

MPMICE2: Single-phase flow in porous media

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Nomenclature

General variables

<u>Variable</u>	<u>Dimensions</u>	<u>Description</u>
V	$[L^3]$	Representative volume
n		Porosity
σ	$[M/L^2]$	Total stress tensor
Δt	$[t]$	Time increment
\mathbf{b}	$[L/t]$	Gravity acceleration
c_v	$[L^2/t^2]$	Constant volume specific heat
f_{fs}	$[ML//t^2]$	Drag forces in momentum exchange term
f^{int}	$[ML//t^2]$	Internal forces
f^{ext}	$[ML//t^2]$	External forces
q_{fs}	$[ML//t^2]$	Heat exchange term
S		Shape function
∇S		Gradient of shape function

Solid phase

<u>Variable</u>	<u>Dimensions</u>	<u>Description</u>
m_s	$[M]$	Solid mass
ρ_s	$[M/L^3]$	Solid density
$\bar{\rho}_s$	$[M/L^3]$	Average Solid density
\mathbf{x}_s	$[L]$	Solid Position vector
\mathbf{U}_s	$[L/t]$	Solid Velocity vector
\mathbf{U}_s	$[L/t]$	Solid Velocity gradient vector
\mathbf{a}_s	$[L/t^2]$	Solid Acceleration vector
σ'	$[M/L^2]$	Effective Stress tensor
e_s	$[L^2/t^2]$	Solid Internal energy
T_s	$[T]$	Solid Temperature
\mathbf{F}_s		Solid Deformation gradient
V_s	$[L^3]$	Volume

Fluid phase

<u>Variable</u>	<u>Dimensions</u>	<u>Description</u>
m_f	$[M]$	Fluid mass
ρ_f	$[M/L^3]$	Fluid density
$\bar{\rho}_f$	$[M/L^3]$	Average Fluid density
\mathbf{U}_f	$[L/t]$	Fluid Velocity vector
σ_f	$[M/L^2]$	Fluid stress tensor
τ_f	$[M/L^2]$	Fluid shear stress tensor
p_f	$[M/L^2]$	Isotropic pressure
e_f	$[L^2/t^2]$	Fluid Internal energy ($c_v T_f$) of the material per unit mass
T_f	$[T]$	Fluid Temperature
ν_f	$[L^3/M]$	Fluid Specific volume $\frac{1}{\rho_f}$
α_f	$[1/T]$	Thermal expansion

Superscript

<u>Variable</u>	<u>Dimensions</u>	<u>Description</u>
n		Current time step
L		Lagrangian values
$n + 1$		Next time step
Subscript		
c		Cell-centered quantity
p		Particle quantity
i		Node quantity
FC		Face-centered quantity
L, R		Left and Right cell faces

Introduction

This report aims to present the detailed description of the governing equations and numerical implementation of single-phase flow in porous media based on the version of Uintah MPMICE code.

Theory and formulation

This section lay out the theoretical framework for the single-phase flow model.

Assumptions

Some assumptions have been made:

1. Solid phase (MPM) is described in a Lagrangian formulation while fluid phase (ICE) are described in an Eulerian formulation in the framework of continuum mechanics and mixture theory.
2. Solid grains are incompressible while the fluid phase is compressible.
3. There is no mass exchange between solid and fluid phases.
4. Terzaghi's effective stress and Darcy's law are valid.

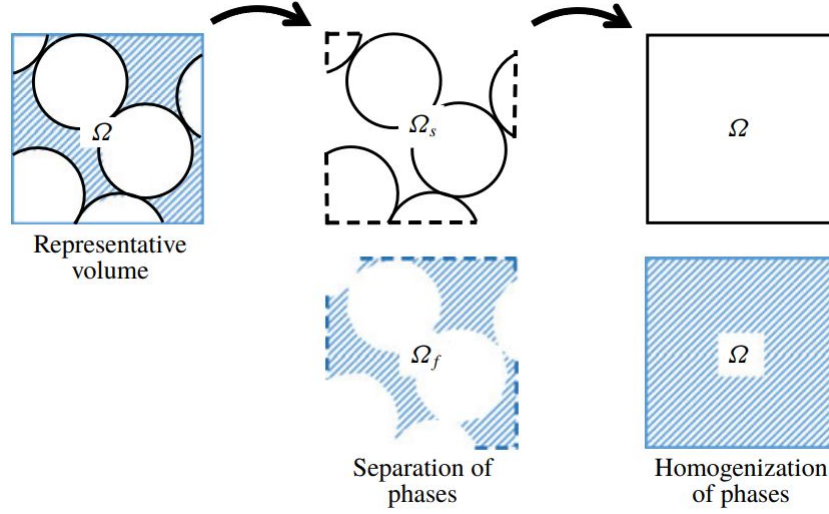


Figure 1: Homogenization of phases.

A representative element volume Ω is decomposed by two domains: solid domain Ω_s and fluid domain Ω_f . Then, the two domains are homogenized into two overlapping continua (see Figure.1 from Baumgarten and Kamrin (2019)). Considering the true (or Eulerian) porosity $n = \Omega_f / \Omega$ of the representative element volume, the average density of solid and fluid phase are defined as:

$$\bar{\rho}_s = (1 - n)\rho_s, \quad \bar{\rho}_f = n\rho_f \quad (1)$$

The mass of solid and fluid phase are:

$$m_s = \int_{\Omega} \rho_s dV = \bar{\rho}_s V, \quad m_f = \int_{\Omega} \rho_f dV = \bar{\rho}_f V \quad (2)$$

Reviewing the Terzaghi's effective stress concept for the saturated porous media, the total stress $\boldsymbol{\sigma}$ is calculated by:

$$\boldsymbol{\sigma} = \boldsymbol{\sigma}' - p_f \mathbf{I} \quad (3)$$

Governing equations

The balance equations are derived based on the mixture theory. The average thermodynamic state of the fluid phase is given by the vector $[m_f, \mathbf{U}_f, e_f, T_f, v_f]$ which are mass, velocity, internal energy, temperature, specific volume. The average state of the solid phase is given by the vector $[m_s, \mathbf{U}_s, e_s, T_s, \boldsymbol{\sigma}']$ which are mass, velocity, internal energy, temperature, effective stress. Here, we summarize the final form of the equations while the derivation is presented in detail in the Appendix.

