1 Overview of implicit ICE 03/31/05

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

-Form RHS
$$B = -\beta (P^{\text{iter}} - P^{\text{old}}) - \sum_{m=1}^{N} \text{Advection } (\theta_m \vec{U_m}^{*f})$$

while |outer residual| < convergence criteria do

-Compute *A* matrix

$$\begin{aligned} A_{r} &= \frac{\Delta t^{2}}{\Delta x^{2}} \sum_{m=1}^{N} \frac{\widehat{\Theta_{m}}}{\langle \rho_{m}^{o} \rangle} \bigg|_{r} \quad A_{l} &= \frac{\Delta t^{2}}{\Delta x^{2}} \sum_{m=1}^{N} \frac{\widehat{\Theta_{m}}}{\langle \rho_{m}^{o} \rangle} \bigg|_{l} \\ A_{t} &= \frac{\Delta t^{2}}{\Delta y^{2}} \sum_{m=1}^{N} \frac{\widehat{\Theta_{m}}}{\langle \rho_{m}^{o} \rangle} \bigg|_{t} \quad A_{b} &= \frac{\Delta t^{2}}{\Delta y^{2}} \sum_{m=1}^{N} \frac{\widehat{\Theta_{m}}}{\langle \rho_{m}^{o} \rangle} \bigg|_{b} \\ A_{f} &= \frac{\Delta t^{2}}{\Delta z^{2}} \sum_{m=1}^{N} \frac{\widehat{\Theta_{m}}}{\langle \rho_{m}^{o} \rangle} \bigg|_{f} \quad A_{bk} &= \frac{\Delta t^{2}}{\Delta z^{2}} \sum_{m=1}^{N} \frac{\widehat{\Theta_{m}}}{\langle \rho_{m}^{o} \rangle} \bigg|_{bk} \\ A_{p} &= \beta + (A_{r} + A_{l} + A_{l} + A_{b} + A_{f} + A_{bk}) \end{aligned}$$

- –Solve for δP
- -Update pressure $P^{\text{iter}} = P^{\text{iter}-1} + \delta P$, set boundary condition on P^{iter}
- –Compute $\vec{U_m}^{*^f}$ (add Exchange contribution, set boundary conditions on $\vec{U_m}^{*^f}$, compute $\langle \rho_m^o \rangle$)

–Form RHS
$$B = -\beta(P^{\text{iter}} - P^{\text{old}}) - \sum_{m=1}^{N} \text{Advection } (\theta_m \vec{U_m}^{*f}),$$

where outer residual =
$$Max(RHS^2)$$
, $\beta = \sum_{m=1}^{N} \frac{\theta_m}{\rho_m^o c_m^2}$

end while

-Compute $\Delta P = P^{\text{iter}} - P^{Old}$

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 $P^{\text{iter}} = P^{\text{iter}-1} + \delta P$, $\Delta P = P^{\text{iter}} - P^{\text{old}}$ and $\beta = \sum_{m=1}^{N} \frac{\theta_m}{\rho_m^o c_m^2}$

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

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

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

Now factor out δP

$$\beta \delta P - \Delta t^{2} \nabla \cdot \sum_{m=1}^{N} \frac{\widehat{\Theta_{m}}}{\langle \rho_{m}^{o} \rangle} \nabla \delta P = \beta (P^{\text{iter}} - P^{old}) + \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{V \rho_{m}^{o}}$$
$$- \Delta t \nabla \cdot \sum_{m=1}^{N} \widehat{\Theta_{m}} \left(\left\langle \frac{\rho_{m} \vec{U}_{m}}{\rho_{m}} \right\rangle - \frac{\Delta t}{\langle \rho_{m}^{o} \rangle} \nabla^{f} P^{\text{iter}} + \text{Exch} + \Delta t \vec{g} \right)$$

The ODE we have to solve is

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

Step 2: Integrate eq. 3 over a cell volume

$$\begin{split} \int_{V} \beta \delta P dV - \Delta t^{2} \int_{V} \nabla \cdot \sum_{m=1}^{N} \frac{\widehat{\theta_{m}}}{\langle \rho_{m}^{o} \rangle} \nabla \delta P dV &= -\int_{V} \beta (P^{\text{iter}} - P^{old}) dV \\ &+ \int_{V} \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{V \rho_{m}^{o}} \\ &- \Delta t \int_{V} \nabla \cdot \left(\sum_{m=1}^{N} \widehat{\theta_{m}} \overrightarrow{U_{m}}^{*f} \right)^{\text{iter}} dV \end{split}$$

