1 Overview of implicit ICE 12/14/05

–Compute $\vec{U}_m^{*f}$ (add Exchange contribution, set boundary conditions on $\vec{U}_m^{*f}$)

–Form RHS $B = -\text{Advection}\ (\theta_m \vec{U}_m^{*f})$

while $|\text{outer residual}| < \text{convergence criteria}$ **do**

–Compute A matrix

$$A_r = \frac{\Delta y \Delta z \Delta t^2}{\Delta x} \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle}\Bigg|_r \qquad A_l = \frac{\Delta y \Delta z \Delta t^2}{\Delta x} \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle}\Bigg|_l$$

$$A_t = \frac{\Delta x \Delta z \Delta t^2}{\Delta y} \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle}\Bigg|_t \qquad A_b = \frac{\Delta x \Delta z \Delta t^2}{\Delta y} \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle}\Bigg|_b$$

$$A_f = \frac{\Delta x \Delta y \Delta t^2}{\Delta z} \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle}\Bigg|_f \qquad A_{bk} = \frac{\Delta x \Delta y \Delta t^2}{\Delta z} \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle}\Bigg|_{bk}$$

$$A_p = V \sum_{m=1}^{N} \theta_m \kappa_m + (A_r + A_l + A_t + A_b + A_f + A_{bk})$$

–Solve for δP

–Update pressure $\Delta P = \sum_{n=1}^{iter} \delta P, \quad P = P^{Old} + \Delta P$, set boundary condition on P and δP

–Recompute $\vec{U}_m^{*f}$ (using δp), add Exchange contribution, set boundary conditions on $\vec{U}_m^{*f}$, compute $\langle \rho_m^o \rangle$)

–Form RHS $B = -V \sum_{m=1}^{N} \theta_m \kappa_m \Delta P - \sum_{m=1}^{N} \text{VAdvection}\ (\theta_m \vec{U}_m^{*f})$,

where outer residual = $Max(RHS), \kappa_m = \frac{v_m^o}{c_m^2}$

end while

2 Derivation of the matrix stencil

Step 1: Derive the implicit form of the pressure, starting with change equation

$$\frac{dP}{dt} = \frac{\sum_{m=1}^{N} \frac{\dot{m}}{V\rho_m^o} - \sum_{m=1}^{N} \nabla \cdot \widehat{\theta_m \vec{U}_m}^{*f}}{\sum_{m=1}^{N} \frac{\theta_m}{\rho_m^o c_m^2}} \tag{1}$$

and the face-centered velocity

$$\vec{U_m}^{*f} = \left\langle \frac{\rho_m \vec{U}_m}{\rho_m} \right\rangle - \frac{\Delta t}{\langle \rho_m^o \rangle} \nabla^f P^{\text{ iter}} + \text{Exchange term} + \Delta t \vec{g}$$

Write eq.1 in terms of $P^{\text{ iter}} = P^{\text{ iter}-1} + \delta P$, $\Delta P = P^{\text{ iter}} - P^{old}$

$$\sum_{m=1}^{N} \theta_m \kappa_m (P^{\text{ iter}} - P^{old}) = \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{V\rho_m^o} - \Delta t \nabla \cdot \widehat{\theta_m} \left(\left\langle \frac{\rho_m \vec{U}_m}{\rho_m} \right\rangle - \frac{\Delta t}{\langle \rho_m^o \rangle} \nabla^f P^{\text{ iter}} + \text{Exch} + \Delta t \vec{g} \right) \tag{2}$$

Substitite in for$P^{\text{ iter}} = P^{\text{ iter}-1} + \delta P$

$$\sum_{m=1}^{N} \theta_m \kappa_m ((P^{\text{ iter}-1} + \delta P) - P^{old}) = \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{V\rho_m^o} - \Delta t \nabla \cdot \widehat{\theta_m} \left(\left\langle \frac{\rho_m \vec{U}_m}{\rho_m} \right\rangle - \frac{\Delta t}{\langle \rho_m^o \rangle} \nabla^f (P^{\text{ iter}-1} + \delta P) + \text{Exch} + \Delta t \vec{g} \right)$$

Now factor out δP

$$\begin{aligned}\sum_{m=1}^{N} \theta_m \kappa_m \delta P - \Delta t^2 \nabla \cdot \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \nabla \delta P = \sum_{m=1}^{N} \theta_m \kappa_m (P^{\text{ iter}} - P^{old}) + \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{V\rho_m^o} \\ - \Delta t \nabla \cdot \sum_{m=1}^{N} \widehat{\theta_m} \overbrace{\left(\left\langle \frac{\rho_m \vec{U}_m}{\rho_m} \right\rangle - \frac{\Delta t}{\langle \rho_m^o \rangle} \nabla^f P^{\text{ iter}} + \text{Exch} + \Delta t \vec{g} \right)}^{\vec{U_m}^{*f}}\end{aligned}$$

The ODE we have to solve is

$$\sum_{m=1}^{N} \theta_m \kappa_m \delta P - \Delta t^2 \nabla \cdot \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \nabla \delta P = - \sum_{m=1}^{N} \theta_m \kappa_m (P^{\text{ iter}} - P^{old}) + \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{V\rho_m^o} - \Delta t \nabla \cdot \left(\sum_{m=1}^{N} \widehat{\theta_m \vec{U}_m}^{*f} \right)^{\text{iter}} \tag{3}$$