Mass Conservation

The mass balance equations for both fluid and solid phase are

$$\frac{1}{V} \frac{D_f m_f}{Dt} = 0, \quad \frac{1}{V} \frac{D_s m_s}{Dt} = 0 \quad (4)$$

Solving the solid mass and the fluid mass balance equation leading to the rate of the specific volume as

$$\bar{\rho}_f \frac{D_f v_f}{Dt} = \nabla \cdot ((1-n)\mathbf{U}_s + n\mathbf{U}_f) \quad (5)$$

Momentum Conservation

The momentum balance equation for the fluid phase is

$$\frac{1}{V} \frac{D_f (m_f \mathbf{U}_f)}{Dt} = -n \nabla p_f + \nabla \cdot \boldsymbol{\tau}_f + \bar{\rho}_f \mathbf{b} + \mathbf{f}_{sf} \quad (6)$$

The momentum balance equation for the solid phase is

$$\frac{1}{V} \frac{D_s (m_s \mathbf{U}_s)}{Dt} = \nabla \cdot (\boldsymbol{\sigma}') - (1-n) \nabla p_f + \bar{\rho}_s \mathbf{b} - \mathbf{f}_{sf} \quad (7)$$

Energy Conservation

The internal energy balance equation for the fluid phase is

$$\frac{1}{V} \frac{D_f (m_f e_f)}{Dt} = -\bar{\rho}_f p \frac{D_f v_f}{Dt} + \boldsymbol{\tau}_f : \nabla \mathbf{U}_f + \nabla \cdot \mathbf{q}_f + q_{sf} \quad (8)$$

The internal energy balance equation for the solid phase is

$$\frac{1}{V} \frac{D_s (m_s e_s)}{Dt} = \boldsymbol{\sigma}' : \nabla \mathbf{U}_s + \nabla \cdot \mathbf{q}_s - q_{sf} \quad (9)$$

Furthermore, to close the systems of the equations, it requires the additional models: (1) An equation of state to establish relations between thermodynamics variables $[P_{eq}, \rho_f, T_f]$. (2) A constitutive equation to describe the stress - strain behaviour of solid phase. (3) Exchange momentum model. (4) Energy exchange model. (5) Optional turbulent model to compute the viscous shear stress $\boldsymbol{\tau}_f$.

Equation of state for fluid phase

The equation of state establishes relations between thermodynamics variables $[P_{eq}, \rho_f, T_f]$. Here, P_{eq} is "equilibrium" pressure which is defined as pressure enables mass of fluid material to fills in an entire porosity volume with no ongoing compression or expansion with given true density ρ_f and temperature T_f . The choice of the equation of state depends on the types of the fluid materials. For example, for the air, it is possible to assume the equation of state for the perfect gas which obeys:

$$P_{eq} = \rho_f R T_f \quad (10)$$

where R is the gas constant. For the water, the equation of state from Thomsen Hartka water model (Thomsen and Hartka (1962)) can be used to obtain the relations between the thermodynamic properties of the water. The model uses a Gibbs function which is given as follow

$$g = 0.5b(T_f - T_o)^2 + (T_f - T_o)(c_o + bT_o) + (P_{eq} - 0.5k_o P_{eq}^2)v_o + P_{eq}((1/3)a^2 P_{eq}^2 + aP(T_f - T_o) + (T_f - T_o)^2)\lambda v_o + T_f(-c_o - bT_o)\log(T_f/T_o) \quad (11)$$

The corresponds equilibrium pressure can be computed from the temperature T and density ρ_f as

$$P_{eq} = (1/(2a^2\lambda v_o \rho_f))((k_o + 2a(-T_f + T_o)\lambda)v_o \rho_f - \sqrt{v_o \rho_f(k_o^2 v_o \rho_f + 4a\lambda(a - (a + k_o(T_f - T_o))v_o \rho_f))}); \quad (12)$$

Constitutive soil model

The constitutive model is used to compute the stress-strain behaviour for the soil state. The detailed of the constitutive soil model will be presented later.

By the nature of the explicit MPM formulation, we can derive the constitutive law in the updated Lagrangian framework of "small strain - large deformation". Therefore, considering the rotation of the particles (representative element volume) by manipulating the rotation of the Cauchy stress tensor. First, the deformation gradient is decomposed into the polar rotation tensor \mathbf{R}_s^{n+1} and sketch tensor \mathbf{V}_s^{n+1} as

$$\mathbf{F}_s^{n+1} = \mathbf{V}_s^{n+1} \mathbf{R}_s^{n+1} \quad (13)$$

Then, before calling the constitutive model, the stress and strain rate tensor are rotated to the reference configuration as

$$\boldsymbol{\sigma}'^{n*} = (\mathbf{R}_s^{n+1})^T \boldsymbol{\sigma}'^{n*} \mathbf{R}_s^{n+1} \quad (14)$$

$$\delta \boldsymbol{\epsilon}^{n*} = (\mathbf{R}_s^{n+1})^T \delta \boldsymbol{\epsilon}^{n*} \mathbf{R}_s^{n+1} \quad (15)$$

Using the constitutive model with the input tensors $\boldsymbol{\sigma}'^{n*}, \delta \boldsymbol{\epsilon}^{n*}$ to compute the Cauchy stress tensor at the advanced time step $\boldsymbol{\sigma}'^{n+1*}$ then rotating it back to current configuration

$$\boldsymbol{\sigma}'^{n+1} = \mathbf{R}_s^{n+1} \boldsymbol{\sigma}'^{n+1*} (\mathbf{R}_s^{n+1})^T \quad (16)$$

Exchange momentum and energy model

Currently, the energy exchange coefficient is assumed to be constant for the sake of simplicity. For the momentum exchange, we can either select the Darcy's law for laminar flow or other models for non laminar flow

Darcy law

The drag force following the Darcy law is given by

$$\mathbf{f}_{fs} = n^2 \frac{\mu}{\kappa} (\mathbf{U}_s - \mathbf{U}_f) \quad (17)$$

where μ is the fluid viscosity, κ is the intrinsic permeability of soil which can be calculated using Kozeny-Carman equation for sand

$$\kappa = A \frac{D_p^2 n^3}{(1-n)^2} \quad (18)$$

where D_p is average diameter of sand grains and A is empirical parameter considering the tortuosity effect.

Forcheimer law for non-Darcy flow

Several models are developed for non-laminar flow (see Yazdchi and Luding (2012) for the summary). For example, the drag force following the Forcheimer law is given by

$$\mathbf{f}_{fs} = n^2 \frac{\mu}{\kappa} (\mathbf{U}_s - \mathbf{U}_f) + \beta n^3 |\mathbf{U}_s - \mathbf{U}_f| (\mathbf{U}_s - \mathbf{U}_f) \quad (19)$$

where $\beta = B(1-n)/(n^3 D_p)$ with B is the empirical parameter.