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.

$$\begin{split} V\beta\delta P - \Delta t^2 \int_{S} \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \nabla \delta P \cdot d\vec{s} &= -V\beta (P^{\text{iter}} - P^{old}) + \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{\rho_m^o} \\ - \Delta t \int_{S} \left(\sum_{m=1}^{N} \widehat{\theta_m} \vec{U_m}^{*f} \right)^{\text{iter}} \cdot d\vec{S} \end{split}$$

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

$$\Delta t^{2} \int_{S} \sum_{m=1}^{N} \frac{\widehat{\theta_{m}}}{\langle \rho_{m}^{o} \rangle} \nabla \delta P \cdot d\vec{s} = \Delta t^{2} \left[\sum_{m=1}^{N} \frac{\widehat{\theta_{m}}}{\langle \rho_{m}^{o} \rangle} \Big|_{R} \Delta y \Delta z \frac{(\delta P_{R} - \delta P)}{\Delta x} - \sum_{m=1}^{N} \frac{\widehat{\theta_{m}}}{\langle \rho_{m}^{o} \rangle} \Big|_{L} \Delta y \Delta z \frac{(\delta P - \delta P_{L})}{\Delta x} \right]$$

$$+ \sum_{m=1}^{N} \frac{\widehat{\theta_{m}}}{\langle \rho_{m}^{o} \rangle} \Big|_{T} \Delta x \Delta z \frac{(\delta P_{T} - \delta P)}{\Delta y} - \sum_{m=1}^{N} \frac{\widehat{\theta_{m}}}{\langle \rho_{m}^{o} \rangle} \Big|_{B} \Delta x \Delta z \frac{(\delta P - \delta P_{B})}{\Delta y}$$

$$+ \sum_{m=1}^{N} \frac{\widehat{\theta_{m}}}{\langle \rho_{m}^{o} \rangle} \Big|_{F} \Delta x \Delta y \frac{(\delta P_{F} - \delta P)}{\Delta z} - \sum_{m=1}^{N} \frac{\widehat{\theta_{m}}}{\langle \rho_{m}^{o} \rangle} \Big|_{BK} \Delta x \Delta y \frac{(\delta P - \delta P_{BK})}{\Delta z} \Big]$$

$$(4)$$

Form the stencil of Matrix A from eq. 4

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

$$V\beta\delta P - \Delta t^{2} \left[A_{R}(\delta P_{R} - \delta P) - A_{L}(\delta P - \delta P_{L}) + A_{T}(\delta P_{T} - \delta P) - A_{B}(\delta P - \delta P_{B}) \right]$$

$$+ A_{T}(\delta P_{T} - \delta P) - A_{B}(\delta P - \delta P_{B})$$

$$A_{F}(\delta P_{F} - \delta P) - A_{BK}(\delta P - \delta P_{BK}) = -V\beta(P^{\text{iter}} - P^{old}) + \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{\rho_{m}^{o}} - \Delta t \text{Advection} \left(\sum_{m=1}^{N} \widehat{\theta_{m}} \overrightarrow{U_{m}}^{*f} \right)^{\text{iter}}$$

$$+ \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{\rho_{m}^{o}} - \Delta t \text{Advection} \left(\sum_{m=1}^{N} \widehat{\theta_{m}} \overrightarrow{U_{m}}^{*f} \right)^{\text{iter}}$$

Factor out δP and divide by V to nondimensionalize the equation

$$\beta - \frac{\Delta t^2}{V} \left[A_R + A_L + A_T + A_B + A_F + A_{BK} \right] \delta p - \frac{\Delta t^2}{V} \left[A_R \delta P_R + A_L \delta P_L + A_T \delta P_T + A_B \delta P_B + A_F \delta P_F + A_{BK} \delta P_{BK} \right] = -\beta (P^{\text{iter}} - P^{\text{old}}) + \frac{\Delta t}{V} \sum_{m=1}^{N} \frac{\dot{m}}{\rho_m^o} - \frac{\Delta t}{V} \text{Advection} \left(\sum_{m=1}^{N} \widehat{\theta_m} \vec{U_m}^* \right)^{\text{iter}}$$

3 Nomenclature

<u>Variable</u>	<u>Dimensions</u>	Description
Δt	[t]	Timestep
ρ	$[M/L^3]$	Density of material
$\langle ho_m^o angle$	$[M/L^3]$	Microscopic density at the face center
$ec{U}$	[L/t]	Velocity vector
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
0		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