Multi-Material Uintah:ICE

Todd Harman

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Contents

Nomenclature

Variable	Dimensions	Description
α_m		Volume fraction of material m, $\frac{V_k}{V}$
$\dot{\alpha}_m$	$[1/t]$	time rate of change of volume fraction of material m
c_m	$[L/t]$	Speed of sound of material m
Δt	$[t]$	Time increment
υ	$[L^3/M]$	Specific volume $\frac{1}{\rho}$
ρ	$[M/L^3]$	Density of material
T	$[T]$	Temperature
E	$[ML^2/t^2T]$	Total energy
e	$[L^2/t^2]$	Internal energy $(c_v T)$ of the material per unit mass
V	$[L^3]$	Volume
$\vec{U}$	$[L/t]$	Velocity vector
c_v	$[L^2/t^2]$	Constant volume specific heat
$\vec{S}_i$	$[L^2]$	Surface vector of side i (area * outward normal)
p	$[M/L^2]$	Pressure
K	$[M/L^3t]$	Momentum exchange coefficient
R	[??]	Heat exchange coefficient between materials
θ_m		Expected volume fraction of material m
$u,\ v,\ w$	$[L/t]$	x, y, z velocity components
$\vec{g}$	$[L/t^2]$	Gravity
Δx	$[L]$	Size of grid cell in x-direction
Δy	$[L]$	Size of grid cell in y-direction
Δz	$[L]$	Size of grid cell in z-direction
γ		Ratio of specific heats for a ideal gas
ε		Rate of strain tensor
q		Dummy variable
d		Dummy variable

Superscript		
n		Current time step
$*$		Quantities that have been interpolated from the cell-center to the face-center
L		Lagrangian values
c		Cell-centered quantity
f		Face-centered quantity
v		Vertex location
e		Edge location
$\prime$		Instantaneous value

Subscript		
m		Material type
o		Pure material
i,j,k		Grid indices in the x, y and z direction
L,R		Left and Right cell faces
T,B		Top and bottom cell faces
FR,BK		Front and back cell faces

Caveat Emptor

This document provides details on the main algorithmic steps in Uintah:ICE. However, as with most documentation, it is out of date, missing key steps and incorrect with certain details. Specifically, it is missing the evolution equation for the specific volume, provides a poor description of the solution of the time advanced pressure and the discretized equations for advection are incorrect. Uintah:ICE does not use corner coupling volumes in the advection routines. This document is still very useful and provides the reader with a basis of the algorithm.

Introduction

The purpose of this report is to give the reader a complete description of the governing equations and numerical techniques used in the single material version of the Uintah ICE CFD code. In essence, this document is a regurgitation and clarification of the algorithm and discussion from Kashiwa et al. (1994) and the relevant references Kashiwa (1987), Kashiwa and Rauenzahn (1994), Kashiwa (1999). This document is broken down into three main parts. In the first section the starting equations and assumptions used in this development are stated. The second part contains a description of the algorithm at the continuum level and in the final section is the discretized equations that will be coded.

The ICE method is a compressible, conservative, finite volume technique with all of the principal variables $(T,\ p,\ m,\ \vec{U}\ldots)$ located at the cell-center. The state variables are the total mass, momentum and total energy of each of the different materials $(m_m,\ (m_m\vec{U}_m),\ E_m)$. Finite volume techniques have the advantage over finite difference methods since the conservation of mass, momentum and internal energy is guaranteed within a single cell. With a conservative formulation no special treatment is need to take care of shock waves. To satisfy the conservation equations, the flux of mass, momentum and energy is needed across each face of the cell. As a result, velocity and pressure must be interpolated from the cell-center out to the face-center. The calculation of the auxiliary quantities is where this implementation of the ICE method differs from the more traditional staggered-grid ICE method.

Part 1: Starting equations

We begin by simply stating the governing equations for the mass, momentum and energy for a compressible multimaterial flow as shown in Kashiwa and Rauenzahn (1994). Although the multimaterial equations are listed, we are only concerned with a subset of these equations, namely the single material case.

Mass

$$\frac{\partial \rho_m}{\partial t} + \nabla \cdot \rho_m \vec{U}_m = \overbrace{\rho_o \dot{\alpha}_m}^{\text{Net source of } m \text{ mass}} \tag{1}$$

Momentum

$$\begin{aligned}\frac{\partial \rho_m \vec{U}_m}{\partial t} + \nabla \cdot \rho_m \vec{U}_m \vec{U}_m = &\overbrace{\rho_o \vec{U}_o \dot{\alpha}_m}^{\text{Net source of } m \text{ momentum due to mass conversion}} - \overbrace{\nabla \cdot (\alpha_m \rho_o \vec{U}'_m \vec{U}'_m)}^{\text{Multiphase Reynolds Stress}} - \overbrace{\theta_m \nabla p}^{\text{Acceleration by the equilibration pressure}} \\ &+ \underbrace{\rho_m \vec{g}}_{\text{Gravitational body force}} - \underbrace{\nabla \theta_m (p_m^o - p)}_{\text{Acceleration by the non-equilibrium pressure}} + \underbrace{\nabla \cdot (\alpha_m \tau_o)}_{\text{Acceleration due to average material stress}} \\ &+ \underbrace{(p_o - p)I - \tau_o \cdot \nabla \alpha_m}_{\text{Momentum exchange}}\end{aligned} \tag{2}$$

where the momentum exchange term can be modeled by

$$\sum_l \theta_m \theta_l K_{m,l} (\vec{U}_l - \vec{U}_m) \tag{3}$$

Energy

$$\begin{aligned}\frac{\partial \rho_m e_m}{\partial t} + \nabla \cdot \rho_m e_m \vec{U}_m = &\overbrace{\rho_o e_m \dot{\alpha}_m}^{\text{Net source of } m \text{ energy due to mass conversion}} - \overbrace{\nabla \cdot (\alpha_m \rho_o e_o \vec{U}'_m)}^{\text{Multiphase fluctuational transport of energy}} - \overbrace{p_m \nabla \cdot \vec{U}^f}^{\text{Average multiphase work}} \\ &+ \underbrace{\alpha_m \gamma_o^{-1} (\dot{p_o - p})}_{\text{Fluctuational work}} + \underbrace{\frac{\alpha_m \tau_o : \varepsilon_o}{2}}_{\text{Average viscous dissipation}} - \underbrace{\nabla \cdot \alpha_m q_o}_{\text{Thermal transport by conduction}} + \underbrace{q_o \nabla \alpha_m}_{\text{Energy exchange by conduction}}\end{aligned} \tag{4}$$

where energy exchange by conduction term can be modeled by

$$\sum_l \theta_m \theta_l R_{m,l} (T_l - T_m) \tag{5}$$

Additional relations include

$$\theta_m = \rho_m \upsilon_m$$

$$1-\sum_m \rho_m \upsilon_m = 0$$
$$p_m = \theta_m p$$
$$p_m = \theta_m p_m^o$$
$$\dot{p^{n^c}} = -(\rho c^2)\nabla\cdot\vec{U}^{n+1^{*f}} \tag{6}$$

Assumptions used

Below is a list of the assumptions used in the integration and the discretization of the governing equations.

1. To simplify the problem, the terms related to the multiphase Reynolds stress and nonequilibrium pressure in the momentum equations are assumed to be zero.
2. The multiphase fluctuational transport of internal energy, fluctuational work, average viscous dissipation, and thermal transport by conduction terms in the energy equation $= 0$.
3. The mesh is a structured grid.
4. The mesh velocity $\vec{U}_{mesh} = 0$.
5. The fluid is a perfect fluid $\frac{\partial p}{\partial \rho} |_s = c^2$.
6. The mesh spacing $\Delta x,\ \Delta y,\ \Delta z$ is constant.
7. The ratio of specific heats γ is constant.
8. Inside of a cell volume $\rho_m, \vec{U}_m, \dot{\alpha_m}\ \upsilon_m, p_m^o, \dot{p}$ are assumed to be constant. See the appendix for the impact of this assumption on the integration of the mass momentum and energy source terms.
9. The time derivatives are represented by first-order finite difference representations.

Part II: Algorithm description at the continuum level

In this section the basic algorithm for solving the time advanced quantities is presented to give the reader an overview of the solution procedure. A small note on notation, superscripts c and f represent cell-centered and face-centered quantities respectively. The steps for the solution of a single time step consist of the following

1. Use the equation of state to calculate p at the cell center (explicit)

2. Calculate the fluxing velocity $\vec{U}^{n+1^{*f}}$ and a linear approximation to the pressure $p^{n+1^{L^c}}$ using the approximate projection method of Casulli and Greenspan (1984) This entails calculating the change in the equilibration pressure Δp^{n+1^c} (pointwise implicit).

3. Determine the face-centered pressure $p^{n+1^{*f}}$ (explicit).

4. Using Δp^{n+1^c} and $p^{n+1^{*f}}$ calculate the source terms (Δ) of momentum and energy. In the single material case this is explicit.

5. Determine the Lagrangian values $m^{n+1^L}, (m\vec{U})^{n+1^L}, e^{n+1^L}$, using the results of step 4.

6. Calculate the advection of $m, (m\vec{U}), (mc_vT)$ with the fluxing velocity $\vec{U}^{n+1^{*f}}$ (explicit)

7. Finally, update quantities for mass, momentum and energy (explicit).

in other words

1. Use EOS to get p at the cell center.

2. Use Euler's equation thingy to solve for the n+1 Lagrangian pressure (cell centered) and the $n+1$ face centered fluxing velocity.

3. Compute face centered pressure using the continuity of acceleration principle.

4. Compute sources of mass, momentum and energy. For the mass, this consists of mass conversion from other types. For momentum, there are momentum sources due to mass conversion, gravity, pressure, divergence of the stress and momentum exchange.

5. Compute Lagrangian values for volume, mass, momentum and energy. "Lagrangian" values are the sum of the time n values and the sources computed in 4.