Solving momentum exchange with an implicit solve

In this study, we apply the Darcy's law to compute the momentum exchange term. The derivation of the implicit integration for the momentum exchange is presented in the section 'Momentum exchange with an implicit solve'. The linear equations has the form:

$$\begin{vmatrix} (1 + \beta_{12}) & -\beta_{12} \\ -\beta_{21} & (1 + \beta_{21}) \end{vmatrix} \begin{vmatrix} \Delta \mathbf{U}_f \\ \Delta \mathbf{U}_s \end{vmatrix} = \begin{vmatrix} \beta_{12} (\mathbf{U}_s^* - \mathbf{U}_f^*) \\ \beta_{21} (\mathbf{U}_f^* - \mathbf{U}_s^*) \end{vmatrix}$$

where the intermediate velocity can be calculated by

$$\begin{aligned} \mathbf{U}_f^* &= \mathbf{U}_f^n + \Delta t \left(-\frac{\nabla P_f^{n+1}}{\bar{\rho}_f^n} + \frac{\nabla \cdot \boldsymbol{\tau}_f^n}{\bar{\rho}_f^n} + \mathbf{b} \right) \\ \mathbf{U}_s^* &= \mathbf{U}_s^n + \Delta t \left(\frac{\nabla \cdot \boldsymbol{\sigma}'^n}{\bar{\rho}_s^n} - \frac{\nabla P_f^{n+1}}{\bar{\rho}_s^n} + \mathbf{b} \right) \end{aligned} \quad (20)$$

Also, the momentum exchange coefficient can be computed at every time step as $\beta_{12} = K/\bar{\rho}_f^n$ and $\beta_{21} = K/\bar{\rho}_s^n$ with Cauchy coefficient $K = (n^n)^2 \mu / \kappa^n$.

Smagorinsky turbulent model

The turbulent effect is modelled using a statistical approach namely large-eddy simulation. In this approach, the micro-scale turbulent influence in the dynamics of the macro-scale motion is computed through simple models like Smagorinsky model. the concept is

1. the velocity is split to a filtered component $\bar{\mathbf{U}}$ representing the motion of large eddies, and a residual component \mathbf{U}' .
2. The filtered velocity is computed by solving the filtered Navier-Stokes equation which derived from the original Navier-Stokes equation.
3. The residual stress tensor is calculated using the Smagorinski model.

In the Smagorinsky mode, the residual stress tensor is:

$$\tau_{ij} = 2\mu_{eff}(\bar{S}_{ij} - \frac{1}{3}\delta_{ij}\bar{S}_{kk}) + \frac{1}{3}\delta_{ij}\tau_{kk} \quad (21)$$

where the the strain rate tensor is given by

$$\bar{S}_{ij} = \frac{1}{2}(\frac{\delta \bar{U}_i}{\delta x_j} + \frac{\delta \bar{U}_j}{\delta x_i}) \quad (22)$$

and the effective viscosity is sum of molecular viscosity and turbulent viscosity $\mu_{eff} = \mu + \mu_t$ in which the turbulent viscosity μ_t is calculated by

$$\mu_t = (C_s \Delta)^2 \sqrt{2\bar{S}_{ij}\bar{S}_{ij}} \quad (23)$$

where C_s is the Smagorinsky constant and $\Delta = \sqrt[3]{dxdydz}$ is the grid size that defines the subgrid length scale.

Numerical Implementation

The fluid phase is discretized in the grid with the state variables stored at the centroid of the cells $[\rho_{fc}, \mathbf{U}_{fc}, T_{fc}, \mathbf{v}_{fc}]$ while the solid phase is discretized in the particles with the state variables $[m_{sp}, \mathbf{U}_{sp}, T_{sp}, \boldsymbol{\sigma}'_{sp}]$. The numerical implementation based on the MP-MICE implementation in Uintah from Guilkey et al. (2007). The weak forms of the governing equation are solved using the following steps:

Interpolation from Solid Particle to Grid

The nodal values of the solid state (mass, velocity, temperature, volume) are:

$$\begin{aligned} m_{si}^n &= \sum S_{ip} m_{sp} \\ \mathbf{U}_{si}^n &= \frac{\sum S_{ip} (m\mathbf{U})_{sp}^n}{m_{si}^n} \\ T_{si}^n &= \frac{\sum S_{ip} (mT)_{sp}^n}{m_{si}^n} \\ V_{si}^n &= \frac{\sum S_{ip} (mV)_{sp}^n}{m_{si}^n} \\ \boldsymbol{\sigma}_{si}^n &= \frac{\sum S_{ip} (\boldsymbol{\sigma}V)_{sp}^n}{V_{si}^n} \end{aligned} \quad (24)$$

The nodal internal forces is calculated by

$$\mathbf{f}_{si}^{int,n} = - \sum \nabla S_{ip} (\boldsymbol{\sigma}'_{sp})^n V_{sp}^n \quad (25)$$

The nodal external forces $\mathbf{f}_{si}^{ext,n}$ and extra momentum from contact forces are computed here. The nodal velocity and nodal temperature are applied boundary conditions.

Then we compute the solid cell variables as:

$$\begin{aligned} m_{sc}^n &= \sum S_{ci} m_{si} \\ \rho_{sc}^n &= \frac{m_{sc}^n}{V} \\ \mathbf{U}_{sc}^n &= \sum S_{ci} \mathbf{U}_{si}^n \\ T_{sc}^n &= \sum S_{ci} T_{si}^n \\ V_{sc}^n &= \sum S_{ci} V_{si}^n \\ \boldsymbol{\sigma}_{sc}^n &= \sum S_{ci} \boldsymbol{\sigma}_{si}^n \end{aligned} \quad (26)$$

Compute the porosity and the momentum exchange coefficient

The nodal porosity can be computed by:

$$n_c^n = 1 - \frac{m_{sc}^n}{(\rho_s V_{sc}^n)} \quad (27)$$

The permeability can be computed from porosity using the Kozeny-Carman formula as below:

$$k_c^n = C \frac{(n_c^n)^3}{(1 - n_c^n)^2} \quad (28)$$

Finally, the momentum exchange coefficients are computed for cell-centered and face-centered as

$$\begin{aligned} \beta_{12c} &= \Delta t \frac{(n_c^n)^2 \mu_f}{k_c^n \bar{\rho}_{fc}^n} \\ \beta_{21c} &= \Delta t \frac{(n_c^n)^2 \mu_f}{k_c^n \bar{\rho}_{sc}^n} \\ \beta_{12,FC} &= \Delta t \frac{(\bar{\rho} \beta_{12c})_{f,R}^n + (\bar{\rho} \beta_{12c})_{f,L}^n}{\bar{\rho}_{f,L}^n + \bar{\rho}_{f,R}^n} \\ \beta_{21,FC} &= \Delta t \frac{(\bar{\rho} \beta_{12c})_{f,R}^n + (\bar{\rho} \beta_{12c})_{f,L}^n}{\bar{\rho}_{f,L}^n + \bar{\rho}_{f,R}^n} \end{aligned} \quad (29)$$

Compute equation of state for fluid phase

For the air, it is possible to assume the equation of state for the perfect gas which obeys:

$$P_{eq} = \rho RT \quad (30)$$

where R is the gas constant. For the water, the equation of state (Thomsen Hartka water model) can be used to obtain the relations between the thermodynamic properties of the water.

