

1. Compute Thermodynamic/Transport Properties  $c_v, k, \mu, \gamma$ 2. Compute the equilibration pressure  $P_{eq}, c_m, \rho_m^o, \theta_m, f_m^\theta, \kappa_m$ , such that  $\sum_{m=1}^N \theta_m = 1$ , see attached for details.3. Compute the mass exchange between materials  $S_{m_m}^{r \leftrightarrow m}, S_{(m\vec{U})_m}^{r \leftrightarrow m}, S_{(me)_m}^{r \leftrightarrow m}, S_{(mv^o)_m}^{r \leftrightarrow m}$ 4. Compute the face-centered velocities

$$\begin{aligned} \vec{U}_m^{*f} &= \left\langle \frac{\rho_m \vec{U}_m}{\rho_m} \right\rangle^{n^f} - \frac{\Delta t}{\langle \rho_m^o \rangle^f} \nabla^f P_{eq} + \sum_{n=1}^N \left\langle \frac{\Delta t \theta_n K_{n,m}}{\rho_m} \right\rangle^f (\vec{U}_n^{*f} - \vec{U}_m^{*f}) + \Delta t \vec{g} \\ &= \frac{(\rho \vec{U})_{m_R} + (\rho \vec{U})_{m_L}}{\rho_{m_R} + \rho_{m_L}} - \Delta t \frac{2.0(v_{m_L}^o v_{m_R}^o)}{v_{m_L}^o + v_{m_R}^o} \left( \frac{P_{eq_R} - P_{eq_L}}{\Delta x} \right) + \text{Exchange Contribution} + \Delta t \vec{g} \end{aligned}$$

The exchange contribution involves a pointwise implicit solve, see attached for details.

5. Update the volume fraction

$$\begin{aligned} V_{total} &= \sum_{m=1}^N (\rho_m V v_m^o) \\ V_m^{new} &= \theta_m V_{total} v_m^o + S_{(mv^o)_m}^{r \leftrightarrow m} \\ \theta_m &= \frac{V_m^{new}}{V_{total}}, \sum_{m=1}^N \theta_m \kappa_m \end{aligned}$$

6. Compute  $\Delta P$ 

$$\Delta P = \Delta t \frac{\sum_{r=1}^N S_{(mv^o)_r}^{r \leftrightarrow m} - \overbrace{\sum_{m=1}^N \nabla \cdot \theta_m \vec{U}_m^{*f}}^{\text{Advection}(\theta, \vec{U}_m^{*f})}}{\sum_{m=1}^N (\theta_m) \kappa_m}$$

where  $P^{n+1} = P_{eq} + \Delta P, S_{\theta_m}^{r \leftrightarrow m} = \frac{S_{(mv^o)_m}^{r \leftrightarrow m}}{V}$  and  $\kappa_m = \frac{v_m^o}{c_m^o}$ .

7. Compute the face centered pressure

$$P^{*f} = \frac{\frac{P}{\sum_{m=1}^N \rho_m} + \frac{P_{adj}}{\sum_{m=1}^N \rho_{m,adj}}}{\frac{1}{\sum_{m=1}^N \rho_m} + \frac{1}{\sum_{m=1}^N \rho_{m,adj}}} = \frac{P \sum_{m=1}^N \rho_{m,adj} + P_{adj} \sum_{m=1}^N \rho_m}{\sum_{m=1}^N \rho_m + \sum_{m=1}^N \rho_{m,adj}}$$

### 8. Accumulate sources

$$\Delta(m\vec{U})_m = -\Delta t V \theta_m \nabla P^{*f} + \Delta t V \sum_{l=1}^N \theta_m \theta_l K_{ml} (\vec{U}_l^{n+1L} - \vec{U}_m^{n+1L}) + \Delta t \nabla \cdot (\theta_m^{*f} \vec{\tau}_m^{*f}) + m_m \vec{g} \Delta t$$

$$\Delta(me)_m = V \theta_m \kappa_m P \Delta P_{\text{Dilata}} - \Delta t \nabla (\theta^{*f} q_m^{*f}) + \Delta t V \sum_{l=1}^N \theta_m \theta_l R_{ml} (T_l^{n+1L} - T_m^{n+1L})$$

where  $q^{*f} = -k^f \nabla T$  and  $\theta^{*f} =$  Computed during the advection of  $\theta_m$

