 - \delta y_1) + \frac{|\vec{p}|}{|\vec{q}|}(z_3 - z_1)(\delta z_3 - \delta z_1)\end{array}\right\}\vec{p}_n \times \vec{q}_n$$

$$\Rightarrow \frac{1}{2}\left\{\begin{array}{l}\left[\frac{|\vec{q}|}{|\vec{p}|}(x_2 - x_1) + \frac{|\vec{p}|}{|\vec{q}|}(x_3 - x_1)\right](-\delta x_1) + \left[\frac{|\vec{q}|}{|\vec{p}|}(y_2 - y_1) + \frac{|\vec{p}|}{|\vec{q}|}(y_3 - y_1)\right](-\delta y_1) \\ + \left[\frac{|\vec{q}|}{|\vec{p}|}(z_2 - z_1) + \frac{|\vec{p}|}{|\vec{q}|}(z_3 - z_1)\right](-\delta z_1) + \frac{|\vec{q}|}{|\vec{p}|}(x_2 - x_1)\delta x_2 + \frac{|\vec{q}|}{|\vec{p}|}(y_2 - y_1)\delta y_2 \\ + \frac{|\vec{q}|}{|\vec{p}|}(z_2 - z_1)\delta z_2 + \frac{|\vec{p}|}{|\vec{q}|}(x_3 - x_1)\delta x_3 + \frac{|\vec{p}|}{|\vec{q}|}(y_3 - y_1)\delta x_3 + \frac{|\vec{p}|}{|\vec{q}|}(z_3 - z_1)\delta x_3\end{array}\right\}\vec{p}_n \times \vec{q}_n$$

$$= A \cdot \vec{p}_n \times \vec{q}_n$$

then $\left|\delta\vec{A}\right| = A \cdot |\vec{p}_n \times \vec{q}_n| = A \cdot \frac{|\vec{p}_n \times \vec{q}_n|}{|\vec{p}||\vec{q}|}$, since $\vec{p}_n = \frac{\vec{p}}{|\vec{p}|}, \vec{q}_n = \frac{\vec{q}}{|\vec{q}|}$

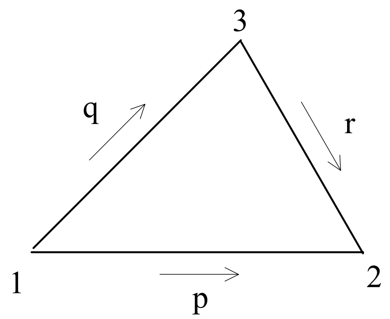
so, we have

$$\delta A = -\frac{1}{2}\left[\frac{|\vec{p}\times\vec{q}|}{|\vec{p}|^2}(x_2 - x_1) + \frac{|\vec{p}\times\vec{q}|}{|\vec{q}|^2}(x_3 - x_1)\right]\delta x_1 - \frac{1}{2}\left[\frac{|\vec{p}\times\vec{q}|}{|\vec{p}|^2}(y_2 - y_1) + \frac{|\vec{p}\times\vec{q}|}{|\vec{q}|^2}(y_3 - y_1)\right]\delta y_2$$

$$-\frac{1}{2}\left[\frac{|\vec{p}\times\vec{q}|}{|\vec{p}|^2}(z_2 - z_1) + \frac{|\vec{p}\times\vec{q}|}{|\vec{q}|^2}(z_3 - z_1)\right]\delta z_3 + \frac{1}{2}\frac{|\vec{p}\times\vec{q}|}{|\vec{p}|^2}(x_2 - x_1)\delta x_2 + \frac{1}{2}\frac{|\vec{p}\times\vec{q}|}{|\vec{p}|^2}(y_2 - y_1)\delta y_2$$

$$+\frac{1}{2}\frac{|\vec{p}\times\vec{q}|}{|\vec{p}|^2}(z_2 - z_1)\delta z_2 + \frac{1}{2}\frac{|\vec{p}\times\vec{q}|}{|\vec{q}|^2}(x_3 - x_1)\delta x_3 + \frac{1}{2}\frac{|\vec{p}\times\vec{q}|}{|\vec{q}|^2}(y_3 - y_1)\delta y_3 + \frac{1}{2}\frac{|\vec{p}\times\vec{q}|}{|\vec{q}|^2}(z_3 - z_1)\delta z_3 = f_i \delta x_i$$