Compute faced-centered velocity

Following the derivation in the Appendix: Advanced Fluid Pressure, we first compute the fluid face-centered velocity as

$$\mathbf{U}_{f,FC}^* = \frac{(\bar{\rho} \mathbf{U})_{f,FC}^n}{\bar{\rho}_{f,FC}^n} + \Delta t \left(-\frac{\nabla^{FC} P_{eq}}{\bar{\rho}_{f,FC}^n} + \frac{\nabla^{FC} \cdot \boldsymbol{\tau}^n}{\bar{\rho}_{s,FC}} + \mathbf{b} \right) \quad (31)$$

The equation (31) is discretized in three dimension (noted that $\nabla^{FC} \cdot \boldsymbol{\tau} = 0$), for example the discretized equation in the x direction is

$$U_{fx}^* = \frac{(\bar{\rho} U)_{fx,R}^n + (\bar{\rho} U)_{fx,L}^n}{\bar{\rho}_{fx,L}^n + \bar{\rho}_{fx,R}^n} + \Delta t \left(-\frac{2(v_{fx,L}^n v_{fx,R}^n)}{v_{fx,L}^n + v_{fx,R}^n} \frac{P_{eqx,R} - P_{eqx,L}}{\Delta x} + b_x \right) \quad (32)$$

The face-centered solid velocity can be calculated as

$$\mathbf{U}_{s,FC}^* = \frac{(\bar{\rho} \mathbf{U})_{s,FC}^n}{\bar{\rho}_{s,FC}^n} + \Delta t \left(\frac{\nabla^{FC} \cdot \boldsymbol{\sigma}_c'^n}{\bar{\rho}_{s,FC}} - \frac{\nabla^{FC} P_{eq}}{\rho_s} + \mathbf{b} \right) \quad (33)$$

The equation (33) is discretized in three dimension (noted that $\nabla^{FC} \cdot \sigma_{ij} = 0$ with $i \neq j$), for example the discretized equation in the x direction is

$$U_{sx}^* = \frac{(\bar{\rho}U)_{sx,R}^n + (\bar{\rho}U)_{sx,L}^n}{\bar{\rho}_{sx,L}^n + \bar{\rho}_{sx,R}^n} + \Delta t \left(\frac{2(\sigma_{xx,R} - \sigma_{xx,L})}{(\bar{\rho}_{sx,L}^n + \bar{\rho}_{sx,R}^n)\Delta x} - \frac{P_{eqx,R} - P_{eqx,L}}{\rho_s \Delta x} + b_x \right) \quad (34)$$

Computing the modified faced-centered velocity \mathbf{U}_{FC}^L considering the momentum exchange

$$\begin{aligned} \mathbf{U}_{f,FC}^L &= \mathbf{U}_{f,FC}^* + \Delta \mathbf{U}_{f,FC} \\ \mathbf{U}_{s,FC}^L &= \mathbf{U}_{s,FC}^* + \Delta \mathbf{U}_{s,FC} \end{aligned} \quad (35)$$

By solving the linear equation below to obtain the increment of velocity

$$\begin{vmatrix} (1 + \beta_{12,FC}) & -\beta_{12,FC} \\ -\beta_{21,FC} & (1 + \beta_{21,FC}) \end{vmatrix} \begin{vmatrix} \Delta \mathbf{U}_{f,FC} \\ \Delta \mathbf{U}_{s,FC} \end{vmatrix} = \begin{vmatrix} \beta_{12,FC}(\mathbf{U}_{s,FC}^* - \mathbf{U}_{f,FC}^*) \\ \beta_{21,FC}(\mathbf{U}_{f,FC}^* - \mathbf{U}_{s,FC}^*) \end{vmatrix}$$

Compute advanced fluid pressure (implicit scheme)

We solve the generalized Poisson's equation below by employing a preconditioned conjugate gradient technique with a multi-grid pre-conditioner

$$\left(\kappa - \nabla^c \frac{\Delta t}{\bar{\rho}_{f,FC}} \cdot \nabla^{FC} \right) \Delta P_c^n = -\nabla^c \cdot \mathbf{U}_{f,FC}^L \quad (36)$$

The advanced fluid pressure at cell center is

$$P_c^{n+1} = P_{eq} + \Delta P_c^n \quad (37)$$

Finally, the faced-centered advanced fluid pressure is

$$P_{f,FC}^{n+1} = \left(\frac{P_{f,L}^{n+1}}{\bar{\rho}_{f,L}^n} + \frac{P_{f,R}^{n+1}}{\bar{\rho}_{f,R}^n} \right) / \left(\frac{1}{\bar{\rho}_{f,L}^n} + \frac{1}{\bar{\rho}_{f,R}^n} \right) = \left(\frac{P_{f,L}^{n+1} \bar{\rho}_{f,R}^n + P_{f,R}^{n+1} \bar{\rho}_{f,L}^n}{\bar{\rho}_{f,L}^n \bar{\rho}_{f,R}^n} \right) \quad (38)$$

Compute viscous shear stress term of the fluid phase

This part compute the viscous shear stress $\Delta(m\mathbf{U})_{fc,\tau}$ for a single viscous compressible Newtonian fluid and optionally shear stress induced by the turbulent model.

Compute nodal internal temperature of the solid phase

The nodal internal temperature rate is computed based on the heat conduction model

$$dT_{si}^L = \frac{(\Delta W_{si}^n + \nabla^i \cdot \mathbf{q}_{si}^n)}{m_{si}^n} \quad (39)$$

where $\Delta W_{si}^n = \boldsymbol{\sigma}' : \nabla \mathbf{U}_s$ is the mechanical work rate computed from the constitutive model. The nodal internal temperature is calculated by

$$T_{si}^L = T_{si}^n + dT_{si}^L \quad (40)$$

Compute and integrate acceleration of the solid phase

After interpolating from material points to the nodes, the nodal acceleration and velocity are calculate by

$$\mathbf{a}_{si}^{L-} = \frac{\mathbf{f}_{si}^{int,n} + \mathbf{f}_{si}^{ext,n}}{m_{si}^n} + \mathbf{g} \quad (41)$$

$$\mathbf{U}_{si}^{L-} = \mathbf{U}_{si}^n + \mathbf{a}_{si}^{L-} \Delta t \quad (42)$$