6. Compute the advection of mass, momentum and energy. These quantities are advected using the face centered fluxing velocities from 2.

7. Compute time advanced values for mass, momentum and energy. "Time advanced" means the sum of the "Lagrangian" values, found in 5, and the advection contribution, from 6.

The steps for one time step will now be discussed in reverse order in the same fashion as Kashiwa et al. (1994).

Step: 1 Equation of state

In order to close the system of equations we need to establish relations between the thermodynamic variables (p, ρ, T, e, h) as well as to relate the transport properties (μ, k) to the thermodynamic variables. For example, for a compressible flow there are three momentum equations, a continuity equation and an energy equation that need to be solved. These equations contain seven unknowns ρ, p, e, T, u, v, w provided that the transport coefficients μ, k can be related to the thermodynamic properties in the list of unknowns Tannehill, Anderson, and Pletcher (1997). It is obvious that two additional equations are needed to close the system of equations. These two additional equations are obtained by determining relations that exist between the thermodynamic variables. For most problems it is possible to assume a perfect gas which obeys,

$$p = \rho R T \tag{7}$$

where R is the gas constant. For a calorically perfect gas, constant specific heats, the following relations exist:

$$e = c_v T \quad h = c_p T \quad \gamma = \frac{c_p}{c_v} \quad c_v = \frac{R}{\gamma - 1} \quad c_p = \frac{\gamma R}{\gamma - 1} \tag{8}$$

For constant specific heats and a ideal gas the equations of state are

$$p = (\gamma - 1)\rho e \qquad T = \frac{(\gamma - 1)}{R} \tag{9}$$

Step: 2 Fluxing Velocity $(\vec{U}^{n+1^{*f}})$ and approximate pressure $(p^{n+1^{L^c}})$

To calculate the Lagrangian volume and the advection of mass, momentum and energy we need the face-centered fluxing velocity. Additionally, we also need $p^{n+1^{*f}}$ and Δp^{n+1^c} to calculate some of the source terms in the momentum and energy equations. The governing equation for the fluxing or face-centered velocity is the solution to the reduced Lagrangian momentum equation at the cell face, at time $t^n + \Delta t$ (Kashiwa et al. 1994).

$$(m \dot{\vec{U}}^f) = \frac{\Delta (m\vec{U})^f}{\Delta t} = -V \nabla p^c + m\vec{g}$$

discretizing in time

$$\frac{m^{n+1^{*f}} \vec{U}^{n+1^f} - m^{n^f} \vec{U}^{n^f}}{\Delta t} = -V^{n^f} \nabla^f p^{n+1^{L^c}} + m^{n^f} \vec{g} \tag{10}$$

Using assumption 9 to eliminate the density in the last term of eq. (10) and solving for $\vec{U}^{n+1^{*f}}$, we get eq. 4.9 of Kashiwa et al. (1994).

$$\vec{U}^{n+1^{*f}} = \overbrace{\frac{(\rho\vec{U})^{n^f}}{\rho^{n^f}}}^{\text{(Cell-centered data from adjacent cells interpolated to the face center)}} - \overbrace{\frac{\Delta t}{\rho^{n^f}} \nabla^f p^{n+1^{L^c}}}^{\text{(pressure gradient)}} + \overbrace{\vec{g}\Delta t}^{\text{(body force)}} \tag{11}$$

In order to compute the pressure gradient term of eq. (11) we need an expression for the cell-centered pressure $p^{n+1^{L^c}}$ at time $n+1$. As prescribed by Kashiwa et al. (1994) we turn to the pressure equation for a single ideal fluid,

$$(\dot{p}^{n+1^c}) = \frac{\Delta p^{n+1^c}}{\Delta t} = -(\rho^c c^2) \nabla \cdot \vec{U}^{n+1^{*f}} \tag{12}$$

Solution strategy

To solve eqs. (11-12) we will employ a preconditioned conjugate gradient technique with a multigrid preconditioner. This method solves a generalized Poissons equation that is obtaind by combining eqs. (11 - 12)

$$\left[\frac{1}{\rho \Delta t c^2} - \nabla^c \cdot \frac{\Delta t}{\rho^f} \nabla^f\right] \Delta p^{n+1^c} = -\nabla^c \cdot \hat{\hat{U}}^{n^f} \tag{13}$$

See the appendix for details.

Step: 3 Face-Centered Pressure $(p^{n+1^{*f}})$

Now we will calculate the last auxiliary quantity $p^{n+1^{*f}}$, the face-centered pressure, by applying the "Continuity of Acceleration" along a line normal to the cell face of interest, Kashiwa (1999). This is analogous to a constant heat flux at the interface of two materials. Suppose that we are interested in the face pressure between cell-center i and $i+1$ we can write the Lagrangian momentum equations

$$\left.\frac{\partial u^f}{\partial t}\right|_R = -\frac{1}{\rho}\left.\frac{\partial p}{\partial x}\right|_f + g_x \Delta t$$

$$\left.\frac{\partial u^f}{\partial t}\right|_L = -\frac{1}{\rho}\left.\frac{\partial p}{\partial x}\right|_f + g_x \Delta t$$

Note at the face between the two cells

$$\left.\frac{\partial u^f}{\partial t}\right|_R = \left.\frac{\partial u^f}{\partial t}\right|_L \tag{14}$$

In discretized form eq. (14) becomes

$$\frac{p^{*f} - p_i^c}{\rho_i^c (\Delta x/2)} = \frac{p_{i+1}^c - p^{*f}}{\rho_{i+1}^c (\Delta x/2)} \tag{15}$$

and solving for p^* we get

$$p^{*f} = \frac{\frac{p_{i+1}^c}{\rho_{i+1}^c} + \frac{p_i^c}{\rho_i^c}}{\frac{1}{\rho_i^c} + \frac{1}{\rho_{i+1}^c}} \tag{16}$$

For multiple materials the form is correct but there are some additional terms.

Step: 4 Source/Sink Terms

The source/sink terms (Δ), shown in eqs. (33 - 35) represents the right hand side of the conservation equations for mass, momentum and energy. It should be emphasized that the superscript f and c represents values residing on the cell-face and cell-center of the control volume respectively. The source terms are

Mass source/sink term

$$\Delta(m_m)^{n+1} = \Delta t \langle m_m^n \dot{\alpha}_m \rangle \quad \text{source of mass resulting from the conversion from other mass types} \tag{17}$$

Momentum source/sink terms

$$\begin{aligned}
\Delta(m_m \vec{U}_m^n)^{n+1} =& \Delta t \langle m_m^n \vec{U}_m^n \dot{\alpha}_m \rangle && \text{net source of } m \text{ momentum due to } m \text{ mass conversion} && (18)\\
& + m_m^n \vec{g} \Delta t && \text{gravity} && (19)\\
& - \Delta t \int_A \theta_m p^{n+1^{*f}} \, d\vec{S} && \text{equilibration pressure} && (20)\\
& + \Delta t V^n \sum_l \theta_m \theta_l K_{m,l} (\vec{U}_l^{n+1^L} - \vec{U}_m^{n+1^L}) && \text{interactions between materials } m \text{ and } l. \text{ For a single fluid this term} =0 && (21)\\
& + \Delta t \int_A \tau_m^f \cdot d\vec{S} && \text{material stresses} && (22)\\
& + \text{other terms}
\end{aligned}$$

For a single viscous compressible Newtonian fluid in cartesian coordinates the stress components are

$$\tau_{xx}^f = 2\mu \frac{\partial u^{n^c}}{\partial x} - \frac{2}{3}\mu(\nabla \cdot \vec{U}^{n^c}) \tag{23}$$

$$\tau_{yy}^f = 2\mu \frac{\partial v^{n^c}}{\partial y} - \frac{2}{3}\mu(\nabla \cdot \vec{U}^{n^c}) \tag{24}$$

$$\tau_{zz}^f = 2\mu \frac{\partial w^{n^c}}{\partial z} - \frac{2}{3}\mu(\nabla \cdot \vec{U}^{n^c}) \tag{25}$$

$$\tau_{xy}^f = \tau_{yx}^f = \mu(\frac{\partial u^{n^c}}{\partial y} + \frac{\partial v^{n^c}}{\partial x}) \tag{26}$$

$$\tau_{yz}^f = \tau_{zy}^f = \mu(\frac{\partial v^{n^c}}{\partial z} + \frac{\partial w^{n^c}}{\partial y}) \tag{27}$$

$$\tau_{zx}^f = \tau_{xz}^f = \mu(\frac{\partial w^{n^c}}{\partial x} + \frac{\partial u^{n^c}}{\partial z}) \tag{28}$$

Energy Source Terms

$$\begin{aligned}
\Delta(m_m e_m)^{n+1} =& \Delta t \langle m_m^n e_m^n \dot{\alpha}_m \rangle && \text{source/sink of } m \text{ internal energy due to mass conversion} && (29)\\
& + \Delta t p_m^o \nabla \cdot \vec{U}^f && \text{Valid for perfect materials only There are issues with this term that are still not resolved} && (30)\\
& + \Delta t V^n \sum_l \theta_m \theta_l R_{m,l} (T_l^{n+1^L} - T_m^{n+1^L}) && \text{Energy exchange between materials. For a single material this} = 0 && (31)\\
& + \text{other terms} && && (32)
\end{aligned}$$

In the case of multiple materials the Lagrangian temperature and velocity is solved for in a pointwise implicit manner.

Step: 5 Lagrangian $\rho^L, (m\vec{U})^L, e^L$

The equations for calculating the Lagrangian contribution of the total mass, momentum, and energy are

Mass:

$$m_m^{n+1^L} = \rho_m^n V^n + \overbrace{\Delta(m_m)^{n+1}}^{\text{source/sink}} \tag{33}$$

Momentum:

$$(m\vec{U})_m^{n+1^L} = (m\vec{U})_m^n - \overbrace{\vec{U}_m^n \Delta(m_m)^{n+1}}^{\text{source/sink due to phase change}} + \overbrace{\Delta(m_m \vec{U}_m)^{n+1}}^{\text{source/sink}} \tag{34}$$

Energy: (The contribution from the kinetic energy is currently missing)

$$(me)_m^{L^{n+1}} = me_m^n - \overbrace{e_m^n \Delta(m_m)^{n+1}}^{\text{source/sink due to phase change}} + \overbrace{\Delta(m_m e_m)^{n+1}}^{\text{source/sink}} \tag{35}$$

where $e_m^n = (c_v T)_m^n$.

