Uintah:ICE Multi-material code

- **Equation of state,** p^{n+1}, θ^{n+1}

- **Calculate the chemistry effects, phase change and energy release,** (explicit)

- **Solve the "pressure equations" for** $\vec{U}^{{n+1}^{*^f}}, \Delta p^{{n+1}^{c}}, p^{{n+1}^{*^f}}$ (implicit, approximate projection method)

- **Evaluate the pressure acceleration, body forces and stresses,** (explicit). **For multiple materials, calculate the momentum and energy exchange,** (implicit). **Add the Lagrangian effects into** $\vec{U}_m^{{n+1}^L}, T_m^{{n+1}^L}, \rho_m^{{n+1}^L}$

- **Advect** $\vec{U}_m^n,\ T_m^n,\ \rho_m^n$

- **Advance in time** $\rho_m^{{n+1}^C},\ \vec{U}_m^{{n+1}^C}, T_m^{{n+1}^C}$

The steps for a single time step are:

1. **Calculate the cell-centered pressure using the equation of state**, p^{n+1}, θ_m^{n+1}

2. **Calculate effects of a chemical reaction, phase change and energy release**, $\langle m_m^n \dot{\alpha_m} \rangle, \langle m_m^n \vec{U}_m^n \dot{\alpha_m} \rangle, \langle m_m^n e_m^n \dot{\alpha_m} \rangle$

3. **Solve the "pressure equations" for $\Delta p^{{n+1}^c}$. Using $\Delta p^{{n+1}^c}$ calculate the cell-centered velocity of material m, $U_m^{n^c}$ to the face-center $U_m^{*^f}$**

$$\vec{U}^{{n+1}^{*^f}} = \overbrace{\frac{(\rho\vec{U})^{n^f}}{\rho^{n^f}}}^{\text{(Cell-centered data from adjacent cells interpolated to the face center)}} - \overbrace{\frac{\Delta t}{\rho^{n^f}} \nabla^f (p^{n^c} + \Delta p^{{n+1}^c})}^{\text{(Linear approximation to the time advance pressure)}} + \overbrace{\vec{g}\Delta t}^{\text{(body force term)}}$$

$+$ Multimaterial coupling term

4. **Calculate the face-centered pressure $p^{*^{n^f}}$ at each of the faces with the surrounding cell-centered pressures.**

$$p^{*^f} = \frac{\frac{p^c_{I+1}}{\rho^c_{I+1}} + \frac{p^c_I}{\rho^c_I}}{\frac{1}{\rho^c_I} + \frac{1}{\rho^c_{I+1}}}$$

5. **With the face-centered U_m^f ,$p^{n^{*f}}$ calculate the source terms for the energy and momentum equations.**

Mass source/sink term

$$\Delta(m_m)^{n+1} = \Delta t\langle m_m^n \dot{\alpha_m}\rangle$$ (source of mass resulting from phase change)

Velocity source/sink terms

$$\frac{\Delta(m_m\vec{U}_m)^{n+1}}{m_m^{n+1^L}} = \frac{\Delta t\langle m_m^n \vec{U}_m^n \dot{\alpha_m}\rangle}{m_m^{n+1^L}}$$ (net source of m momentum due to m mass conversion)

$$+ \frac{V^n \vec{g}\Delta t}{V_m^{n+1^L}}$$ (acceleration due to gravity)

$$- \frac{\upsilon_m \Delta t \int_A p^{n+1^{*f}}\, d\vec{S}}{V_m^{n+1^L}}$$ (acceleration due to the equilibration pressure)

$$+ \frac{\upsilon_m \theta_l \Delta t V^n K(\vec{U}_l^{n^L} - \vec{U}_m^{n^L})}{V_m^{n+1^L}}$$ (interactions between materials m and l. For a single fluid this term =0)

$$+ \frac{\Delta t \int_A \tau_m^f \cdot d\vec{S}}{m_m^{n+1^L}}$$ (acceleration due to material stresses)

$+$ other terms

Energy Source Terms

$$\frac{\Delta(m_m e_m)^{n+1}}{m_m^{n+1^L}} = \frac{\Delta t\langle m_m^n e_m^n \dot{\alpha_m}\rangle}{m_m^{n+1^L}}$$ (source/sink of k internal energy due to mass conversion)

$$+ \frac{(\frac{\upsilon_m}{c_m})^2 (p_m^o \Delta p^{n+1^c})}{V_m^{n+1^L}}$$

$$+ \frac{\upsilon_k \theta_l \Delta t V_m^n R(T_l^{n^L} - T_m^{n^L})}{V_m^{n+1^L}}$$ (Energy exchange between materials. For a single material this = 0)

$+$ other terms

6. **Calculate the Lagrangian values**

Lagrangian Volume:

$$V_m^{n+1^L} = V^n + \Delta t \sum_i^{cell\ faces} (\vec{S} \cdot \vec{U}^{n+1^{*^f}})_i$$

Lagrangian Mass:

$$\rho_m^{n+1^L} = \frac{\rho_m^n V_m^n + \overbrace{\Delta(m_m)^{n+1}}^{\text{source/sink due to phase change}}}{V_m^{n+1^L}}$$

$$m_m^{n+1^L} = \rho_m^{n+1} V_m^{n+1^L}$$

Lagrangian Velocity:

Note: in the source/sink of this equation there is a exchange term which contains the $\vec{U}_m^{n+1^L}$. This must be solved for implicitly.

$$\vec{U}_m^{n+1^L} = \vec{U}_m^n [1 - \frac{\overbrace{\Delta m_m{}^{n+1}}^{\text{source/sink due to phase change}}}{m_m^{n+1^L}}] + \frac{\overbrace{\Delta(m_m \vec{U}_m)^{n+1}}^{\text{source/sink}}}{m_m^{n+1^L}}$$

Lagrangian Temperature:

Note: in the source/sink of this equation there is a exchange term which contains the $T_m^{n+1^L}$. This must be solved for implicitly.

$$T_m^{n+1^L} = T_m^n [1 - \frac{\overbrace{\Delta(m_m e_m)^{n+1}}^{\text{source/sink due to phase change}}}{c_v m_m^{n+1^L}}] + \frac{\overbrace{\Delta(m_m e_m)^{n+1}}^{\text{source/sink}}}{c_v m_m^{n+1^L}}$$

7. **Advection of ρ_m^n,$\vec{U}_m^n$, T_m^n**

8. **Finally, calculate the time advanced quanties for mass, velocity, and temperature.**

$$\rho_m^{n+1} = \frac{{\rho_m^{\mathrm{n+1}}}^L {V_m^{\mathrm{n+1}}}^L - \Delta t \mathsf{Advection}(\rho_m^n)}{V}, \tag{1}$$

$$\vec{U}_m^{n+1} = \frac{{\vec{U}_m^{\mathrm{n+1}}}^L {V_m^{\mathrm{n+1}}}^L - \Delta t \mathsf{Advection}(\vec{U}_m^n)}{V}, \tag{2}$$

$$T_m^{n+1} = \frac{{T_m^{\mathrm{n+1}}}^L {V_m^{\mathrm{n+1}}}^L - \Delta t \mathsf{Advection}(T_m^n)}{V} \tag{3}$$