

1 Overview of implicit ICE 10/27/05

–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 |outer residual| < convergence criteria **do**

–Compute A matrix

$$\begin{aligned} A_r &= \frac{\Delta t^2}{\Delta x^2} \sum_{m=1}^N \frac{\widehat{\theta}_m}{\langle \rho_m^o \rangle} \Big|_r & A_l &= \frac{\Delta t^2}{\Delta x^2} \sum_{m=1}^N \frac{\widehat{\theta}_m}{\langle \rho_m^o \rangle} \Big|_l \\ A_t &= \frac{\Delta t^2}{\Delta y^2} \sum_{m=1}^N \frac{\widehat{\theta}_m}{\langle \rho_m^o \rangle} \Big|_t & A_b &= \frac{\Delta t^2}{\Delta y^2} \sum_{m=1}^N \frac{\widehat{\theta}_m}{\langle \rho_m^o \rangle} \Big|_b \\ A_f &= \frac{\Delta t^2}{\Delta z^2} \sum_{m=1}^N \frac{\widehat{\theta}_m}{\langle \rho_m^o \rangle} \Big|_f & A_{bk} &= \frac{\Delta t^2}{\Delta z^2} \sum_{m=1}^N \frac{\widehat{\theta}_m}{\langle \rho_m^o \rangle} \Big|_{bk} \\ A_p &= \sum_{m=1}^N \theta_m \kappa_m + (A_r + A_l + A_t + A_b + A_f + A_{bk}) \end{aligned}$$

–Solve for δP

–Update pressure $\Delta P = \sum_{n=1}^{iter} \delta P$, $P = P^{Old} + \Delta P$, 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 $B = -\sum_{m=1}^N \theta_m \kappa_m \Delta P - \sum_{m=1}^N \text{Advection}(\theta_m \vec{U}_m^{*f})$,

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

end while

2 Derivation of the matrix stencil

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

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

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 $P^{\text{iter}} = P^{\text{iter}-1} + \delta P$, $\Delta P = P^{\text{iter}} - P^{\text{old}}$

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

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

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

Now factor out δP

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

The ODE we have to solve is

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

Step 2: Integrate eq. 3 over a cell volume

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

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.

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

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

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

Form the stencil of Matrix A from eq. 4

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

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

Factor out δP and divide by V to nondimensionalize the equation

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

3 Nomenclature

<u>Variable</u>	<u>Dimensions</u>	<u>Description</u>
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
<u>Superscript</u>		
old		Previous timestep
n		Current timestep
$iter$		outer iteration number
<u>Subscript</u>		
m		Material index
o		Pure material
l, r, t, b, f, bk		Left, right, top and bottom, front and back cell faces
<u>Misc</u>		
$\langle \rangle$		value averaged to the face