Step: 6 Advection Operator

The compatible advection operator comes exclusively from VanderHeyden and Kashiwa (1998). To begin the governing equation for the advection of q is

$$-\Delta t \text{Advection}((q), \vec{U}^{n+1^{*f}}) = -\sum_{outflux} \langle q \rangle_o \Delta V_o + \sum_{influx} \langle q \rangle_{in} \Delta V_{in}, \tag{36}$$

where ΔV are the fluxed volumes into and out of cell i, j, k. This fluxed volume is the volume of material which passes through each surface section in the time increment Δt. The quantity q can be either ρ, $\rho\vec{u}$ or $\rho c_v T$ and the fluxes of q associated with fluxed volumes are determined using

$$\langle q \rangle = q_{ijk} + (\nabla q)_{ijk} \cdot \langle \mathbf{r_v} \rangle \tag{37}$$

where $\langle \mathbf{r_v} \rangle$ is the volume centroid of flux of volume ΔV. The angle brackets denote the average of the quantity over the fluxed volume at time t. The gradients shown in eq. (37) are limited in a Van Leer fashion using

$$(\nabla q)_{ijk} = \alpha_{ijk} (\nabla q)_{ijk}, \tag{38}$$

$$\alpha_{ijk} = min\left(1, \alpha_{max}, \alpha_{min}\right), \tag{39}$$

$$\alpha_{max} = max\left(0, \frac{\bar{q}_{max} - q_{ijk}}{max[q^v] - q_{ijk}}\right), \tag{40}$$

$$\alpha_{min} = max\left(0, \frac{\bar{q}_{min} - q_{ijk}}{min[q^v] - q_{ijk}}\right), \tag{41}$$

where $\bar{q}_{max}$, $\bar{q}_{min}$ are the max. and min. values of the surrounding cell-centered data. q^v are the values of q interpolated to the cell vertices using the linear expansion

$$q^v = q_{ijk} + (\nabla q)_{ijk} \cdot (\mathbf{r^v} - \mathbf{r_{ijk}}). \tag{42}$$

Step: 7 Time Advanced

We will begin by examining the equations for the time advanced, mass, momentum and energy, see the appendix for the derivation.

$$m_m^{n+1} = m_m^{n+1^L} - \Delta t \text{Advection}(\rho_m^{n+1^L}, \vec{U}^{n+1^{*f}}) \tag{43}$$

$$(m\vec{U})_m^{n+1} = (m\vec{U})_m^{n+1^L} - \Delta t \text{Advection}((\rho\vec{U})_m^{n+1^L}, \vec{U}^{n+1^{*f}}) \tag{44}$$

$$(mc_vT)_m^{n+1} = (mc_vT)_m^{n+1^L} - \Delta t \text{Advection}((\rho c_v T)_m^{n+1^L}), \vec{U}^{n+1^{*f}}) \tag{45}$$

The Lagrangian values $\rho_m^{n+1^L}$, $V_m^{n+1^L}$, $(m\vec{U})_m^{n+1^L}$, $(mc_vT)_m^{n+1^L}$ in eqs. (43- 45) represent **all** of the physical changes inside of a control volume that are not accounted for by the advection operator. As a convention, we will think of these quantities as being determined at time $n+1$.

Part III: Discretized Equations

In this section the discretized governing equations are shown for a single compressible viscous fluid but before we proceed a small note on notation. The indices used to denote the x, y and z direction are i, j and k respectively, and the fourth index represents the face of interest. The grid layout in 2 and 3-dimensions is shown in fig. 1. For example the y-component of the face-centered velocity across the top face of cell i, j, k is $v^{*f}_{i,j,k,t}$ Additionally, there are two layers of ghost cells that surround the domain.

Step: 1 Discretized Equation of state

If the energy equation is not included then the discretized equations of state is

$$\rho_{i,j,k} = \frac{p_{i,j,k}}{RT_{i,j,k}} \tag{46}$$

where R is the gas constant. For constant specific heats and a ideal gas the equations of state are

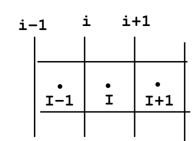
$$p^{n}_{i,j,k} = (\gamma - 1)\rho^{n^c}_{i,j,k} e^{n^c}_{i,j,k} \qquad T^{n^c}_{i,j,k} = \frac{(\gamma-1)e^{n^c}_{i,j,k}}{R} \tag{47}$$

Step: 2a Discretized Face-centered Velocity $\vec{U}^{n+1^{*f}}$

The discretized form of the face-centered velocity eq. (11) in the x, y and z directions is

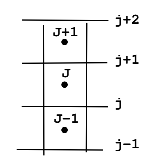
<u>x-component</u>

$$u^{n+1^{*f}}_{i,j,k,L} = \frac{(\rho u^{n^c})_{i-1,j,k} + (\rho u^{n^c})_{i,j,k}}{\rho^{n^c}_{i-1,j,k} + \rho^{n^c}_{i,j,k}} - \frac{2\Delta t\left(p^{n+1^{L^c}}_{i,j,k} - p^{n+1^{L^c}}_{i-1,j,k}\right)}{\Delta x(\rho^{n^c}_{i-1,j,k} + \rho^{n^c}_{i,j,k})} + g_x \Delta t$$



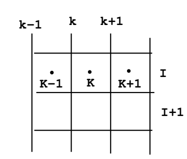
<u>y-component</u>

$$v^{n+1^{*f}}_{i,j,k,B} = \frac{(\rho v^{n^c})_{i,j,k} + (\rho v^{n^c})_{i,j-1,k}}{\rho^{n^c}_{i,j,k} + \rho^{n^c}_{i,j-1,k}} - \frac{2\Delta t\left(p^{n+1^{L^c}}_{i,j,k} - p^{n+1^{L^c}}_{i,j-1,k}\right)}{\Delta y(\rho^{n^c}_{i,j,k} + \rho^{n^c}_{i,j-1,k})} + g_y \Delta t$$



<u>z-component</u>

$$w^{n+1^{*f}}_{i,j,k,BK} = \frac{(\rho w^{n^c})_{i,j,k-1} + (\rho w^{n^c})_{i,j,k}}{\rho^{n^c}_{i,j,k-1} + \rho^{n^c}_{i,j,k}} - \frac{2\Delta t\left(p^{n+1^{L^c}}_{i,j,k} - p^{n+1^{L^c}}_{i,j,k-1}\right)}{\Delta z(\rho^{n^c}_{i,j,k-1} + \rho^{n^c}_{i,j,k})} + g_z \Delta t$$



Step: 2b Discretized change in the cell-centered equilibration pressure

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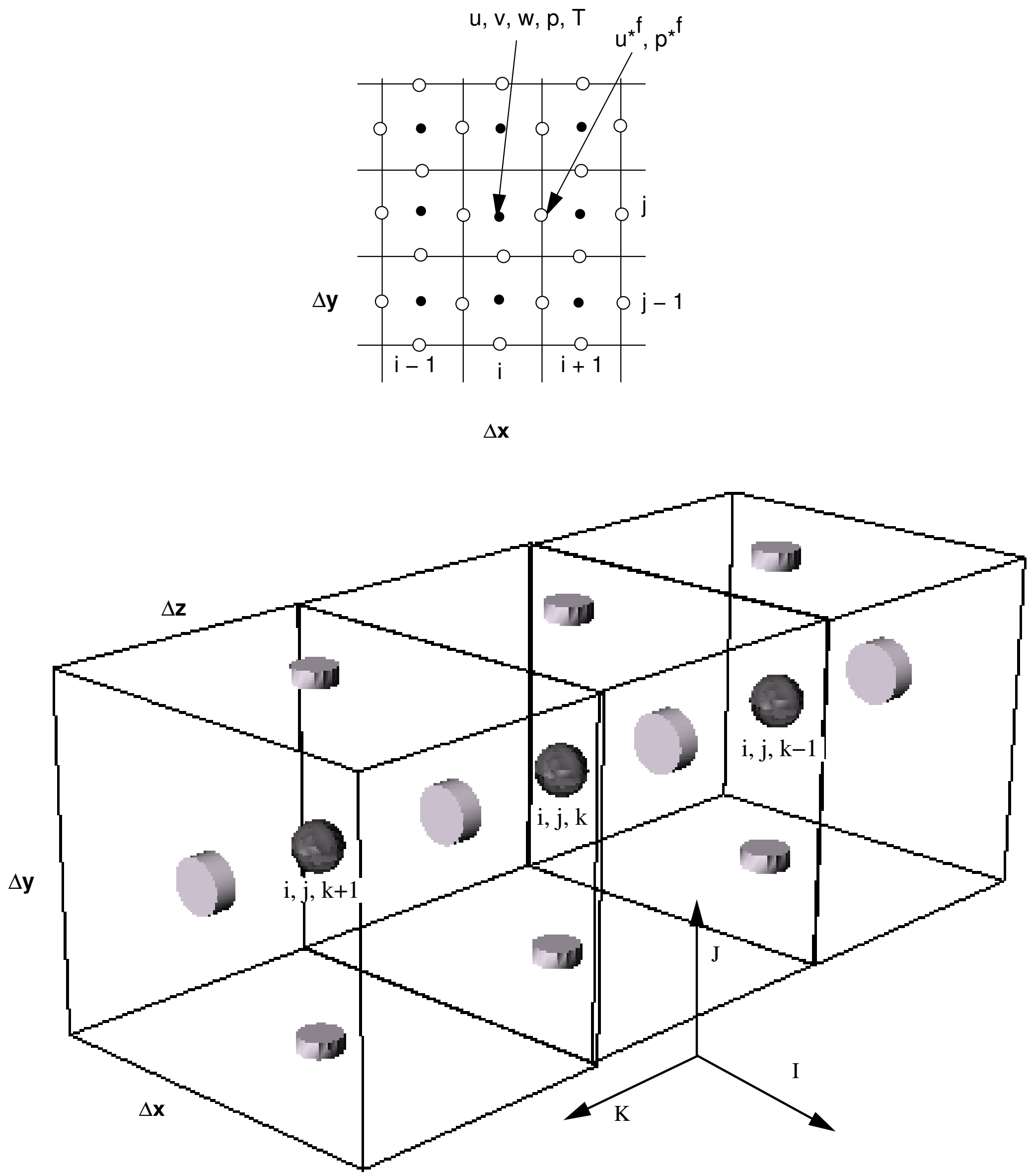
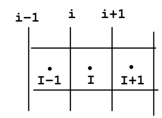


Figure 1: Two-Dimensional grid showing the location of the primary and auxiliary variables.

