1 Overview of implicit ICE 10/04/04

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

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

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

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

–Compute A matrix

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

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

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

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

–Solve for δP

–Update pressure $P^{\text{ iter}} = P^{\text{ iter}-1} + \delta P$, set boundary condition on $P^{\text{ iter}}$

end while

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

–Compute $\vec{U}_m^{*f}$ add exchange contribution, 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 $\beta = \sum_{m=1}^{N} \frac{\theta_m}{\rho_m^o c_m^2}$

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

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

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

Now factor out δP

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

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

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

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

Form the stencil of Matrix A from eq. 4

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

$$V\beta\delta P - \Delta t^2\Big[A_R(\delta P_R-\delta P) - A_L(\delta P-\delta P_L) \quad (5)$$
$$+A_T(\delta P_T-\delta P) - A_B(\delta P-\delta P_B)$$
$$A_F(\delta P_F-\delta P) - A_{BK}(\delta P-\delta P_{BK})\Big] = -V\beta(P^{\,\text{iter}}-P^{old}) + \Delta t\sum_{m=1}^{N}\frac{\dot{m}}{\rho_m^o} - \Delta t\,\text{Advection}\left(\sum_{m=1}^{N}\widehat{\theta_m\vec{U}_m}^{*f}\right)^{\text{iter}}$$

Factor out δP and divide by V to nondimensionalize the equation

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

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
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