### 9. Compute Lagrangian quantities

$$m_m^L = \rho_m V + S_{m_m}^{r \leftrightarrow m}$$

$$(m\vec{U})_m^L = (m\vec{U})_m + \Delta(m\vec{U})_m + S_{(m\vec{U})_m}^{r \leftrightarrow m}$$

$$(me)_m^L = (me)_m + \Delta(me)_m + S_{(me)_m}^{r \leftrightarrow m}$$

Note this includes the pointwise implicit solve for the momentum and energy exchange

#### **Evolution of specific volume**

$$(mv^o)_m^L = (mv^o)_m + \Delta t f_m^0 V \nabla \cdot \vec{U}_m^{*f} + \Delta t V [\theta_m \alpha_m \dot{T}_m - f_m^0 \sum_{s=1}^N \theta_s \alpha_s \dot{T}_s] \quad \text{where } \alpha = 0(\text{mpm}) = 1/T(\text{ice})$$

$$\text{Note } \Delta t f_m^0 V \nabla \cdot \vec{U}_m^{*f} = \theta_m \kappa_m V \Delta p$$

$$\dot{T}_m = \frac{(T_{\text{After Exchange Process}} - T_{\text{Top of the time step}})}{\Delta t}$$

### 10. Advect and Advance in time

$$m_m^{n+1} = m_m^L - \Delta t \text{Advection}(m_m^L, \vec{U}_m^{*f})$$

$$(m\vec{U})_m^{n+1} = (m\vec{U})_m^L - \Delta t \text{Advection}((m\vec{U})_m^L, \vec{U}_m^{*f})$$

$$(me)_m^{n+1} = (me)_m^L - \Delta t \text{Advection}((\rho e)_m^L, \vec{U}_m^{*f})$$

$$(mv^o)_m^{n+1} = (mv^o)_m^L - \Delta t \text{Advection}((\rho v^o)_m^L, \vec{U}_m^{*f})$$

## Calculation of the equilibration pressure

Initial Guess

$eos(T_m, P)$  compute  $\rightarrow \rho_m^o$

$$\theta_m = \frac{\rho_m}{\rho_m^o}$$

$eos(T_m, \rho_m^o)$  compute  $\rightarrow P_{eos_m}, \frac{dP}{d\rho_m^o}, \frac{dP}{de}$

$$c_m = \sqrt{\frac{\left( \frac{dP}{d\rho_m^o} + \frac{dP}{de} * P_{eos_m} \right)}{\rho_m^{o^2}}}$$

**while**  $|1 - \sum \theta_m| < \text{convergence criteria}$  **do**

**for**  $m = 1$  to All Matls **do**

$eos(T_m, \rho_m^o m)$  compute  $\rightarrow P_{eos_m}, \frac{dP}{d\rho_m^o}$

$$Q_m + = P - P_{eos_m}$$

$$y_m + = \frac{dP}{d\rho_m^o} \frac{\rho_m}{\theta_m^2}$$

**end for**

$$\Delta p = \frac{\sum \theta_m - \theta_{closed\ packed} - \sum \frac{Q_m}{y_m}}{\sum \frac{1}{y_m}}$$

$$P_{eq} = P_{eq} + \Delta p$$

**for**  $m = 1$  to All Matls **do**

$eos(P, T_m)$  compute  $\rightarrow \rho_m^o$

$eos(\rho_m^o, T_m)$  compute  $\rightarrow P_{eos_m}, \frac{dP}{d\rho_m^o}, \frac{dP}{de}$

$$c_m = \sqrt{\frac{\left( \frac{dP}{d\rho_m^o} + \frac{dP}{de} * P_{eos_m} \right)}{\rho_m^{o^2}}}$$

$$\theta_m = \frac{\rho_m}{\rho_m^o}$$

**end for**

**end while**

BulletProofing( $P, \rho_m^o, \theta_m$ )

$$\text{compute } \kappa_m = \frac{v_m^o}{c_m^2}, f_m^\theta = \frac{\theta_m \kappa_m}{\sum_{s=1}^N \theta_s \kappa_s}, \quad v_m^o = \frac{1}{\rho_m^o}$$