Step: 3 Discretized change in the face-centered pressure

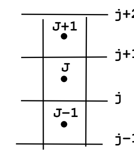
The discretized face-centered equilibration pressure eq. (16) is, (Kashiwa et al. 1994)
x-direction

$$p^{n+1^{*f}}_{i,j,k,L} = \left(\frac{\upsilon^{n^c}_{i,j,k} p^{n+1^{Lc}}_{i,j,k} + \upsilon^{n^c}_{i-1,j,k} p^{n+1^{Lc}}_{i-1,j,k}}{\upsilon^{n^c}_{i,j,k} + \upsilon^{n^c}_{i-1,j,k}} \right)$$



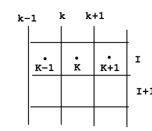
y-direction

$$p^{n+1^{*f}}_{i,j,k,B} = \left(\frac{\upsilon^{n^c}_{i,j,k} p^{n+1^{Lc}}_{i,j,k} + \upsilon^{n^c}_{i,j-1,k} p^{n+1^{Lc}}_{i,j-1,k}}{\upsilon^{n^c}_{i,j,k} + \upsilon^{n^c}_{i,j-1,k}} \right)$$



z-direction

$$p^{n+1^{*f}}_{i,j,k,BK} = \left(\frac{\upsilon^{n^c}_{i,j,k} p^{n+1^{Lc}}_{i,j,k} + \upsilon^{n^c}_{i,j,k-1} p^{n+1^{Lc}}_{i,j,k-1}}{\upsilon^{n^c}_{i,j,k} + \upsilon^{n^c}_{i,j,k-1}} \right)$$



Step: 4 Discretized Source/Sink Terms

Now performing the surface integrals, for a viscous compressible fluid in Cartesian coordinates we get the following velocity source/sink terms. Figure 2 shows the diffusion of the x-component of momentum in and out of a control volume.
x-component source terms

$$\begin{aligned}
\Delta(mu)^{n+1}_{i,j,k} &= \Delta t (m^n u^n \dot{\alpha})_{i,j,k} - \Delta t (p^{n+1^{*f}}|_{i,j,k,R} - p^{n+1^{*f}}|_{i,j,k,L}) \Delta y \Delta z \\
&+ \Delta t \Bigg((\tau^f_{xx}|_{i,j,k,R} - \tau^f_{xx}|_{i,j,k,L}) \Delta y \Delta z + (\tau^f_{yx}|_{i,j,k,T} - \tau^f_{yx}|_{i,j,k,B}) \Delta x \Delta z \\
&+ (\tau^f_{zx}|_{i,j,k,FR} - \tau^f_{zx}|_{i,j,k,BK}) \Delta x \Delta y \Bigg) + m_{i,j,k} g_x \Delta t
\end{aligned}$$

y-component source terms

$$\begin{aligned}
\Delta(mv)^{n+1} &= \Delta t \langle m^n v^n \dot{\alpha} \rangle - \Delta t (p^{n+1^{*f}}|_{i,j,k,T} - p^{n+1^{*f}}|_{i,j,k,B}) \Delta x \Delta z \\
&+ \Delta t \Bigg((\tau^f_{xy}|_{i,j,k,R} - \tau^f_{xy}|_{i,j,k,L}) \Delta y \Delta z + (\tau^f_{yy}|_{i,j,k,T} - \tau^f_{yy}|_{i,j,k,B}) \Delta x \Delta z \\
&+ (\tau^f_{zy}|_{i,j,k,FR} - \tau^f_{zy}|_{i,j,k,BK}) \Delta x \Delta y \Bigg) + m_{i,j,k} g_y \Delta t
\end{aligned}$$

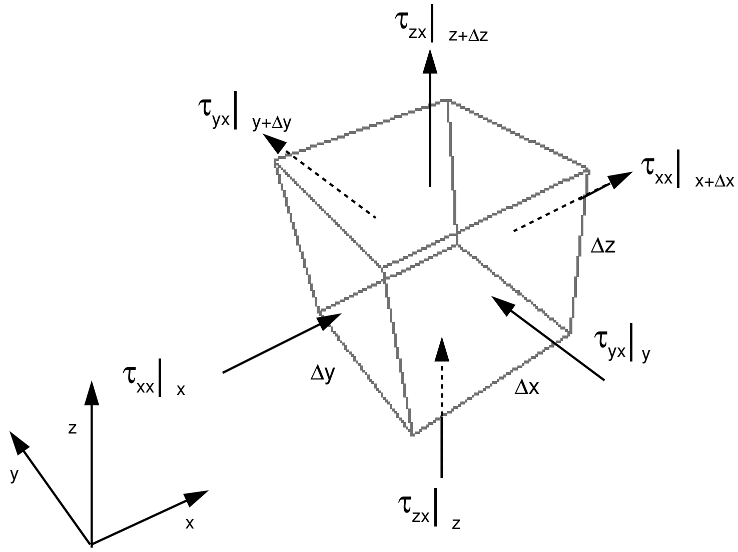


Figure 2: Volume element with arrows indicating the direction in which the x-component of momentum is transported through the surfaces.

<u>z-component source terms</u>

$$
\begin{aligned}
\Delta(mw)^{\mathrm{n+1}} = {} & \Delta t \langle m^n w^n \dot{\alpha} \rangle - \Delta t V^n \left(p^{\mathrm{n+1}^{*f}}|_{j,k,k,FR} - p^{\mathrm{n+1}^{*f}}|_{i,j,k,BK}\right)\Delta x \Delta y \\
& + \Delta t \Bigg((\tau^f_{xz}|_{i,j,k,R} - \tau^f_{xz}|_{i,j,k,L})\Delta y \Delta z + (\tau^f_{yz}|_{i,j,k,T} - \tau^f_{yz}|_{i,j,k,B})\Delta x \Delta z \\
& + (\tau^f_{zz}|_{i,j,k,FR} - \tau^f_{zz}|_{i,j,k,BK})\Delta x \Delta y \Bigg) + m_{i,j,k} g_z \Delta t
\end{aligned}
$$

Now for the stress components we will discretize eqs. (23 - 28) using second-order finite-difference centered representation of the derivatives. For a multimaterial problem we define an effective viscosity across the right face of cell i,j,k

$$
\mu^{*f}_{i,j,k,R} = \frac{2\mu_i \mu_{i+1}}{\mu_i + \mu_{i+1}}
$$

All of the transport coefficients have this form. For each face an edge velocity, which is simply the average of the four nearest neighbors. The naming convection is shown in fig. 3.

$$
\begin{aligned}
\tau^f_{xx}|_{left} = {} & 2\mu^{*f} \frac{(u^{n^c}_{i,j,k} - u^{n^c}_{i-1,j,k})}{\Delta x} \\
& - \frac{2}{3}\mu^{*f} \left(\frac{(u^{n^c}_{i,j,k} - u^{n^c}_{i-1,j,k})}{\Delta x} + \frac{(v^{n^e}|^{left}_{top,z} - v^{n^e}|^{left}_{bottom,z})}{\Delta y} + \frac{(w^{n^e}|^{left}_{front,y} - w^{n^e}|^{left}_{back,y})}{\Delta z} \right)
\end{aligned}
$$

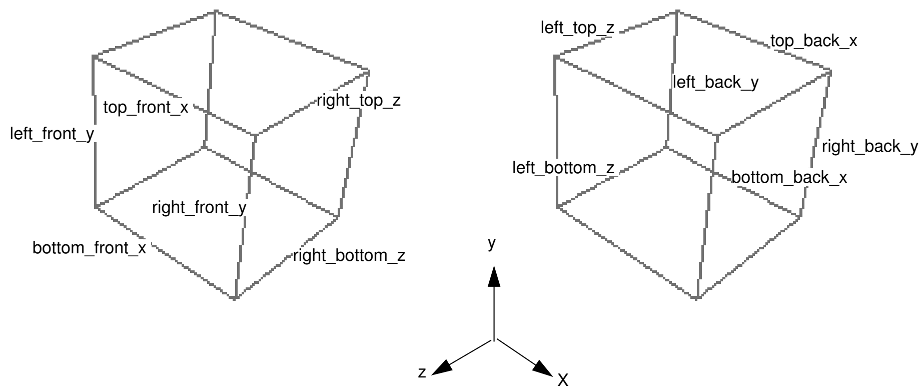


Figure 3: Naming convention for the edge velocities.

