I C E, explicit pressure, single material 11/7/14

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

2. Compute the pressure using an equation of state (ideal Gas).

   $P_{eq} = (\gamma - 1)C_v\rho T$

   $c = \sqrt{\frac{dP}{d\rho} + \frac{dP}{de}\frac{P_{eq}}{\rho^2}}$

   where $\frac{dP}{d\rho} = (\gamma - 1)C_v T$ and $\frac{dP}{de} = (\gamma - 1)\rho$

   set boundary conditions on P_{eq}

   Compute the compressibility $\kappa = \frac{v^o}{c^2}$

3. Compute the face-centered velocities

   $\vec{U}^{*^f} = \left\langle \frac{\rho\vec{U}}{\rho} \right\rangle^{n^f} - \frac{\Delta t}{<\rho^o>^f}\nabla^f P_{eq} + \Delta t\vec{g}$

   $= \frac{(\rho\vec{U})_R + (\rho\vec{U})_L}{\rho_R + \rho_L} - \Delta t\frac{2.0(v_L^o v_R^o)}{v_L^o + v_R^o}\left(\frac{P_{eq_R} - P_{eq_L}}{\Delta x}\right) + \Delta t\vec{g}$

   Set boundary conditions on $\vec{U}^{*^f}$

4. Compute the change in pressure ΔP

   $\Delta P = \frac{-\Delta t \quad \overbrace{\nabla \cdot \theta\vec{U}^{*^f}}^{\text{Advection}(\theta, \vec{U}^{*^f})}}{\kappa}$

   where $P^{n+1} = P_{eq} + \Delta P$ for a single material $\theta = 1.0$ Set boundary conditions on P^{n+1}

5. Compute the face centered pressure

   $P^{*^f} = \frac{\frac{P}{\rho} + \frac{P_{adj}}{\rho_{adj}}}{\frac{1}{\rho} + \frac{1}{\rho_{adj}}} = \frac{P\rho_{adj} + P_{adj}\rho}{\rho + \rho_{adj}}$

6. Accumulate sources of momentum and internal energy

   $\Delta(m\vec{U}) = -\Delta t V \nabla P^{*^f} + \nabla\cdot(\tau^{*^f}) + m\vec{g}\Delta t$

   $\Delta(me) = V\kappa P\Delta P - \nabla q^{*^f}$

   where $q^{*^f} = -k^f\nabla T$

7. Compute Lagrangian quantities

   $m^L = \rho V$

   $(m\vec{U})^L = (m\vec{U}) + \Delta(m\vec{U})$

   $(me)^L = (me) + \Delta(me)$

8. Advect and advance in time

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

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

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

9. Compute primitive Variables from n+1 conserved quantities

   $\rho^{n+1} = m^{n+1}/V$

   $\vec{U}^{n+1} = \frac{(m\vec{U})^{n+1}}{m^{n+1}}$

   $T^{n+1} = \frac{(me)^{n+1}}{m^{n+1}C_v}$

   Set boundary conditions on the primitive variables $(\vec{U}, \rho, T)$.

Advection Operator

The governing equation for the advection of q is

$$-\Delta t \text{Advection}((q), \vec{U}^{\text{n+1}^{*f}}) = -\sum_{outflux} \langle q \rangle_o \Delta V_o + \sum_{influx} \langle q \rangle_{in} \Delta V_{in},$$

where ΔV are the fluxed volumes into and out of cell i, j, k. This fluxed volume is the volume of material which passes through each cell face in Δt. The quantity q is ρ, $\rho\vec{u}$ or $\rho c_v T$ and the fluxes of q associated with fluxed volumes are determined using

$$\langle q \rangle = q_{ijk} + (\nabla q)_{ijk} \cdot \langle \mathbf{r_v} \rangle \tag{1}$$

where $\langle \mathbf{r_v} \rangle$ is the volume centroid of flux of volume ΔV. The angle brackets denote the average of the quantity over the fluxed volume at time t. The gradients shown in Eq.(1) are limited in a Van Leer fashion using

$$(\nabla q)_{ijk} = \alpha_{ijk} (\nabla q)_{ijk},$$

$$\alpha_{ijk} = min\left(1, \alpha_{max}, \alpha_{min}\right),$$

$$\alpha_{max} = max\left(0, \frac{\bar{q}_{max} - q_{ijk}}{max[q^v] - q_{ijk}}\right),$$

$$\alpha_{min} = max\left(0, \frac{\bar{q}_{min} - q_{ijk}}{min[q^v] - q_{ijk}}\right),$$

where $\bar{q}_{max}$, $\bar{q}_{min}$ are the max. and min. values of the surrounding cell-centered data. q^v are the values of q interpolated to the cell vertices using the linear expansion

$$q^v = q_{ijk} + (\nabla q)_{ijk} \cdot (\mathbf{r^v} - \mathbf{r_{ijk}}).$$