1. Rearrange the starting momentum Equation in the x-direction

$$(mu)_m^{n+1L} = (mu)_m^n + \text{sources /Sinks} + \Delta t V \sum_n \theta_m \theta_n K_{m,n} (u_n^{n+1L} - u_m^{n+1L})$$

Divide through by the mass

$$u_m^{n+1L} = \frac{(mu)_m^n}{m_m^{n+1L}} + \frac{\text{sources /Sinks}}{m_m^{n+1L}} + \frac{\Delta t V \sum_n \theta_m \theta_n K_{m,n} (u_n^{n+1L} - u_m^{n+1L})}{m_m^{n+1L}}$$

Now assume that  $m_m^{n+1L} = m_m^n$  and using  $\theta_m = \frac{\rho_m}{\rho_m^o}$

$$u_m^{n+1L} = \underbrace{u_m^n}_a - \underbrace{\frac{\text{sources /Sinks}}{m_m^n}}_b + \underbrace{\Delta t \sum_n \frac{\theta_n K_{m,n}}{\rho_m^o}}_{\beta} (u_n^{n+1L} - u_m^{n+1L})$$

$$u_m^{n+1L} = a + b + \beta_{mn} (u_n^{n+1L} - u_m^{n+1L})$$

2. Let

$$u_m^{n+1L} = \underbrace{\tilde{u}_m^{nL}}_{\text{base vel FC}} + \underbrace{\Delta u_m^{nL}}_{\text{contribution due momentum exchange}}$$

3. For two materials we have

$$\begin{aligned} \tilde{u}_1^{nL} + \Delta u^{L1} &= a_1 + b_1 + \beta_{12} \left[ (\tilde{u}_2^{nL} + \Delta u^{L2}) - (\tilde{u}_1^{nL} + \Delta u^{L1}) \right] \\ \tilde{u}_2^{nL} + \Delta u^{L2} &= a_2 + b_2 + \beta_{21} \left[ (\tilde{u}_1^{nL} + \Delta u^{L1}) - (\tilde{u}_2^{nL} + \Delta u^{L2}) \right] \end{aligned}$$

Note that  $\tilde{u}_2^{nL} = a_1 + b_1$ , and rearranging

$$\Delta u^{L1} (1 + \beta_{12}) - \beta_{12} \Delta u^{L2} = \beta_{12} (\tilde{u}_2^{nL} - \tilde{u}_1^{nL})$$

$$-\beta_{21} \Delta u^{L1} - \Delta u^{L2} (1 + \beta_{21}) = \beta_{21} (\tilde{u}_1^{nL} - \tilde{u}_2^{nL})$$

$$\begin{vmatrix} (1 + \beta_{12}) & -\beta_{12} \\ -\beta_{21} & (1 + \beta_{21}) \end{vmatrix} \begin{vmatrix} \Delta u^{L1} \\ \Delta u^{L2} \end{vmatrix} = \begin{vmatrix} \beta_{12} (\tilde{u}_2^{nL} - \tilde{u}_1^{nL}) \\ \beta_{21} (\tilde{u}_1^{nL} - \tilde{u}_2^{nL}) \end{vmatrix}$$