$$
\begin{aligned}
\tau^f_{xx}|_{right} = {} & 2\mu^{*f}\,\frac{(u^{n^c}_{i+1,j,k} - u^{n^c}_{i,j,k})}{\Delta x} \\
& - \frac{2}{3}\mu^{*f}\left(\frac{(u^{n^c}_{i+1,j,k} - u^{n^c}_{i,j,k})}{\Delta x} + \frac{(v^{n^e}|^{right}_{top,z} - v^{n^e}|^{right}_{bottom,z})}{\Delta y} + \frac{(w^{n^e}|^{right}_{front,y} - w^{n^e}|^{right}_{back,y})}{\Delta z}\right)
\end{aligned}
$$

$$
\begin{aligned}
\tau^f_{yy}|_{bottom} = {} & 2\mu^{*f}\,\frac{(v^{n^c}_{i,j,k} - v^{n^c}_{i,j-1,k})}{\Delta y} \\
& - \frac{2}{3}\mu^{*f}\left(\frac{(u^{n^e}|^{bottom}_{right,z} - u^{n^e}|^{bottom}_{left,z})}{\Delta x} + \frac{(v^{n^c}_{i,j,k} - v^{n^c}_{i,j-1,k})}{\Delta y} + \frac{(w^{n^e}|^{bottom}_{front,x} - w^{n^e}|^{bottom}_{back,x})}{\Delta z}\right)
\end{aligned}
$$

$$
\begin{aligned}
\tau^f_{yy}|_{top} = {} & 2\mu^{*f}\,\frac{(v^{n^c}_{i,j+1,k} - v^{n^c}_{i,j,k})}{\Delta y} \\
& - \frac{2}{3}\mu^{*f}\left(\frac{(u^{n^e}|^{top}_{right,z} - u^{n^e}|^{top}_{left,z})}{\Delta x} + \frac{(v^{n^c}_{i,j+1,k} - v^{n^c}_{i,j,k})}{\Delta y} + \frac{(w^{n^e}|^{top}_{front,x} - w^{n^e}|^{top}_{back,x})}{\Delta z}\right)
\end{aligned}
$$

$$
\begin{aligned}
\tau^f_{zz}|_{back} = {} & 2\mu^{*f}\,\frac{(w^{n^c}_{i,j,k} - w^{n^c}_{i,j,k-1})}{\Delta z} \\
& - \frac{2}{3}\mu^{*f}\left(\frac{(u^{n^e}|^{back}_{right,y} - u^{n^e}|^{back}_{left,y})}{\Delta x} + \frac{(v^{n^e}|^{back}_{top,x} - v^{n^e}|^{back}_{bottom,x})}{\Delta y} + \frac{(w^{n^c}_{i,j,k} - w^{n^c}_{i,j,k-1})}{\Delta z}\right)
\end{aligned}
$$

$$\tau_{zz}^{f}|_{front} = 2\mu^{*f}\,\frac{(w^{n^c}_{i,j,k+1} - w^{n^c}_{i,j,k})}{\Delta z}$$

$$-\frac{2}{3}\mu^{*f}\left(\frac{(u^{n^e}|^{front}_{right,y} - u^{n^e}|^{front}_{left,y})}{\Delta x} + \frac{(v^{n^e}|^{front}_{top,x} - v^{n^e}|^{front}_{bottom,x})}{\Delta y} + \frac{(w^{n^c}_{i,j,k+1} - w^{n^c}_{i,j,k})}{\Delta z}\right)$$

$$\tau_{xy}^{f}|_{left} = \mu^{*f}\left(\frac{(u^{n^e}|^{left}_{top,z} - u^{n^e}|^{left}_{bottom,z})}{\Delta y} + \frac{(v^{n^c}_{i,j,k} - v^{n^c}_{i-1,j,k})}{\Delta x}\right)$$

$$\tau_{xy}^{f}|_{right} = \mu^{*f}\left(\frac{(u^{n^e}|^{right}_{top,z} - u^{n^e}|^{right}_{bottom,z})}{\Delta y} + \frac{(v^{n^c}_{i+1,j,k} - v^{n^c}_{i,j,k})}{\Delta x}\right)$$

$$\tau_{xz}^{f}|_{left} = \mu^{*f}\left(\frac{(u^{n^e}|^{left}_{front,y} - u^{n^e}|^{left}_{back,y})}{\Delta z} + \frac{(w^{n^c}_{i,j,k} - w^{n^c}_{i-1,j,k})}{\Delta x}\right)$$

$$\tau_{xz}^{f}|_{right} = \mu^{*f}\left(\frac{(u^{n^e}|^{right}_{front,y} - u^{n^e}|^{right}_{back,y})}{\Delta z} + \frac{(w^{n^c}_{i+1,j,k} - w^{n^c}_{i,j,k})}{\Delta x}\right)$$

$$\tau_{yx}^{f}|_{bottom} = \mu^{*f}\left(\frac{(u^{n^c}_{i,j,k} - u^{n^c}_{i,j-1,k})}{\Delta y} + \frac{(v^{n^e}|^{bottom}_{right,z} - v^{n^e}|^{bottom}_{left,z})}{\Delta x}\right)$$

$$\tau_{yx}^{f}|_{top} = \mu^{*f}\left(\frac{(u^{n^c}_{i,j+1,k} - u^{n^c}_{i,j,k})}{\Delta y} + \frac{(v^{n^e}|^{top}_{right,z} - v^{n^e}|^{top}_{left,z})}{\Delta x}\right)$$

$$\tau_{yz}^{f}|_{bottom} = \mu^{*f}\left(\frac{(v^{n^e}|^{bottom}_{front,x} - v^{n^e}|^{bottom}_{back,x})}{\Delta z} + \frac{(w^{n^c}_{i,j,k} - w^{n^c}_{i,j,k-1})}{\Delta y}\right)$$

$$\tau_{yz}^{f}|_{top} = \mu^{*f}\left(\frac{(v^{n^e}|^{top}_{front,x} - v^{n^e}|^{top}_{back,x})}{\Delta z} + \frac{(w^{n^c}_{i,j+1,k} - w^{n^c}_{i,j,k})}{\Delta y}\right)$$

$$\tau_{zx}^{f}|_{back} = \mu^{*f}\left(\frac{(u^{n^c}_{i,j,k} - u^{n^c}_{i,j,k-1})}{\Delta z} + \frac{(w^{n^e}|^{back}_{right,y} - w^{n^e}|^{back}_{left,y})}{\Delta x}\right)$$

$$\tau_{zx}^{f}|_{front} = \mu^{*f}\left(\frac{(u^{n^c}_{i,j,k+1} - u^{n^c}_{i,j,k})}{\Delta z} + \frac{(w^{n^e}|^{front}_{right,y} - w^{n^e}|^{front}_{left,y})}{\Delta x}\right)$$

$$\tau_{zy}^{f}|_{back} = \mu^{*f}\left(\frac{(v^{n^c}_{i,j,k} - v^{n^c}_{i,j,k-1})}{\Delta z} + \frac{(w^{n^e}|^{back}_{top,x} - w^{n^e}|^{back}_{bottom,x})}{\Delta y}\right)$$

$$\tau_{zy}^{f}|_{front} = \mu^{*f}\left(\frac{(v^{n^c}_{i,j,k+1} - v^{n^c}_{i,j,k})}{\Delta z} + \frac{(w^{n^e}|^{front}_{top,x} - w^{n^e}|^{front}_{bottom,x})}{\Delta y}\right)$$

Energy equation source terms

$$\Delta(me)^{n+1}_{ijk} = \Delta t(\nabla\cdot\vec{U})_{ijk} \tag{48}$$

Step: 5 Discretized Lagrangian $\rho^L, (m\vec{U})^L, e^L$

The equations for calculating the Lagrangian contribution of the total mass, momentum, and energy are

Mass:

$$m_{i,j,k}^{\text{n+1}^L} = \rho_{i,j,k}^n V_{i,j,k}^n + \overbrace{\Delta(m_m)_{i,j,k}^{\text{n+1}}}^{\text{source/sink}} \tag{49}$$

Momentum:

$$(mu)_{i,j,k}^{\text{n+1}^L} = (mu)_{i,j,k}^{n^c} - \overbrace{u_{i,j,k}^{n^c}\Delta(m)_{i,j,k}^{\text{n+1}}}^{\text{source/sink due to phase change}} + \overbrace{\Delta(mu)_{i,j,k}^{\text{n+1}}}^{\text{source/sink}} \tag{50}$$

$$(mv)_{i,j,k}^{\text{n+1}^L} = (mv)_{i,j,k}^{n^c} - \overbrace{v_{i,j,k}^{n^c}\Delta(m)_{i,j,k}^{\text{n+1}}}^{\text{source/sink due to phase change}} + \overbrace{\Delta(mv)_{i,j,k}^{\text{n+1}}}^{\text{source/sink}} \tag{51}$$

$$(mw)_{i,j,k}^{\text{n+1}^L} = (mw)_{i,j,k}^{n^c} - \overbrace{w_{i,j,k}^{n^c}\Delta(m)_{i,j,k}^{\text{n+1}}}^{\text{source/sink due to phase change}} + \overbrace{\Delta(mw)_{i,j,k}^{\text{n+1}}}^{\text{source/sink}} \tag{52}$$

Energy: (The contribution from the kinetic energy is currently missing)

$$e_{i,j,k}^{L^{\text{n+1}}} = e_{i,j,k}^n - \overbrace{e_{i,j,k}^n\Delta(m)_{i,j,k}^{\text{n+1}}}^{\text{source/sink due to phase change}} + \overbrace{\Delta(me)_{i,j,k}^{\text{n+1}}}^{\text{source/sink}} \tag{53}$$

where $e^n = (c_v T)^n_.$

Step: 6 Discretized Advection Operator

This section is out of date. We do not use the corner coupling volumes (2 and 3)

Below is the advection operator, eq. (36), with the influx and outflux summation terms expanded, assuming $u = v = 1.0$, see Fig(4).

$$
\begin{aligned}
&-\Delta t \text{Advection}((q), \vec{U}^{n+1^{*f}}) = \\
&\overbrace{-\left[\langle q\rangle_{1,i,j}\Delta V_{1,i,j} + \langle q\rangle_{2,i,j}\Delta V_{2,i,j} + \langle q\rangle_{3,i,j}\Delta V_{3,i,j} + \langle q\rangle_{4,i,j}\Delta V_{4,i,j}\right]}^{outflux} \\
&\overbrace{+\left[\langle q\rangle_{1,i,j}\Delta V_{1,i,j-1} + \langle q\rangle_{2,i,j}\Delta V_{2,i-1,j-1} + \langle q\rangle_{3,i,j}\Delta V_{3,i-1,j-1} + \langle q\rangle_{4,i,j}\Delta V_{4,i-1,j}\right]}^{influx}
\end{aligned} \tag{54}
$$