Compute Lagrangian value (mass, momentum and energy)

For the fluid phase, the linear momentum rate, the energy rate are

$$\Delta(m\mathbf{U})_{fc} = V n_c^n \nabla^c P_{fc}^{n+1} + \Delta(m\mathbf{U})_{fc,\tau} + V \bar{\rho}_{fc}^n \mathbf{g} \quad (43)$$

$$\Delta(me)_{fc} = V n_c^n P_{fc}^{n+1} \nabla^c \cdot \mathbf{U}_{f,FC}^* + \nabla^c \cdot \mathbf{q}_{fc}^n \quad (44)$$

The Lagrangian value of the mass, linear momentum and energy of fluid phase without momentum exchange are

$$m_{fc}^L = V \bar{\rho}_{fc}^n \quad (45)$$

$$(m\mathbf{U})_{fc}^{L-} = V \bar{\rho}_{fc}^n \mathbf{U}_{fc}^n + \Delta(m\mathbf{U})_{fc} \quad (46)$$

$$(me)_{fc}^{L-} = V \bar{\rho}_{fc}^n T_{fc}^n c_v + \Delta(me)_{fc} \quad (47)$$

For the solid phase, the Lagrangian value of the linear momentum and energy of solid phase are

$$m_{sc}^L = m_{sc}^n \quad (48)$$

$$(m\mathbf{U})_{sc}^{L-} = \sum S_{ci} m_{si}^n \mathbf{U}_{si}^{L-} + V (1 - n_c^n) \nabla^c P_{fc}^{n+1} \quad (49)$$

$$(me)_{sc}^{L-} = \sum S_{ci} m_{si}^n T_{si}^L \quad (50)$$

To consider the momentum exchange, the Lagrangian velocity is modified as

$$\begin{aligned} \mathbf{U}_{fc}^L &= \mathbf{U}_{fc}^{L-} + \Delta \mathbf{U}_{fc} \\ \mathbf{U}_{sc}^L &= \mathbf{U}_{sc}^{L-} + \Delta \mathbf{U}_{sc} \end{aligned} \quad (51)$$

where the cell-centered intermediate velocity can be calculated by

$$\begin{aligned} \mathbf{U}_{fc}^{L-} &= \frac{(m\mathbf{U})_{fc}^{L-}}{m_{fc}^L} \\ \mathbf{U}_{sc}^{L-} &= \frac{(m\mathbf{U})_{sc}^{L-}}{m_{sc}^L} \end{aligned} \quad (52)$$

And the increment of the velocity can be computed by solving the linear equation below

$$\begin{vmatrix} (1 + \beta_{12,c}) & -\beta_{12,c} \\ -\beta_{21,c} & (1 + \beta_{21,c}) \end{vmatrix} \begin{vmatrix} \Delta \mathbf{U}_{fc} \\ \Delta \mathbf{U}_{sc} \end{vmatrix} = \begin{vmatrix} \beta_{12,c} (\mathbf{U}_{sc}^{L-} - \mathbf{U}_{fc}^{L-}) \\ \beta_{21,c} (\mathbf{U}_{fc}^{L-} - \mathbf{U}_{sc}^{L-}) \end{vmatrix}$$

Finally, we obtain the cell-centered solid acceleration and temperature rate as

$$d\mathbf{U}_{sc}^L = \frac{(\mathbf{m}\mathbf{U})_{sc}^L - (\mathbf{m}\mathbf{U})_{sc}^n}{m_{sc}^L \Delta t} \quad (53)$$

$$dT_{sc}^L = \frac{(me)_{sc}^L - (me)_{sc}^n}{m_{sc}^L c_v \Delta t} \quad (54)$$

Compute Lagrangian specific volume of the fluid phase

To compute the Lagrangian value of the specific volume of the fluid phase, we need to compute the Lagrangian temperature rate as below

$$T_{fc}^{n+1} = \frac{(me)_{fc}^L}{m_{fc}^L c_v} \quad (55)$$

$$\frac{D_f T_{fc}}{Dt} = \frac{T_{fc}^{n+1} - T_{fc}^n}{\Delta t} \quad (56)$$

As such, the Lagrangian specific volume rate is

$$\Delta(m\mathbf{v})_{fc} = V \nabla^c \cdot ((1 - n_c^n) \mathbf{U}_{sc}^L + n_c^n \mathbf{U}_{fc}^L) \quad (57)$$

Finally, the Lagrangian specific volume is

$$(m\mathbf{v})_{fc}^L = V \bar{\rho}_{fc}^n \mathbf{v}_{fc}^n + \Delta(m\mathbf{v})_{fc} \quad (58)$$

Compute advection term and advance in time

The time advanced mass, linear momentum, energy and specific volume are:

$$m_{fc}^{n+1} = m_{fc}^L - \Delta t \text{Advection}(\bar{\rho}_{fc}^L, \mathbf{U}_{f,FC}^L) \quad (59)$$

$$(\mathbf{m}\mathbf{U})_{fc}^{n+1} = (\mathbf{m}\mathbf{U})_{fc}^L - \Delta t \text{Advection}((\bar{\rho}\mathbf{U})_{fc}^L, \mathbf{U}_{f,FC}^L) \quad (60)$$

$$(me)_{fc}^{n+1} = (me)_{fc}^L - \Delta t \text{Advection}((\bar{\rho}c_v T)_{fc}^L, \mathbf{U}_{f,FC}^L) \quad (61)$$

$$(m\mathbf{v})_{fc}^{n+1} = (m\mathbf{v})_{fc}^L - \Delta t \text{Advection}((\bar{\rho}\mathbf{v})_{fc}^L, \mathbf{U}_{f,FC}^L) \quad (62)$$

Finally, the state variables of the fluid phase of the next time step are

$$\bar{\rho}_{fc}^{n+1} = \frac{m_{fc}^{n+1}}{V} \quad (63)$$

$$\mathbf{U}_{fc}^{n+1} = \frac{(\mathbf{m}\mathbf{U})_{fc}^{n+1}}{m_{fc}^{n+1}} \quad (64)$$

$$T_{fc}^{n+1} = \frac{(me)_{fc}^{n+1}}{m_{fc}^{n+1}} \quad (65)$$

$$\mathbf{v}_{fc}^{n+1} = \frac{(m\mathbf{v})_{fc}^{n+1}}{m_{fc}^{n+1}} \quad (66)$$