4. Solve for  $\Delta u^{L1}$  and add it to  $\tilde{u}_m^{nL}$  to get  $u_m^{n+1L}$

1. Rearrange the starting momentum Equation in the x-direction

$$(mu)_m^{n+1*f} = \left\langle (mu)_m \right\rangle^{n^f} - \Delta t V \theta_m \nabla^f P_{eq} + \Delta t V \sum_n \left\langle \theta_m \theta_n K_{m,n} \right\rangle^f (u_n^{n+1*f} - u_m^{n+1*f}) + \Delta t m_m \vec{g}$$

where  $\theta = \frac{\rho_m}{\rho_m^o} = v_m^o$  and  $m_m = \rho_m V$  so

$$(mu)_m^{n+1*f} = \left\langle (mu)_m \right\rangle^{n^f} - \Delta t \left\langle \frac{m_m}{\rho_m^o} \right\rangle^f \nabla^f P_{eq} + \Delta t \sum_n \left\langle \frac{m_m \theta_n K_{m,n}}{\rho_m^o} \right\rangle^f (u_n^{n+1*f} - u_m^{n+1*f}) + \Delta t \left\langle m_m \right\rangle^f \vec{g}$$

Now assume that  $(m)_m^{n+1*f} = \left\langle m \right\rangle_m^{n*f}$  and divide through.

$$(u)_m^{n+1*f} = \underbrace{\left\langle \frac{(\rho u)_m}{\rho_m} \right\rangle^{n^f}}_a - \underbrace{\Delta t \left\langle \frac{1}{\rho_m^o} \right\rangle^f}_b \nabla^f P_{eq} + \underbrace{\Delta t \sum_n \left\langle \frac{\theta_n K_{m,n}}{\rho_m^o} \right\rangle^f}_\beta (u_n^{n+1*f} - u_m^{n+1*f}) + \underbrace{\Delta t \vec{g}}_c$$

$$(u)_m^{n+1*f} = a - b \nabla^f P_{eq} + \beta_{mn} (u_n^{n+1*f} - u_m^{n+1*f}) + c$$

2. Let

$$u_m^{n+1*f} = \underbrace{\tilde{u}_m^{n*f}}_{\text{base vel FC}} + \underbrace{\Delta u^{*f}}_{\text{contribution due momentum exchange}}$$

3. For two materials we have

$$\begin{aligned} \tilde{u}_1^{n*f} + \Delta u_1^{*f} &= a_1 - b_1 \nabla^f P_{eq} + \beta_{12} \left[ (\tilde{u}_2^{n*f} + \Delta u_2^{*f}) - (\tilde{u}_1^{n*f} + \Delta u_1^{*f}) \right] + c \\ \tilde{u}_2^{n*f} + \Delta u_2^{*f} &= a_2 - b_2 \nabla^f P_{eq} + \beta_{21} \left[ (\tilde{u}_1^{n*f} + \Delta u_1^{*f}) - (\tilde{u}_2^{n*f} + \Delta u_2^{*f}) \right] + c \end{aligned}$$

Note that  $\tilde{u}_1^{n*f} = a_1 - b_1 \nabla^f P_{eq} + c$ , and rearranging

$$\Delta u_1^{*f} (1 + \beta_{12}) - \beta_{12} \Delta u_2^{*f} = \beta_{12} (\tilde{u}_2^{n*f} - \tilde{u}_1^{n*f})$$

$$-\beta_{21} \Delta u_1^{*f} - \Delta u_2^{*f} (1 + \beta_{21}) = \beta_{21} (\tilde{u}_1^{n*f} - \tilde{u}_2^{n*f})$$

$$\begin{vmatrix} (1 + \beta_{12}) & -\beta_{12} \\ -\beta_{21} & (1 + \beta_{21}) \end{vmatrix} \begin{vmatrix} \Delta u_1^{*f} \\ \Delta u_2^{*f} \end{vmatrix} = \begin{vmatrix} \beta_{12} (\tilde{u}_2^{n*f} - \tilde{u}_1^{n*f}) \\ \beta_{21} (\tilde{u}_1^{n*f} - \tilde{u}_2^{n*f}) \end{vmatrix}$$

4. Solve for  $\Delta u_1^{*f}$  and add it to  $\tilde{u}_m^{n*f}$  to get  $(u)_m^{n+1*f}$