The discretized equation for outflux of q eq. (37) is

$$\langle q\rangle_{1,i,j,k} = q_{i,j,k} + \frac{\partial q_{i,j,k}}{\partial x}\mathbf{r_{x,1}} + \frac{\partial q_{i,j,k}}{\partial y}\mathbf{r_{y,1}} \tag{55}$$

$$\langle q\rangle_{2,i,j,k} = q_{i,j,k} + \frac{\partial q_{i,j,k}}{\partial x}\mathbf{r_{x,2}} + \frac{\partial q_{i,j,k}}{\partial y}\mathbf{r_{y,2}} \tag{56}$$

$$\langle q\rangle_{3,i,j,k} = q_{i,j,k} + \frac{\partial q_{i,j,k}}{\partial x}\mathbf{r_{x,3}} + \frac{\partial q_{i,j,k}}{\partial y}\mathbf{r_{y,3}} \tag{57}$$

$$\langle q\rangle_{4,i,j,k} = q_{i,j,k} + \frac{\partial q_{i,j,k}}{\partial x}\mathbf{r_{x,4}} + \frac{\partial q_{i,j,k}}{\partial y}\mathbf{r_{y,4}} \tag{58}$$

where the centroids for each outflux volume are shown below. The differencing scheme used to approximate the gradients of q is discussed in the appendix. Listed below are the equations for the outflow volume fluxes for cell i, j, at time t, and the the associated centroids, Fig. (4) Note that the equations for the centroids vary depending on the velocity direction. The lengths B and H used in the equations below are given by $|u*\Delta t|$ and $|v*\Delta t|$ respectively and $l_1 = \Delta x - B$ and $l_2 = \Delta y - H$ The Courant numbers $\sigma_x = \frac{u\Delta t}{\Delta x}$ and $\sigma_y = \frac{v\Delta t}{\Delta y}$ must satisfy $\sigma_x < 1$ and $\sigma_y < 1$.

<u>($\nearrow, u > 0, v > 0$), cell (i, j), Fig. (4a)</u>

$$\Delta V_{\substack{i,j\\ outflow}} = \Delta V_1 + \Delta V_2 + \Delta V_3 + \Delta V_4$$

$$\mathbf{r}_{x,4} = l_1 + \frac{B}{2} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,4} = \frac{l_2}{2} - \frac{\Delta y}{2}, \quad \mathbf{r}_{x,1} = \frac{l_1}{2} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,1} = l_2 + \frac{H}{2} - \frac{\Delta y}{2}$$

$$\mathbf{r}_{x,2} = l_1 + \frac{B}{3} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,2} = l_2 + \frac{2H}{3} - \frac{\Delta y}{2}, \quad \mathbf{r}_{x,3} = l_1 + \frac{2B}{3} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,3} = l_2 + \frac{H}{3} - \frac{\Delta y}{2}$$

<u>($\searrow, u > 0, v < 0$), cell (i, j), Fig. (4b)</u>

$$\mathbf{r}_{x,4} = l_1 + \frac{B}{2} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,4} = H + \frac{l_2}{2} - \frac{\Delta y}{2}, \quad \mathbf{r}_{x,1} = \frac{l_1}{2} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,1} = \frac{H}{2} - \frac{\Delta y}{2}$$

$$\mathbf{r}_{x,2} = l_1 + \frac{B}{3} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,2} = \frac{H}{3} - \frac{\Delta y}{2}, \quad \mathbf{r}_{x,3} = l_1 + \frac{2B}{3} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,3} = \frac{2H}{3} - \frac{\Delta y}{2}$$

$\underline{(\nwarrow, u < 0, v > 0), \text{ cell } (i, j), \text{ Fig. (4c)}}$

$$\mathbf{r}_{x,4} = \frac{B}{2} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,4} = \frac{l_2}{2} - \frac{\Delta y}{2}, \quad \mathbf{r}_{x,1} = B + \frac{l_1}{2} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,1} = l_2 + \frac{H}{2} - \frac{\Delta y}{2}$$
$$\mathbf{r}_{x,2} = \frac{2B}{3} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,2} = l_2 + \frac{2H}{3} - \frac{\Delta y}{2}, \quad \mathbf{r}_{x,3} = \frac{B}{3} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,3} = l_2 + \frac{H}{3} - \frac{\Delta y}{2}$$

$\underline{(\swarrow, u < 0, v < 0), \text{ cell } (i, j), \text{ Fig. (4d)}}$

$$\mathbf{r}_{x,4} = \frac{B}{2} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,4} = H + \frac{l_2}{2} - \frac{\Delta y}{2}, \quad \mathbf{r}_{x,1} = B + \frac{l_1}{2} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,1} = \frac{H}{2} - \frac{\Delta y}{2}$$
$$\mathbf{r}_{x,2} = \frac{2B}{3} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,2} = \frac{H}{3} - \frac{\Delta y}{2}, \quad \mathbf{r}_{x,3} = \frac{B}{3} - \frac{\Delta x}{2}, \quad \mathbf{r}_{y,3} = \frac{2H}{3} - \frac{\Delta y}{2}$$

In a compact form the outflow volume centroids of cell i, j can be written as

$$\mathbf{r}_{x,4} = C_4 + \frac{B}{2} - \frac{\Delta x}{2} \quad \begin{cases} \nearrow\searrow, \text{or } u > 0, & C_4 = l_1; \quad \text{case 1} \\ \nwarrow\swarrow, \text{or } u < 0, & C_4 = 0; \quad \text{case 2} \end{cases} \tag{59}$$

$$\mathbf{r}_{y,4} = C_4 + \frac{l_2}{2} - \frac{\Delta y}{2} \quad \begin{cases} \nearrow\nwarrow, \text{or } v > 0, & C_4 = 0; \quad \text{case 3} \\ \searrow\swarrow, \text{or } v < 0, & C_4 = H; \quad \text{case 4} \end{cases} \tag{60}$$

$$\mathbf{r}_{x,1} = C_1 + \frac{l_1}{2} - \frac{\Delta x}{2} \quad \begin{cases} \nearrow\searrow, \text{or } u > 0, & C_1 = 0; \quad \text{case 1} \\ \nwarrow\swarrow, \text{or } u < 0, & C_1 = B; \quad \text{case 2} \end{cases} \tag{61}$$

$$\mathbf{r}_{y,1} = C_1 + \frac{H}{2} - \frac{\Delta y}{2} \quad \begin{cases} \nearrow\nwarrow, \text{or } v > 0, & C_1 = l_2; \quad \text{case 3} \\ \searrow\swarrow, \text{or } v < 0, & C_1 = 0; \quad \text{case 4} \end{cases} \tag{62}$$

$$\mathbf{r}_{x,2} = C_2 + \alpha\frac{B}{3} - \frac{\Delta x}{2} \quad \begin{cases} \nearrow\searrow, \text{or } u > 0, & C_2 = l_1; \quad \alpha = 1 \quad \text{case1} \\ \nwarrow\swarrow, \text{or } u < 0, & C_2 = 0; \quad \alpha = 2 \quad \text{case2} \end{cases} \tag{63}$$

$$\mathbf{r}_{y,2} = C_2 + \alpha\frac{H}{3} - \frac{\Delta y}{2} \quad \begin{cases} \nearrow\nwarrow, \text{or } v > 0, & C_2 = l_2; \quad \alpha = 2 \quad \text{case3} \\ \searrow\swarrow, \text{or } v < 0, & C_2 = 0; \quad \alpha = 1 \quad \text{case4} \end{cases} \tag{64}$$

$$\mathbf{r}_{x,3} = C_3 + \alpha\frac{B}{3} - \frac{\Delta x}{2} \quad \begin{cases} \nearrow\searrow, \text{or } u > 0, & C_3 = l_1; \quad \alpha = 2 \quad \text{case1} \\ \nwarrow\swarrow, \text{or } u < 0, & C_3 = 0; \quad \alpha = 1 \quad \text{case2} \end{cases} \tag{65}$$

$$\mathbf{r}_{y,3} = C_3 + \alpha\frac{H}{3} - \frac{\Delta y}{2} \quad \begin{cases} \nearrow\nwarrow, \text{or } v > 0, & C_3 = l_2; \quad \alpha = 1 \quad \text{case3} \\ \searrow\swarrow, \text{or } v < 0, & C_3 = 0; \quad \alpha = 2 \quad \text{case4} \end{cases} \tag{66}$$