Interpolate from cell to node of the solid phase

First we interpolate the acceleration, velocity and temperature to the node

$$\mathbf{a}_{si}^n = \sum S_{ci} d\mathbf{U}_{sc}^L \quad (67)$$

$$\mathbf{U}_{si}^{n+1} = \sum S_{ci} d\mathbf{U}_{sc}^L \Delta t \quad (68)$$

$$dT_{si}^n = \sum S_{ci} dT_{sc}^L \quad (69)$$

Then the boundary condition and contact forces are applied to the nodal velocity and the acceleration is modified by

$$\mathbf{a}_{si}^n = \frac{\mathbf{v}_{si}^{n+1} - \mathbf{v}_{si}^n}{\Delta t} \quad (70)$$

Update the particle variables

The state variables of the solid phase $[\mathbf{U}_{sp}^{n+1}, \mathbf{x}_{sp}^{n+1}, \nabla \mathbf{U}_{sp}^{n+1}, T_{sp}^{n+1}, \mathbf{F}_{sp}^{n+1}, V_{sp}^{n+1}]$ (velocity, position, velocity gradient, temperature, deformation gradient, volume) are updated here

$$\mathbf{U}_{sp}^{n+1} = \mathbf{U}_{sp}^n + \sum S_{sp} \mathbf{a}_{si}^n \Delta t \quad (71)$$

$$\mathbf{x}_{sp}^{n+1} = \mathbf{x}_{sp}^n + \sum S_{sp} \mathbf{U}_{si}^{n+1} \Delta t \quad (72)$$

$$\nabla \mathbf{U}_{sp}^{n+1} = \sum \nabla S_{sp} \mathbf{U}_{si}^{n+1} \quad (73)$$

$$T_{sp}^{n+1} = T_{sp}^n + \sum S_{sp} dT_{si}^n \Delta t \quad (74)$$

$$\mathbf{F}_{sp}^{n+1} = (\mathbf{I} + \nabla \mathbf{U}_{sp}^{n+1} \Delta t) \mathbf{F}_{sp}^n \quad (75)$$

$$V_{sp}^{n+1} = \det(\mathbf{F}_{sp}^{n+1}) V_{sp}^o \quad (76)$$

Finally, the effective stress $(\boldsymbol{\sigma}')^{n+1}$ is updated from the constitutive model.

Appendix

Before deriving the governing equation, we give some definition (following Kashiwa (2001)) as below:

$$-\frac{1}{V} \left[\frac{\partial V}{\partial p} \right] \equiv \kappa_f \quad \text{isothermal compressibility of fluid} \quad (77)$$

$$\frac{1}{V} \left[\frac{\partial V}{\partial T} \right] \equiv \alpha_f \quad \text{constant pressure thermal expansivity of fluid} \quad (78)$$

Then, the rate of volume with incompressible solid grains are calculated as below:

$$\begin{aligned} \frac{1}{V} \frac{D_f V}{Dt} &= \frac{1}{V} \left(\left[\frac{\partial V}{\partial p} \right] \frac{D_f p}{Dt} + \left[\frac{\partial V}{\partial T} \right] \frac{D_f T}{Dt} \right) = \frac{1}{V} \left(-\kappa \frac{D_f p}{Dt} + \alpha \frac{D_f T}{Dt} \right) \\ &= -(-\nabla \cdot \mathbf{U}_f + \alpha_f \frac{D_f T_f}{Dt}) + \alpha_f \frac{D_f T_f}{Dt} = \nabla \cdot \mathbf{U}_f \end{aligned} \quad (79)$$

$$\frac{1}{V} \frac{D_s V}{Dt} = \nabla \cdot \mathbf{U}_s \quad (80)$$

It is also convenient to define the Lagrangian derivative for a state variable f as:

$$\frac{D_f f}{Dt} = \frac{\partial f}{\partial t} + \mathbf{U}_f \cdot \nabla f \quad \frac{D_s f}{Dt} = \frac{\partial f}{\partial t} + \mathbf{U}_s \cdot \nabla f \quad (81)$$

Evolution of porosity

Solving the solid mass balance equation (4) with the definition of solid mass in equation (2), it leads to the rate of porosity as below:

$$\frac{D_s m_s}{Dt} = \frac{D_s ((1-n)\rho_s V)}{Dt} = \rho_s V \frac{D_s (1-n)}{Dt} + (1-n)V \frac{D_s \rho_s}{Dt} + (1-n)\rho_s \frac{D_s V}{Dt} = 0 \quad (82)$$

The soil grains are assumed to be incompressible, therefore, term 2 in the right hand side is zero.

$$V \frac{D_s (1-n)}{Dt} + (1-n) \frac{D_s V}{Dt} = 0 \quad (83)$$

Dividing all terms with V with the equation (79), it leads to:

$$\frac{D_s n}{Dt} = \frac{\partial n}{\partial t} + \mathbf{U}_s \cdot \nabla n = (1-n) \nabla \cdot \mathbf{U}_s \quad (84)$$

Finally, we get:

$$\frac{\partial n}{\partial t} = (1-n) \nabla \cdot \mathbf{U}_s - \mathbf{U}_s \cdot \nabla n \quad (85)$$

Evolution of specific volume

Solving the fluid mass balance equation (4) with the definition of fluid mass in equation (2), it leads to:

$$\frac{D_f m_f}{Dt} = \frac{D_f (n \rho_f V)}{Dt} = \rho_f V \frac{D_f n}{Dt} + n V \frac{D_f \rho_f}{Dt} + n \rho_f \frac{D_f V}{Dt} = 0 \quad (86)$$

Dividing all terms with V and converting the fluid density ρ_f to the specific volume v_f , it becomes:

$$\frac{D_f n}{Dt} - \bar{\rho}_f \frac{D_f v_f}{Dt} + \frac{n}{V} \frac{D_f V}{Dt} = 0 \quad (87)$$

The Lagrangian porosity can be written as:

$$\frac{D_f n}{Dt} = \frac{\partial n}{\partial t} + \mathbf{U}_f \cdot \nabla n \quad (88)$$

Combining equations (79), (85), (87), (88) we get:

$$\bar{\rho}_f \frac{D_f v_f}{Dt} = \nabla \cdot ((1-n)\mathbf{U}_s + n\mathbf{U}_f) \quad (89)$$

Momentum conservation

The linear momentum balance equation for the fluid phase based on mixture theory is:

$$\frac{1}{V} \frac{D_f (m_f \mathbf{U}_f)}{Dt} = \nabla \cdot (-n p_f \mathbf{I}) + \nabla \cdot \boldsymbol{\tau}_f + \bar{\rho}_f \mathbf{b} + \mathbf{f}_{sf} + \mathbf{f}_b \quad (90)$$