Step 2: Integrate eq. 3 over a cell volume

$$\int_V \sum_{m=1}^{N} \theta_m \kappa_m \delta P dV - \Delta t^2 \int_V \nabla \cdot \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \nabla \delta P dV = - \int_V \sum_{m=1}^{N} \theta_m \kappa_m (P^{\text{ iter}} - P^{old}) dV + \int_V \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{V \rho_m^o} - \Delta t \int_V \nabla \cdot \left(\sum_{m=1}^{N} \widehat{\theta_m \vec{U}_m}^{*f} \right)^{\text{iter}} dV$$

Invoke the divergence theorem $\int_V \nabla \cdot \vec{f} dV = \int_S \vec{f} \cdot d\vec{s}$ to convert the volume to surface integrals.

$$V \sum_{m=1}^{N} \theta_m \kappa_m \delta P - \Delta t^2 \int_S \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \nabla \delta P \cdot d\vec{s} = -V \sum_{m=1}^{N} \theta_m \kappa_m (P^{\text{ iter}} - P^{old}) + \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{\rho_m^o} - \Delta t \int_S \left(\sum_{m=1}^{N} \widehat{\theta_m \vec{U}_m}^{*f} \right)^{\text{iter}} \cdot d\vec{S}$$

Step 3: Write out the contributions for each face of the computational cell

$$\begin{aligned} \Delta t^2 \int_S \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \nabla \delta P \cdot d\vec{s} = \Delta t^2 \Bigg[& \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Bigg|_R \Delta y \Delta z \frac{(\delta P_R - \delta P)}{\Delta x} - \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Bigg|_L \Delta y \Delta z \frac{(\delta P - \delta P_L)}{\Delta x} \\ & + \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Bigg|_T \Delta x \Delta z \frac{(\delta P_T - \delta P)}{\Delta y} - \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Bigg|_B \Delta x \Delta z \frac{(\delta P - \delta P_B)}{\Delta y} \\ & + \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Bigg|_F \Delta x \Delta y \frac{(\delta P_F - \delta P)}{\Delta z} - \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Bigg|_{BK} \Delta x \Delta y \frac{(\delta P - \delta P_{BK})}{\Delta z} \Bigg] \end{aligned} \quad (4)$$

Form the stencil of Matrix A from eq. 4

$$A_{R/L} = \frac{\Delta y \Delta z \Delta t^2}{\Delta x} \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Bigg|_{R/L} \quad A_{T/B} = \frac{\Delta x \Delta z \Delta t^2}{\Delta y} \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Bigg|_{T/B} \quad A_{F/BK} = \frac{\Delta y \Delta x \Delta t^2}{\Delta z} \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Bigg|_{F/BK}$$

$$\begin{aligned} V \sum_{m=1}^{N} \theta_m \kappa_m \delta P - \Big[& A_R (\delta P_R - \delta P) - A_L (\delta P - \delta P_L) \\ & + A_T (\delta P_T - \delta P) - A_B (\delta P - \delta P_B) \\ & A_F (\delta P_F - \delta P) - A_{BK} (\delta P - \delta P_{BK}) \Big] = -V \sum_{m=1}^{N} \theta_m \kappa_m (P^{\text{ iter}} - P^{old}) + \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{\rho_m^o} - \Delta t \text{Advection} \left(\sum_{m=1}^{N} \widehat{\theta_m \vec{U}_m}^{*f} \right)^{\text{iter}} \end{aligned} \quad (5)$$

Factor out δP the equation (In impICE.cc we don't normalize by V to make it non-dimensional. We need to keep it dimensional for implicit AMRICE)

$$\left(V \sum_{m=1}^{N} \theta_m \kappa_m + \left[A_R + A_L + A_T + A_B + A_F + A_{BK} \right] \right) \delta p - \left[A_R \delta P_R + A_L \delta P_L + A_T \delta P_T + A_B \delta P_B + A_F \delta P_F + A_{BK} \delta P_{BK} \right] =$$

$$-V \sum_{m=1}^{N} \theta_m \kappa_m (P^{\text{ iter}} - P^{old}) + \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{\rho_m^o} - \Delta t V \text{Advection} \left(\sum_{m=1}^{N} \widehat{\theta_m \vec{U}_m}^{*f} \right)^{\text{iter}}$$

3 Nomenclature

Variable	Dimensions	Description
Δt	$[t]$	Timestep
ρ	$[M/L^3]$	Density of material
$\langle \rho_m^o \rangle$	$[M/L^3]$	Microscopic density at the face center
$\vec{U}$	$[L/t]$	Velocity vector
V	$[L^3]$	Cell Volume
P	$[M/L^2]$	Pressure
θ_m		volume fraction of material m
$\widehat{\theta_m}$		upwinded volume fraction
Superscript		
old		Previous timestep
n		Current timestep
$iter$		outer iteration number
Subscript		
m		Material index
o		Pure material
l, r, t, b, f, bk		Left, right, top and bottom, front and back cell faces
Misc		
$\langle \rangle$		value averaged to the face