A Unified Formulation of the Segregated Class of Algorithms for Multi-Fluid Flow at All Speeds

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Abstract

The class of segregated pressure-based, single-fluid, all speed flow algorithms is extended to multi-fluid flow simulations using a unified, compact, and easy to understand notation. Depending on the constraint equation used to derive the pressure correction equation, the extended multi-fluid flow algorithms are shown to fall under two categories denoted in this work by the Mass Conservation Based Algorithms (MCBA) and the Geometric Conservation Based Algorithms (GCBA). This paper deals with the formulation of both types of algorithms and presents several techniques developed to promote and accelerate their convergence. Moreover, the differences and similarities between the two categories are explained and the mass conservation-based formulation is shown to represent a subset of the geometric-based formulation.

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Nomenclature

$A_P^{(k)}$,..	coefficients in the discretized equation for $\phi^{(k)}$.
$B_P^{(k)}$	source term in the discretized equation for $\phi^{(k)}$.
$\mathbf{B}^{(k)}$	body force per unit volume of fluid/phase k.
$C_\rho^{(k)}$	coefficient equals to $1/R^{(k)}T^{(k)}$.
$\hat{\mathbf{d}}_{\mathrm{f}}$	covariant unit vector (i.e. in the direction of $\mathbf{d}_{\mathrm{f}}$).
$D_P^{(k)}[\phi^{(k)}]$	the *D* operator.
$\tilde{D}_P^{(k)}[\phi^{(k)}]$	the modified *D* operator.
$\mathbf{D}_P^{(k)}[\phi^{(k)}]$	the vector form of the *D* operator.
$\tilde{\mathbf{D}}_P^{(k)}[\phi^{(k)}]$	the vector form of the modified *D* operator.
$g^{(km)}$	drag function (Eq. (4)).
$H_{\mathrm{P}}[\phi^{(k)}]$	the H operator.
$HI_{\mathrm{P}}[\phi^{(k)}]$	the *HI* operator working on $\phi^{(k)}$ ($\phi^{(k)}=u^{(k)},v^{(k)}$, or $w^{(k)}$).
$HP_P[\phi^{(k)}]$	the *HP* operator working on $\phi^{(k)}$ ($\phi^{(k)}=u^{(k)},v^{(k)}$, or $w^{(k)}$).
$\widetilde{HP}_P[\phi^{(k)}]$	the modified *HP* operator working on $\phi^{(k)}$ ($\phi^{(k)}=u^{(k)},v^{(k)}$, or $w^{(k)}$).
$\mathbf{HP}_P[\mathbf{u}^{(k)}]$	the vector form of the *HP* operator.
$\widetilde{\mathbf{HP}}_P[\mathbf{u}^{(k)}]$	the vector form of the modified *HP* operator.
$\mathbf{HI}_P[\mathbf{u}^{(k)}]$	the vector form of the *HI* operator.
$\mathbf{I}^{(k)}$	inter-phase momentum transfer.
$\mathbf{J}_f^{(k)D}$	diffusion flux of $\phi^{(k)}$ across cell face 'f'.
$\mathbf{J}_f^{(k)C}$	convection flux of $\phi^{(k)}$ across cell face 'f'.
$\dot{M}^{(k)}$	mass source per unit volume.
$\tilde{n}_f$	contravariant unit vector (i.e. in the direction of $\mathbf{S}_{\mathrm{f}}$).
P	pressure.
$\mathrm{Pr}^{(k)}, \mathrm{Pr}_t^{(k)}$	laminar and turbulent Prandtl number for fluid/phase k.
$\dot{q}^{(k)}$	heat generated per unit volume of fluid/phase k.
$Q^{(k)}$	general source term of fluid/phase k.
$r^{(k)}$	volume fraction of fluid/phase k.
$R^{(k)}$	gas constant for fluid/phase k.
$\mathbf{S}_{\mathrm{f}}$	surface vector.

t	time.
$T^{(k)}$	temperature of fluid/phase k.
$U_f^{(k)}$	interface flux velocity $\left(\mathbf{v}_f^{(k)}.\mathbf{S}_f\right)$ of fluid/phase k.
$\mathbf{u}^{(k)}$	velocity vector of fluid/phase k.
$u^{(k)}, v^{(k)}$,..	velocity components of fluid/phase k.
x, y,z	Cartesian coordinates.
$\lVert a, b \rVert$	the maximum of a and b.