On the right hand side, the first term is the divergence of partial fluid phase stress, the second term is the body force, the third term is the drag force (momentum exchange) and the fourth term is the buoyant force described in Drumheller (2000) for the immiscible mixtures. The buoyant force is in the form:

$$\mathbf{f}_b = \boldsymbol{\sigma}_f \nabla(n) \quad (91)$$

As a result, the linear momentum balance equation for fluid phase becomes:

$$\frac{1}{V} \frac{D_f (m_f \mathbf{U}_f)}{Dt} = -n \nabla p_f + \nabla \cdot \boldsymbol{\tau}_f + \bar{\rho}_f \mathbf{b} + \mathbf{f}_{sf} \quad (92)$$

The Reynolds stress component can be included in the term $\boldsymbol{\tau}_f$ to consider the turbulent effects if needed. To derive the linear momentum balance equation for the solid phase, we begin with the linear momentum balance equation for the mixture as:

$$\frac{1}{V} \frac{D_f (m_f \mathbf{U}_f)}{Dt} + \frac{1}{V} \frac{D_s (m_s \mathbf{U}_s)}{Dt} = \nabla \cdot (\boldsymbol{\sigma}) + \bar{\rho}_f \mathbf{b} + \bar{\rho}_s \mathbf{b} \quad (93)$$

Combining Terzaghi's equation (3) and subtracting both sides with equation (92), we obtain the linear momentum balance equation for the solid phase as:

$$\frac{1}{V} \frac{D_s (m_s \mathbf{U}_s)}{Dt} = \nabla \cdot (\boldsymbol{\sigma}') - (1-n) \nabla p_f + \bar{\rho}_s \mathbf{b} - \mathbf{f}_{sf} \quad (94)$$

Energy conservation

We adopt the general form of the total energy balance equation for the porous media from Hassanizadeh (1986), the total energy balance equation for the fluid phase is:

$$\frac{1}{V} \frac{D_f(m_f(e_f + 0.5\mathbf{U}_f^2))}{Dt} = \nabla \cdot (-np_f \mathbf{I}) \cdot \mathbf{U}_f + \nabla \cdot \mathbf{q}_f + (\bar{\rho}_f \mathbf{b}) \cdot \mathbf{U}_f + \mathbf{f}_{sf} \cdot \mathbf{U}_f + q_{sf} \quad (95)$$

Applying the product rule $D(m\mathbf{U}^2) = D(m\mathbf{U} \cdot \mathbf{U}) = 2\mathbf{U} \cdot D(m\mathbf{U})$, the left hand side of equation (95) becomes:

$$\frac{1}{V} \frac{D_f(m_f(e_f + 0.5\mathbf{U}_f^2))}{Dt} = \frac{1}{V} \frac{D_f(m_f e_f)}{Dt} + \frac{1}{V} \frac{D_f(m_f \mathbf{U}_f)}{Dt} \cdot \mathbf{U}_f \quad (96)$$

Combining equations (92), (95), (96), we obtain the final form of the internal energy balance equation for the fluid phase as:

$$\frac{1}{V} \frac{D_f(m_f e_f)}{Dt} = -\bar{\rho}_f p \frac{D_f \mathbf{U}_f}{Dt} + \nabla \cdot \mathbf{q}_f + q_{sf} \quad (97)$$

On the right hand side, the terms include the average pressure-volume work, the average viscous dissipation, the thermal transport and the energy exchange between solid and fluid respectively. The heat flux is $\mathbf{q}_f = \bar{\rho}_f \alpha_f \nabla T_f$. To derive the internal energy balance equation for the solid phase, we begin with the total energy balance equation for the mixture based on Hassanizadeh (1986) as:

$$\begin{aligned} \frac{1}{V} \frac{D_f(m_f(e_f + 0.5\mathbf{U}_f^2))}{Dt} + \frac{1}{V} \frac{D_s(m_s(e_s + 0.5\mathbf{U}_s^2))}{Dt} &= \nabla \cdot (-np_f \mathbf{I}) \cdot \mathbf{U}_f \\ &+ \nabla \cdot (\boldsymbol{\sigma}' - (1-n)p_f \mathbf{I}) \cdot \mathbf{U}_s + (-np_f \mathbf{I}) : \nabla \mathbf{U}_f + (\boldsymbol{\sigma}' - (1-n)p_f \mathbf{I}) : \nabla \mathbf{U}_s \\ &+ (\bar{\rho}_f \mathbf{b}) \cdot \mathbf{U}_f + (\bar{\rho}_s \mathbf{b}) \cdot \mathbf{U}_s + \nabla \cdot \mathbf{q}_f + \nabla \cdot \mathbf{q}_s + \mathbf{f}_{sf} \cdot (\mathbf{U}_f - \mathbf{U}_s) \end{aligned} \quad (98)$$

Subtracting equation (98) to equations (95) and (94), we obtained the internal energy balance equation for solid phase as:

$$\frac{1}{V} \frac{D_s(m_s e_s)}{Dt} = \boldsymbol{\sigma}' : \nabla \mathbf{U}_s + \nabla \cdot \mathbf{q}_s - q_{sf} \quad (99)$$

On the right hand side, the terms include the mechanical work, thermal transport and energy exchange between solid and fluid respectively. The heat flux is $\mathbf{q}_s = \bar{\rho}_s \alpha_s \nabla T_s$.

Advanced Fluid Pressure

The discretization of the pressure equation begins with the Lagrangian face-centered velocity and the equation for the pressure

$$\bar{\rho}_{f,FC} \frac{\mathbf{U}_{f,FC}^{n+1} - \mathbf{U}_{f,FC}^n}{dt} = n \nabla^{FC} P_{fc}^{n+1} + \bar{\rho}_{f,FC} \mathbf{b} \quad (100)$$

$$\kappa \frac{dP}{dt} = \nabla^c \cdot \mathbf{U}_{f,FC}^{n+1} \quad (101)$$

The divergence of the equation (100) with $\nabla \cdot \mathbf{b} = 0$ is

$$\nabla^c \cdot \mathbf{U}_{f,FC}^{n+1} - \nabla^c \cdot \mathbf{U}_{f,FC}^n = \nabla^c \frac{\Delta t}{\bar{\rho}_{f,FC}^n} \cdot \nabla^{FC} (P_{fc}^n + \Delta P_{fc}^n) \quad (102)$$

To solve this equation, we define the face-centered intermediate velocity $\mathbf{U}_{f,FC}^*$ as:

$$\bar{\rho}_{f,FC} \frac{\mathbf{U}_{f,FC}^* - \mathbf{U}_{f,FC}^n}{\Delta t} = n \nabla^{FC} P_{fc}^n + \bar{\rho}_{f,FC} \mathbf{b} \quad (103)$$

The divergence of the equation (103) is

$$\nabla^c \cdot \mathbf{U}_{f,FC}^* - \nabla^c \cdot \mathbf{U}_{f,FC}^n = \nabla^c \frac{\Delta t}{\bar{\rho}_{f,FC}^n} \cdot \nabla^{FC} P_{fc}^n \quad (104)$$

Combining equations (101, 102, 104), it leads to

$$\left(\kappa - \nabla^c \frac{\Delta t}{\bar{\rho}_{f,FC}^n} \cdot \nabla^{FC} \right) \Delta P_{fc}^n = -\nabla^c \cdot \mathbf{U}_{f,FC}^* \quad (105)$$

When the fluid is incompressible, κ approaches to zero and the equation (105) becomes the Poisson's equation for the incompressible fluid flow.

