ICE EQ FORM 07/11/05

1. Compute Thermodynamic/Transport Properties c_v, k, μ, γ

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

$$\vec{U}_m^{*f} = \left\langle \frac{\rho_m \vec{U}_m}{\rho_m} \right\rangle^{nf} - \frac{\Delta t}{< \rho_m^o >^f} \nabla^f P_{eq} + \sum_{n=1}^{N} \left\langle \frac{\Delta t \theta_n K_{n,m}}{\rho_m} \right\rangle^f (\vec{U}_n^{*f} - \vec{U}_m^{*f}) + \Delta t \vec{g}$$

$$= \frac{(\rho\vec{U})_{m_R} + (\rho\vec{U})_{m_L}}{\rho_{m_R} + \rho_{m_L}} - \Delta t \frac{2.0(v_{m_L}^o v_{m_R}^o)}{v_{m_L}^o + v_{m_R}^o} \left(\frac{P_{eq_R} - P_{eq_L}}{\Delta x} \right) + \text{Exchange Contribution} + \Delta t \vec{g}$$

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

5. Update the volume fraction

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

6. Compute ΔP

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

where $P^{n+1} = P_{eq} + \Delta P, S_{\theta_m}^{r\leftrightarrow m} = \frac{S_{(mv^o)}^{r\leftrightarrow m}}{V}$ and $\kappa_m = \frac{v_m^o}{c_m^2}$.

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

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

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

where $\theta^{*^f} q^{*^f} = - < \theta k > \nabla T$ and $<\theta k> = (2(\theta k)_{m_R} (\theta k)_{m_L}) / ((\theta k)_{m_R} + (\theta k)_{m_L})$

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

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

Note $\Delta t f_m^\theta V \nabla \cdot \vec{U}_m^{*^f} = \theta_m \kappa_m V \Delta p$
$\dot{T}_m = \frac{(T_{\text{After Exchange Process}} - T_{\text{Top of the time step}})}{\Delta t}$

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 $\rightarrow$ $P_{eos_m}, \frac{dP}{d\rho_m^o}, \frac{dP}{de}$

while $|1 - \sum \theta_m| <$ 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 $\rightarrow$ ρ_m^o

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

    $c_m = \sqrt{\frac{dP}{d\rho_m^o} + \frac{dP}{de} \frac{P_{eos_m}}{\rho_m^{o2}}}$

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

  end for

end while

BulletProofing(P, ρ_m^o, θ_m)

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

Solving for the Lagrangian momentum with an implicit solve

1. Rearrange the starting momentum Equation in the x-direction
   $(mu)_m^{n+1^L} = (mu)_m^n + \text{sources /Sinks} + \Delta t V \sum_n \theta_m \theta_n K_{m,n}(u_n^{n+1^L} - u_m^{n+1^L})$
   Divide through by the mass
   $u_m^{n+1^L} = \frac{(mu)_m^n}{m_m^{n+1^L}} + \frac{\text{sources /Sinks}}{m_m^{n+1^L}} + \frac{\Delta t V \sum_n \theta_m \theta_n K_{m,n}(u_n^{n+1^L} - u_m^{n+1^L})}{m_m^{n+1^L}}$
   Now assume that $m_m^{n+1^L} = m_m^n$ and using $\theta_m = \frac{\rho_m}{\rho_m^o}$
   $$u_m^{n+1^L} = \underbrace{u^n}_{a} - \underbrace{\frac{\text{sources /Sinks}}{m_m^n}}_{b} + \underbrace{\Delta t \sum_n \frac{\theta_n K_{m,n}}{\rho_m^o}}_{\beta}(u_n^{n+1^L} - u_m^{n+1^L})$$
   $$u_m^{n+1^L} = a + b + \beta_{mn}(u_n^{n+1^L} - u_m^{n+1^L})$$

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

3. For two materials we have
   $$\tilde{u}_1^{n^L} + \Delta u^{L_1} = a_1 + b_1 + \beta_{12}\left[(\tilde{u}_2^{n^L} + \Delta u^{L_2}) - (\tilde{u}_1^{n^L} + \Delta u^{L_1})\right]$$
   $$\tilde{u}_2^{n^L} + \Delta u^{L_2} = a_2 + b_2 + \beta_{21}\left[(\tilde{u}_1^{n^L} + \Delta u^{L_1}) - (\tilde{u}_2^{n^L} + \Delta u^{L_2})\right]$$
   Note that $\tilde{u}_2^{n^L} = a_1 + b_1$,and rearranging
   $\Delta u^{L_1}(1+\beta_{12}) - \beta_{12}\Delta u^{L_2} = \beta_{12}(\tilde{u}_2^{n^L} - \tilde{u}_1^{n^L})$
   $-\beta_{21}\Delta u^{L_1} - \Delta u^{L_2}(1+\beta_{21}) = \beta_{21}(\tilde{u}_1^{n^L} - \tilde{u}_2^{n^L})$
   $$\begin{vmatrix} (1+\beta_{12}) & -\beta_{12} \\ -\beta_{21} & (1+\beta_{21}) \end{vmatrix} \begin{vmatrix} \Delta u^{L_1} \\ \Delta u^{L_2} \end{vmatrix} = \begin{vmatrix} \beta_{12}(\tilde{u}_2^{n^L} - \tilde{u}_1^{n^L}) \\ \beta_{21}(\tilde{u}_1^{n^L} - \tilde{u}_2^{n^L}) \end{vmatrix}$$

4. Solve for Δu^{L_1} and add it to $\tilde{u}_m^{n^L}$ to get $u_m^{n+1^L}$

Solving for the Face centered velocities with an implicit solve

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 $\theta = \frac{\rho_m}{\rho_m^o} = \nu_m^o$ 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
   $$\tilde{u}_1^{n^{*f}} + \Delta u_1^{*f} = a_1 - b_1 \nabla^f P_{eq} + \beta_{12} \left[(\tilde{u}_2^{n^{*f}} + \Delta u_2^{*f}) - (\tilde{u}_1^{n^{*f}} + \Delta u_1^{*f}) \right] + c$$
   $$\tilde{u}_2^{n^{*f}} + \Delta u_2^{*f} = a_2 - b_2 \nabla^f P_{eq} + \beta_{21} \left[(\tilde{u}_1^{n^{*f}} + \Delta u_1^{*f}) - (\tilde{u}_2^{n^{*f}} + \Delta u_2^{*f}) \right] + c$$
   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 Δu_1^{*f} and add it to $\tilde{u}_m^{n^{*f}}$ to get $(u)_m^{n+1^{*f}}$