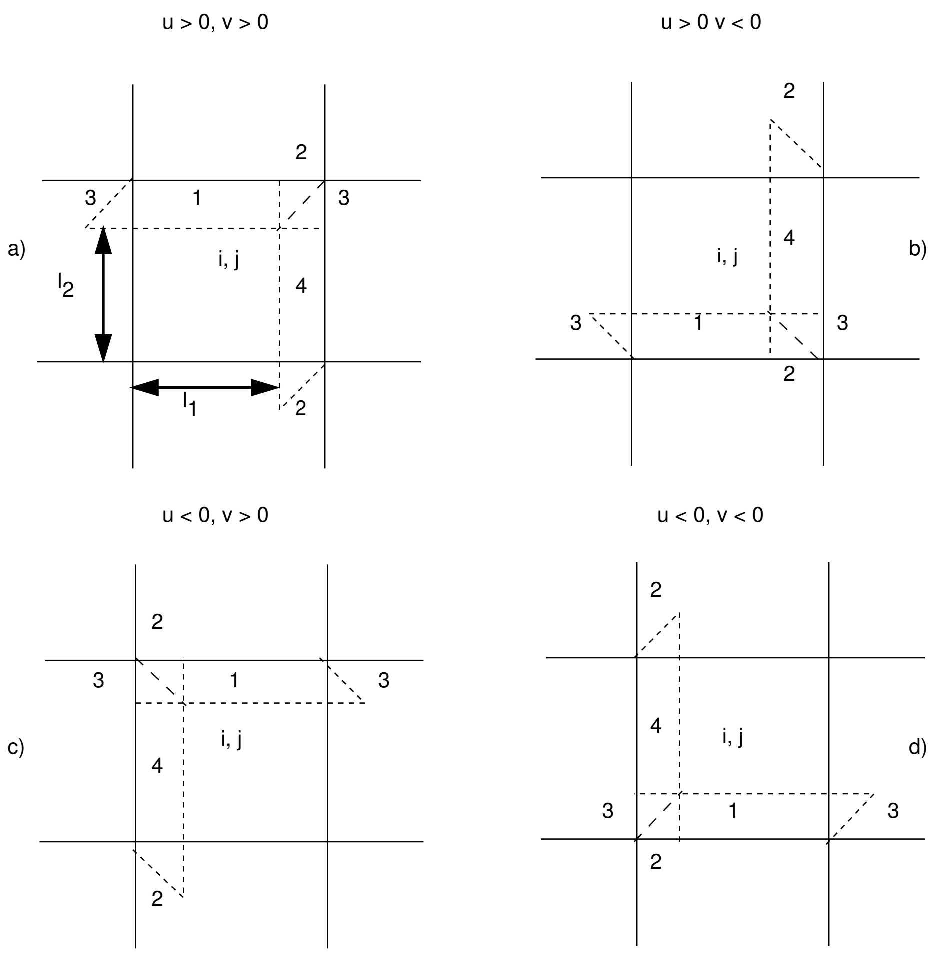


Figure 4: Cell (i, j) with outflow fluxes shown at time t

The equations for the inflow volume fluxes to the surrounding cells and the associated centroids are shown below. Note the coordinate system for each of the surrounding cells is the cell centroid of that particular cell, $\Delta x/2, \Delta y/2$.

<u>$(\nearrow, u > 0, v > 0)$, contribution from cell (i, j), Fig. (4a)</u>

$$\underset{inflow}{\Delta V_{i+1,j}} = \Delta V_{4,i,j} \quad ; \quad \underset{inflow}{\Delta V_{i+1,j+1}} = \Delta V_{2,i,j} + \Delta V_{3,i,j} \quad ; \quad \underset{inflow}{\Delta V_{i,j+1}} = \Delta V_{1,i,j}$$

<u>$(\searrow, u > 0, v < 0)$, contribution from cell (i, j), Fig. (4b)</u>

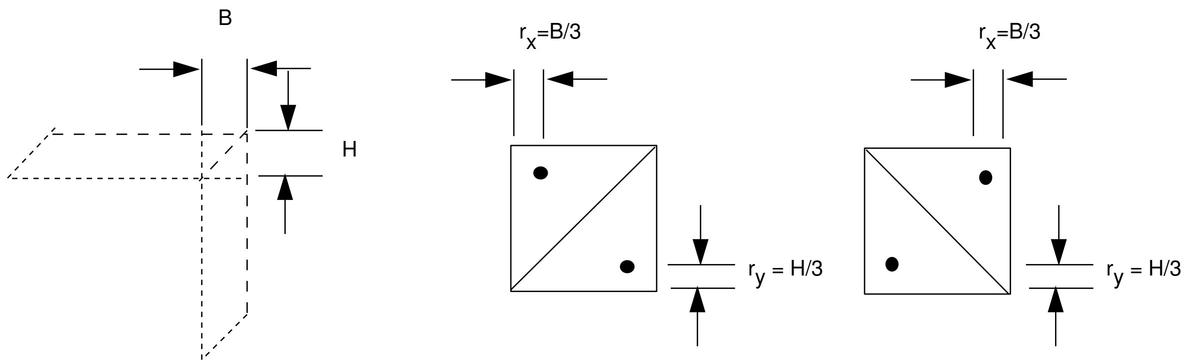


Figure 5: outflow fluxes shown at time t

$$\underset{inflow}{\Delta V_{i+1,j}} = \Delta V_{4,i,j} \quad ; \quad \underset{inflow}{\Delta V_{i+1,j-1}} = \Delta V_{2,i,j} + \Delta V_{3,i,j} \quad ; \quad \underset{inflow}{\Delta V_{i,j-1}} = \Delta V_{1,i,j}$$

<u>($\nwarrow, u < 0, v > 0$), contribution from cell (i, j), Fig. (4c)</u>

$$\underset{inflow}{\Delta V_{i-1,j}} = \Delta V_{4,i,j} \quad ; \quad \underset{inflow}{\Delta V_{i-1,j+1}} = \Delta V_{2,i,j} + \Delta V_{3,i,j} \quad ; \quad \underset{inflow}{\Delta V_{i,j+1}} = \Delta V_{1,i,j}$$

<u>($\swarrow, u < 0, v < 0$), contribution from cell (i, j), Fig. (4d)</u>

$$\underset{inflow}{\Delta V_{i-1,j}} = \Delta V_{4,i,j} \quad ; \quad \underset{inflow}{\Delta V_{i-1,j-1}} = \Delta V_{2,i,j} + \Delta V_{3,i,j} \quad ; \quad \underset{inflow}{\Delta V_{i,j-1}} = \Delta V_{1,i,j}$$

where,

$$\Delta V_3 = \frac{BH}{2} \quad ; \quad \Delta V_2 = \frac{BH}{2}$$

$$\Delta V_4 = (\Delta y - H)(B) \quad ; \quad \Delta V_1 = (\Delta x - B)(H)$$

$$l_2 = \Delta y - H \quad ; \quad l_1 = \Delta x - B$$

Vertex values of q_v

The discretized equations for the vertex values of q interpolated by eq. (42) in 2-dimensions is, Fig. (6).

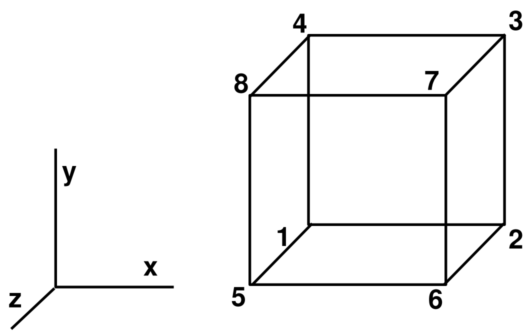


Figure 6: Schematic of a cell with vertices labeled

$$q^1 = q_{ijk} + \frac{\partial q_{ijk}}{\partial x}(-\frac{\Delta x}{2}) + \frac{\partial q_{ijk}}{\partial y}(-\frac{\Delta y}{2}) \tag{67}$$

$$q^2 = q_{ijk} + \frac{\partial q_{ijk}}{\partial x}(\frac{\Delta x}{2}) + \frac{\partial q_{ijk}}{\partial y}(-\frac{\Delta y}{2}) \tag{68}$$

$$q^3 = q_{ijk} + \frac{\partial q_{ijk}}{\partial x}(\frac{\Delta x}{2}) + \frac{\partial q_{ijk}}{\partial y}(\frac{\Delta y}{2}) \tag{69}$$

$$q^4 = q_{ijk} + \frac{\partial q_{ijk}}{\partial x}(-\frac{\Delta x}{2}) + \frac{\partial q_{ijk}}{\partial y}(\frac{\Delta y}{2}) \tag{70}$$

Note: a simple approach may be to use
$q^1 = 0.25(q_{ijk} + q_{i-1jk} + q_{i-1j-1k} + q_{ij-1k})$

The gradients of q are approximated by second-order finite difference

$$\frac{\partial q}{\partial x} = \frac{q_{i+1} - q_{i-1}}{2\Delta x} \tag{71}$$

$$\frac{\partial q}{\partial y} = \frac{q_{j+1} - q_{j-1}}{2\Delta y} \tag{72}$$

Step: 7 Discretized Time Advanced Equations

Below is the discretized equations for the time advanced mass, momentum and internal energy, eq. (43 - 45)

$$(m)^{n+1}_{i,j,k} = m^{n+1^L}_{ijk} - \Delta t \,\text{Advection}(\rho^{n+1^L}_{i,j,k}\vec{U}^{n+1^{*f}}) \tag{73}$$

$$(mu)^{n+1}_{i,j,k} = (mu)^{n+1^L}_{i,j,k} - \Delta t \,\text{Advection}((\rho u)^{n+1^L}_{i,j,k}, \vec{U}^{n+1^{*f}}) \tag{74}$$

$$(mv)^{n+1}_{i,j,k} = (mv)^{n+1^L}_{i,j,k} - \Delta t \,\text{Advection}((\rho v)^{n+1^L}_{i,j,k}, \vec{U}^{n+1^{*f}}) \tag{75}$$

$$(mw)^{n+1}_{i,j,k} = (mw)^{n+1^L}_{i,j,k} - \Delta t \,\text{Advection}((\rho w)^{n+1^L}_{i,j,k}, \vec{U}^{n+1^{*f}}) \tag{76}$$

$$(me)_{i,j,k}^{n+1} = (mc_vT)_{i,j,k}^{\mathrm{n+1}^L} - \Delta t\,\mathrm{Advection}((\rho c_vT)_{i,j,k}^{\mathrm{n+1}^L}, \vec{U}^{\mathrm{n+1}^{*^f}}) \tag{77}$$

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Appendix Derivation of the time advanced equations

In this section we will derive the $n+1$ time equations for the conservation of mass, momentum and energy, eqs. 4.8 of Kashiwa et al. (1994). The goal is to illustrate the steps that were taken from in reducing the governing equations 1 - 4 to the time advanced equations 4.6 in Kashiwa et al. (1994). In doing so we will use the right hand side of eqs. [1 - 4] times the volume as the source terms. Beginning with Reynolds transport theorem, applied to a material volume (Thompson 1972).