Momentum exchange with an implicit solve

Considering the fluid momentum balance equation as

$$(m\mathbf{U})_{f,FC}^{n+1} = (m\mathbf{U})_{f,FC}^n - \Delta t (V n \nabla^{FC} P_{fc}^n + m_f \mathbf{b}) + V K \Delta t (\mathbf{U}_{s,FC}^{n+1} - \mathbf{U}_{f,FC}^{n+1}) \quad (106)$$

Assuming $m_{f,FC}^{n+1} = m_{f,FC}^n$ we get

$$\mathbf{U}_{f,FC}^{n+1} = \mathbf{U}_{f,FC}^n - \Delta t \left(\frac{\nabla^{FC} P_{fc}^n}{\bar{\rho}_{f,FC}^n} + \mathbf{b} \right) + \frac{\Delta t K}{\bar{\rho}_{f,FC}^n} (\mathbf{U}_{s,FC}^{n+1} - \mathbf{U}_{f,FC}^{n+1}) \quad (107)$$

As defined in the section 'Advanced Fluid Pressure', the face-centered intermediate fluid velocity $\mathbf{U}_{f,FC}^* = \Delta t (\nabla^{FC} P_{fc}^n / \bar{\rho}_{f,FC}^n + \mathbf{b})$ leading to

$$\mathbf{U}_{f,FC}^{n+1} = \mathbf{U}_{f,FC}^* + \frac{\Delta t K}{\bar{\rho}_{f,FC}^n} (\mathbf{U}_{s,FC}^{n+1} - \mathbf{U}_{f,FC}^{n+1}) \quad (108)$$

Considering the solid momentum balance equation as

$$(m\mathbf{U})_{s,FC}^{n+1} = (m\mathbf{U})_{s,FC}^n - \Delta t (V \nabla^{FC} \cdot \boldsymbol{\sigma}'^n - V(1-n) \nabla^{FC} P_{fc}^n + m_s \mathbf{b}) - V K \Delta t (\mathbf{U}_{s,FC}^{n+1} - \mathbf{U}_{f,FC}^{n+1}) \quad (109)$$

We define the face-centered intermediate solid velocity as $\mathbf{U}_{s,FC}^* = \Delta t (\nabla^{FC} \cdot \boldsymbol{\sigma}'^n / \bar{\rho}_{s,FC} - \nabla^{FC} P_{fc}^n / \rho_s + \mathbf{b})$ leading to

$$\mathbf{U}_{s,FC}^{n+1} = \mathbf{U}_{s,FC}^* - \frac{\Delta t K}{\bar{\rho}_{s,FC}^n} (\mathbf{U}_{s,FC}^{n+1} - \mathbf{U}_{f,FC}^{n+1}) \quad (110)$$

Combining equation (108) and (110) we get

$$\begin{aligned} \mathbf{U}_{f,FC}^* + \Delta \mathbf{U}_{f,FC} &= \mathbf{U}_{f,FC}^* + \frac{\Delta t K}{\bar{\rho}_{f,FC}^n} (\mathbf{U}_{s,FC}^* + \Delta \mathbf{U}_{s,FC} - \mathbf{U}_{f,FC}^* - \Delta \mathbf{U}_{f,FC}) \\ \mathbf{U}_{s,FC}^* + \Delta \mathbf{U}_{s,FC} &= \mathbf{U}_{s,FC}^* - \frac{\Delta t K}{\bar{\rho}_{s,FC}^n} (\mathbf{U}_{s,FC}^* + \Delta \mathbf{U}_{s,FC} - \mathbf{U}_{f,FC}^* - \Delta \mathbf{U}_{f,FC}) \end{aligned} \quad (111)$$

Rearranging the equation (111), it leads to the linear system of equations

$$\begin{vmatrix} (1 + \beta_{12,FC}) & -\beta_{12,FC} \\ -\beta_{21,FC} & (1 + \beta_{21,FC}) \end{vmatrix} \begin{vmatrix} \Delta \mathbf{U}_{f,FC} \\ \Delta \mathbf{U}_{s,FC} \end{vmatrix} = \begin{vmatrix} \beta_{12,FC} (\mathbf{U}_{s,FC}^* - \mathbf{U}_{f,FC}^*) \\ \beta_{21,FC} (\mathbf{U}_{f,FC}^* - \mathbf{U}_{s,FC}^*) \end{vmatrix}$$

Solving this linear equations with $\beta_{12,FC} = (\Delta t K) / \bar{\rho}_{f,FC}^n$ and $\beta_{21,FC} = (\Delta t K) / \bar{\rho}_{s,FC}^n$. Similar derivation can be performed to computed the cell-center velocity increment leading to

$$\begin{vmatrix} (1 + \beta_{12c}) & -\beta_{12c} \\ -\beta_{21c} & (1 + \beta_{21c}) \end{vmatrix} \begin{vmatrix} \Delta \mathbf{U}_{fc} \\ \Delta \mathbf{U}_{sc} \end{vmatrix} = \begin{vmatrix} \beta_{12c} (\mathbf{U}_{sc}^* - \mathbf{U}_{fc}^*) \\ \beta_{21c} (\mathbf{U}_{fc}^* - \mathbf{U}_{sc}^*) \end{vmatrix}$$

with $\beta_{12c} = (\Delta t K) / \bar{\rho}_{fc}^n$ and $\beta_{21c} = (\Delta t K) / \bar{\rho}_{sc}^n$ and the cell-centered intermediate velocity can be calculated by

$$\begin{aligned} \mathbf{U}_{fc}^* &= \mathbf{U}_{fc}^n + \Delta t \left(-\frac{\nabla P_{fc}^{n+1}}{\bar{\rho}_{fc}^n} + \frac{\nabla \cdot \boldsymbol{\tau}_{fc}^n}{\bar{\rho}_{fc}^n} + \mathbf{b} \right) \\ \mathbf{U}_{sc}^* &= \mathbf{U}_{sc}^n + \Delta t \left(\frac{\nabla \cdot \boldsymbol{\sigma}_c'^n}{\bar{\rho}_{sc}^n} - \frac{\nabla P_{fc}^{n+1}}{\rho_s} + \mathbf{b} \right) \end{aligned} \quad (112)$$

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