Moreover, since the above method will only provide the driving forces acting along $\vec{p}$ and $\vec{q}$. So, we should use the same method to compute the other driving forces along $\vec{r}$



$$A_i = \frac{1}{2}\vec{p}\times\vec{q} \Rightarrow \delta A_i = f_i \delta x_i$$

$$A_j = \frac{1}{2}(-\vec{r})\times(\vec{p}) \Rightarrow \delta A_j = f_j \delta x_j$$

$$A_k = \frac{1}{2}(-\vec{q})\times\vec{r} \Rightarrow \delta A_k = f_k \delta x_k$$

$$then, f_s = \frac{1}{3}(f_i + f_j + f_k)$$

Free Energy Term:

Then consider the term $g\delta v$

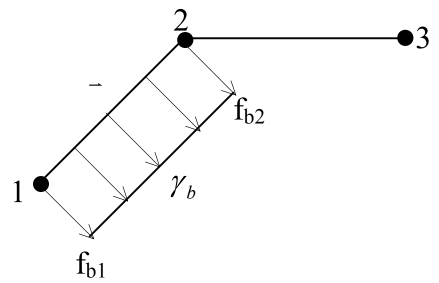
$$\delta v = \frac{1}{3}\left(\delta r_{n1} + \delta r_{n2} + \delta r_{n3}\right)A, \qquad A = \frac{1}{2}\left|\vec{p} \times \vec{q}\right|$$

$$g\delta v = \frac{1}{3} gA\left(\hat{l}\,\delta x_1 + \hat{m}\,\delta y_1 + \hat{n}\,\delta z_1 + \hat{l}\,\delta x_2 + \hat{m}\,\delta y_2 + \hat{n}\,\delta z_2 + \hat{l}\,\delta x_3 + \hat{m}\,\delta y_3 + \hat{n}\,\delta z_3\right)$$

where $\left(\hat{l}, \hat{m}, \hat{n}\right) = \underline{n}$, the unit normal vector of the element surface

Grain Boundary Term:

then this will have general $f_g \delta x$

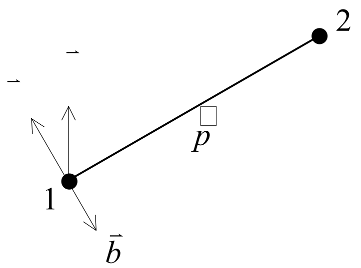


Assume the grain boundary tension γ_b will always perpendicular to the surface and γ_b is uniform distributed along the line between node 1, 2.

Therefore, we should add $f_{b1} = \frac{1}{2}\left|\vec{p}\right| \bullet \gamma_b$ on node 1 and $f_{b2} = \frac{1}{2}\left|\vec{p}\right| \bullet \gamma_b$ on node 2.

From the figure, f_{b1} and f_{b2} have the same direction perpendicular to $\vec{p}$

$\vec{b}$.



$\vec{e}_z$ is the unit vector in z direction.

$\vec{e}_z \times \vec{p} = \vec{t}$

$\vec{t} \times \vec{p} = \vec{b}$, $\vec{b}_n = \frac{\vec{b}}{|\vec{b}|}$ is the unit vector of f_{b1} and f_{b2}

So, the total f term is $f = f_s + f_g + f_b$

Global Matrix Assembly:

Using the assembly method presented by Hughes (relations of ID, IEN and LM arrays). Please refer to reference [3]. Meanwhile, a small arbitrary mass should be added on the diagonal entities, which is for preventing singular problem. The amount of the small arbitrary mass should be chosen carefully (please see the argument in Ref [2] section 3.7).