$$\int_V \frac{\partial ()}{\partial t} dV + \int_A () \vec{U} \cdot d\vec{S} = \frac{d}{dt} \int_V () dV \tag{78}$$

Using eq. (78) and letting $() = m_m$ the equation for the conservation of mass for multiple materials in a control volume becomes

$$\int_V \frac{\partial m_m}{\partial t} dV + \int_A m_m \vec{U}_m \cdot d\vec{S} = \int_v m_m \dot{\alpha}_m dV$$

After integrating the conservation of mass becomes

$$V \frac{\partial m_m}{\partial t} + V \sum_{i=1}^{n} \rho_m \vec{U}_m \cdot \vec{S} = V m_m \dot{\alpha}_m$$

Now replace the time derivative with a first order finite-difference representation and rearranging

$$\boxed{\rho_m^{n+1} V^{n+1} = \underbrace{\Delta t \rho_m^n V^n + \Delta t m_m^n \dot{\alpha}_m}_{\text{Lagrangian change in mass}} - \Delta t \sum_{i=1}^{n} \rho_m^n \vec{U}_m^n \cdot \vec{S}} \tag{79}$$

<u>Momentum</u> For the momentum equation we will assume that the multiphase Reynolds stress and the acceleration by non-equilibrium pressure is zero. If we let $() = \rho_m \vec{U}_m$ and substitute into eq. (78) the momentum equation becomes,

$$\begin{aligned} \int_V \frac{\partial \rho_m \vec{U}_m}{\partial t} dV + \int_A \rho_m \vec{U}_m \vec{U}_m \cdot d\vec{S} = & \int_V \rho_o \vec{U}_o \dot{\alpha}_m dV \\ & + \int_V \rho_m \vec{g} dV \\ & + \int_V \theta_m \nabla p dV \\ & + \int_V \nabla \cdot (\alpha_m \tau_o) dV \\ & + \int_V \sum_l \theta_k \theta_l K_{m,l} (\vec{U}_l - \vec{U}_m) dV \end{aligned}$$

Before this equation can be integrated we need to convert the volume integral for the pressure gradient and the divergence of the deformation tensor into surface integrals.

This is done through the divergence theorem for a scalar a tensor (Bird et al. 1960)

$$\int_V \nabla s dV = \int_A s d\vec{S}$$

$$\int_V \nabla \cdot \tau dV = \int_A \tau \cdot d\vec{S}$$

After making the substitution the momentum equations becomes

$$\begin{aligned}\int_V \frac{\partial \rho_m \vec{U}_m}{\partial t} dV + \int_A \rho_m \vec{U}_m \vec{U}_m \cdot d\vec{S} = \int_V \rho_m \vec{U}_m \dot{\alpha}_m dV + \int_V \rho_m \vec{g}\, dV \\ + \int_A \theta_m p\, d\vec{S} + \int_A \tau_m \cdot d\vec{S} + V \sum_l \theta_k \theta_l K_{m,l} (\vec{U}_l - \vec{U}_m)\end{aligned}$$

We now integrate all of the terms except for those involving the pressure and deviatoric stress tensor

$$\begin{aligned}\frac{\partial \rho_m \vec{U}_m}{\partial t} + \sum_{i=1}^{n} \rho_m \vec{U}_m (\vec{U}_m \cdot \vec{S}) = m_m \vec{U}_m \dot{\alpha}_m + m_m \vec{g} + \int_A \theta_m p\, d\vec{S} \\ + \int_A \tau_m \cdot d\vec{S} + \int_V \sum_l \theta_k \theta_l K_{m,l} (\vec{U}_l - \vec{U}_m)\, dV\end{aligned}$$

Now replace the time derivative with a first order finite-difference representation and rearranging

$$\begin{aligned}(m_m \vec{U}_m)^{n+1} = (m_m \vec{U}_m)^n + \Delta t m_m^n \vec{U}_m^n \dot{\alpha}_m + \Delta t m_m \vec{g} + \Delta t \int_A \theta_m p\, d\vec{S} \\ + \Delta t \int_A \tau_m \cdot d\vec{S} + \Delta t V \sum_l \theta_k \theta_l K_{m,l} (\vec{U}_l^n - \vec{U}_m^n) - \Delta t \sum_{i=1}^{n} \rho_m \vec{U}^n (\vec{U}^n \cdot \vec{S}) \qquad (80)\end{aligned}$$

For the energy equation we start by ignoring the multiphase fluctuational transport of internal energy, fluctuational work, average viscous dissipation, thermal transport by conduction. Letting $() = \rho_m e_m$ in eq. (78) the energy equation reduces to

$$\begin{aligned}\int_V \frac{\partial \rho_m e_m}{\partial t} dV + \int_A \rho_m e_m \vec{U}_m \cdot d\vec{S} = \int_V \rho_o e_o \dot{\alpha}_m dV \\ + \int_V (\frac{p_m \upsilon_m}{c_m^2}) \dot{p}\, dV \\ + \int_V \sum_l \theta_k \theta_l R_{m,l} (T_l - T_m) dV \qquad (81)\end{aligned}$$

Making the substitutions $p_k = \theta_k p_k^o,\ \dot{p} = \frac{\Delta p}{\Delta t}$ and integrating, eq. (81) becomes

$$\begin{aligned}\frac{\partial m_m e_m}{\partial t} + \sum_{i=1}^{n} m_m e_m (\vec{U}_m \cdot \vec{S}) = m_m e_o \dot{\alpha}_m + V (\frac{p_m \upsilon_m}{c_m^2}) \frac{\Delta p}{\Delta t} \\ + V \sum_l \theta_k \theta_l R_{m,l} (T_l - T_m)\end{aligned}$$

Now replace the time derivative with a first order finite-difference representation and rearranging

$$
\begin{aligned}
(m_m e_m)^{n+1} = (m_m e_m)^n + \Delta t m_m^n e_o \dot{\alpha}_m + \Delta t V (\frac{p_m \upsilon_m}{c_m^2})\Delta p \\
+ \Delta t V \sum_l \theta_k \theta_l R_{m,l}(T_l - T_m) - \Delta t \sum_{i=1}^{n} m_m^n e^n (\vec{U}_m \cdot \vec{S})
\end{aligned}
\tag{82}
$$

Appendix: Derivation of the "pressure equation"

The derivation of the pressure equation begins with the Lagrangian face-centered velocity and the equation for the pressure, Kashiwa et al. (1994)

$$\rho \frac{d\vec{U}^f}{dt} = -\nabla^f p^{\mathrm{n+1}^{L^c}} + \rho \vec{g} \tag{83}$$

$$\frac{dp}{dt} = -\rho c^2 \nabla \cdot \vec{U}^{\mathrm{n+1}^{*f}} \tag{84}$$

Discretizing eqs. (83 - 84) in time and rearranging

$$\vec{U}^{\mathrm{n+1}^{*f}} - \left(\frac{\rho^{n^c} \vec{U}^{n^c}}{\rho^{n^c}}\right)^f = -\frac{\Delta t}{\rho^f} \nabla^f p^{\mathrm{n+1}^{L^c}} + \Delta t \vec{g} \tag{85}$$

$$\nabla^c \cdot \vec{U}^{\mathrm{n+1}^{*f}} = -\frac{\Delta p}{\rho \Delta t c^2} \tag{86}$$

is the time n face centered velocity. Now we take the divergence of equation (85)

$$\nabla^c \cdot \vec{U}^{\mathrm{n+1}^{*f}} - \nabla^c \cdot \left(\frac{\rho^{n^c} \vec{U}^{n^c}}{\rho^{n^c}}\right)^f = -\nabla^c \cdot \left[\frac{\Delta t}{\rho^f} \nabla^f p^{\mathrm{n+1}^{L^c}} - \Delta t \vec{g}\right] \tag{87}$$

Now substitute eqs. 86 into 87, multiply through by -1 and note that $p^{\mathrm{n+1}^{L^c}} = p^{n^c} + \Delta p^{\mathrm{n+1}^c}$ and $\nabla^c \cdot \vec{g} = 0$

$$\frac{\Delta p}{\rho \Delta t c^2} + \nabla^c \cdot \left(\frac{\rho^{n^c} \vec{U}^{n^c}}{\rho^{n^c}}\right)^f = \nabla^c \cdot \left[\frac{\Delta t}{\rho^f} \nabla^f (p^{n^c} + \Delta p^{\mathrm{n+1}^c})\right] \tag{88}$$

Now define an approximation to the face-centered velocity at time n as

$$\hat{\vec{U}}^{n^f} = \left(\frac{\rho^{n^c} \vec{U}^{n^c}}{\rho^{n^c}}\right)^f - \frac{\Delta t}{\rho^f} \nabla^f p^{n^c} + \Delta t \vec{g} \tag{89}$$

and its divergence is simply

$$\nabla^c \cdot \hat{\vec{U}}^{n^f} = \nabla^c \cdot \left(\frac{\rho^{n^c} \vec{U}^{n^c}}{\rho^{n^c}}\right)^f - \nabla^c \cdot \left[\frac{\Delta t}{\rho^f} \nabla^f p^{n^c} - \Delta t \vec{g}\right] \tag{90}$$

Rearranging eq. (91)

$$\frac{\Delta p}{\rho \Delta t c^2} + \nabla^c \cdot \left[\frac{\Delta t}{\rho^f} \nabla^f (\Delta p^{\mathrm{n+1}^c})\right] = -\nabla^c \cdot \left(\frac{\rho^{n^c} \vec{U}^{n^c}}{\rho^{n^c}}\right)^f + \nabla^c \cdot \left[\frac{\Delta t}{\rho^f} \nabla^f (p^{n^c})\right] \tag{91}$$

Finally we get the pressure equation

$$\left[\frac{1}{\rho \Delta t c^2} - \nabla^c \cdot \frac{\Delta t}{\rho^f} \nabla^f\right] \Delta p^{\mathrm{n+1}^c} = -\nabla^c \cdot \hat{\vec{U}}^{n^f} \tag{92}$$