1   Overview of implicit ICE   12/16/03

while $|$outer residual$| <$ convergence criteria **do**

–Compute $\vec{U}_m^{*^f}$

–Add Exchange contribution to $\vec{U}_m^{*^f}$, compute $\langle \rho_m^o \rangle$

–Compute A matrix

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

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

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

$$A_p = \beta + (A_r + A_l + A_t + A_b + A_f + A_{bk})$$

where $\beta = \sum_{m=1}^{N} \frac{\theta_m}{\rho_m^o c_m^2}$

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

where outer residual $= Max(RHS^2)$

–Solve for δP

–Update pressure $P^{\text{iter}} = P^{\text{iter}-1} + \delta P$

end while

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

–Compute $\vec{U}_m^{*^f}$ include exchange (set boundary conditions on $\vec{U}_m^{*^f}$)

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

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

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

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

Now factor out δP

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

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

The ODE we have to solve is

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

Step 2: Integrate eq. 3 over a cell volume

$$\int_V \beta \delta P \, dV - \Delta t^2 \int_V \nabla \cdot \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \nabla \delta P \, dV = -\int_V \beta (P^{\text{iter}} - P^{old}) \, dV$$

$$+ \int_V \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{V \rho_m^o}$$

$$- \Delta t \int_V \nabla \cdot \left(\sum_{m=1}^{N} \widehat{\theta_m} \vec{U}_m^{*f} \right)^{\text{iter}} dV$$

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.

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

$$- \Delta t \int_S \left(\sum_{m=1}^{N} \widehat{\theta_m} \vec{U}_m^{*f} \right)^{\text{iter}} \cdot d\vec{S}$$

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

$$\Delta t^2 \int_S \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \nabla \delta P \cdot d\vec{s} = \Delta t^2 \left[\sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \right|_R \Delta y \Delta z \frac{(\delta P_R - \delta P)}{\Delta x} \quad - \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \right|_L \Delta y \Delta z \frac{(\delta P - \delta P_L)}{\Delta x}$$

$$+ \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Big|_T \Delta x \Delta z \frac{(\delta P_T - \delta P)}{\Delta y} \quad - \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Big|_B \Delta x \Delta z \frac{(\delta P - \delta P_B)}{\Delta y}$$

$$+ \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Big|_F \Delta x \Delta y \frac{(\delta P_F - \delta P)}{\Delta z} \quad - \sum_{m=1}^{N} \frac{\widehat{\theta_m}}{\langle \rho_m^o \rangle} \Big|_{BK} \Delta x \Delta y \frac{(\delta P - \delta P_{BK})}{\Delta z} \right] \qquad (4)$$

Form the stencil of Matrix A from eq. 4

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

$$V\beta \delta P - \Delta t^2 \left[A_R(\delta P_R - \delta P) - A_L(\delta P - \delta P_L) \right. \qquad (5)$$

$$+ A_T(\delta P_T - \delta P) - A_B(\delta P - \delta P_B)$$

$$\left. A_F(\delta P_F - \delta P) - A_{BK}(\delta P - \delta P_{BK}) \right] = -V\beta(P^{\text{iter}} - P^{old}) + \Delta t \sum_{m=1}^{N} \frac{\dot{m}}{\rho_m^o} - \Delta t \, \text{Advection} \left(\sum_{m=1}^{N} \widehat{\theta_m} \vec{U}_m^{*f} \right)^{\text{iter}}$$

Factor out δP and divide by V to nondimensionalize the equation

$$\beta - \frac{\Delta t^2}{V} \left[A_R + A_L + A_T + A_B + A_F + A_{BK} \right] \delta p - \frac{\Delta t^2}{V} \left[A_R \delta P_R + A_L \delta P_L + A_T \delta P_T + A_B \delta P_B + A_F \delta P_F + A_{BK} \delta P_{BK} \right] =$$

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

3

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
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