Greek Symbols

$\rho^{(k)}$	density of fluid/phase k.
$\Gamma^{(k)}$	diffusion coefficient of fluid/phase k.
$\Phi^{(k)}$	dissipation term in energy equation of fluid/phase k.
$\phi^{(k)}$	general scalar quantity associated with fluid/phase k.
κ_f	space vector equal to $\left(\hat{\mathbf{n}}_f - \gamma\hat{\mathbf{d}}_f\right)S_f$
$\Delta_P\left[\phi^{(k)}\right]$	the Δ operator.
$\mu^{(k)}, \mu_t^{(k)}$	laminar and turbulent viscosity of fluid/phase k.
Ω	cell volume.
$\beta^{(k)}$	thermal expansion coefficient for phase/fluid k.
δt	time step.
γ	scaling factor.

Subscripts

e, w, .	refers to the east, west, … face of a control volume.
E,W,..	refers to the East, West, … neighbors of the main grid point.
f	refers to control volume face f.
P	refers to the P grid point.

Superscripts

C	refers to convection contribution.
D	refers to diffusion contribution.
(k)	refers to fluid/phase k.
$(k)^*, (k)^{**}$,..	refers to first, second, … updated value at the current iteration.
(k) ◐	refers to values of fluid/phase k from the previous iteration.
$(k)'$	refers to correction field of phase/fluid k.

m	refers to fluid/phase m.
old	refers to values from the previous time step.
sx	refers to SIMPLEX.

Introduction

Over the past two decades important advances have taken place in CFD centered around increasing numerical accuracy through the development of high-resolution schemes [1-14] and improving efficiency through devising better solution algorithms [15-21], better solvers [22,23], and increasing use of multigrid techniques [24-27]. While high-resolution schemes, solvers, and multigrid techniques can be applied indiscriminately to the simulation of single-fluid or multi-fluid flows, nearly all developments in solution algorithms have been directed towards the simulation of incompressible, compressible, and more recently all-speed single-fluid flows [28-32]. In this paper, a solution algorithm denotes the procedure used to solve the coupling between the velocity, pressure, mass fraction, and density (for compressible flow) fields.

For the solution of single-fluid flow, a number of segregated solution algorithms have been developed [15,16-18,20,33,34]. Additionally, several techniques to improve the performance, facilitate the implementation, and extend the capability of these algorithms have been advertised. The use of the Momentum Weighted Interpolation Method (MWIM) [35-39] and the Pressure Weighted Interpolation Method (PWIM) [40-44] that have enabled the implementation of these algorithms with a collocated variable arrangement is an example of such techniques. Another example is the extension of the segregated pressure-based algorithms to simulating flows at all speeds [31,32,45-48].

On the other hand, developments in multi-fluid solution algorithms have lagged behind that of single-fluid algorithms, partly because of the higher computational cost involved, and partly due to the numerical difficulties that had to be first addressed in the simulation of single-fluid flow. While the main difficulty in simulating single-fluid flow stems from the coupling between the momentum and continuity equations, in multi-fluid flow situations, this problem is further complicated by the fact that there are as many sets of continuity and momentum equations as there are fluids, that they are all coupled together in various ways (interchange momentum …), and that the fluids share space.

Despite these complexities, successful segregated pressure-based solution algorithms have been devised. These algorithms can be divided into two groups based on the constraint equation used in deriving the pressure equation. Among these algorithms are the Inter-Phase Slip Algorithm (IPSA) and its variants devised by the Spalding Group at Imperial College [49-52] and the Implicit Multi-Field algorithms (IMF) developed by the Los Alamos Scientific Laboratory (LASL) group [53-62]. However, in contrast with the widespread information available on single-fluid solution algorithms, much less information is available on multi-fluid solution algorithms, a fact that has confined their implementation to a small community, slowed their development, and isolated them from the newer developments in single-fluid flow algorithms (PWIM, all speed flows,…).

From the above, it is obvious that the segregated class of algorithms and the many techniques developed for single-fluid flow, have neither been fully extended nor applied to the simulation of multi-fluid flow. The main objective of this work is to extend the applicability of single-fluid algorithms to multi-fluid flow simulations, and to derive these algorithms using a unified, compact, and easy to understand notation that can be expanded systematically to yield the coefficients of the pressure correction equation, thus facilitating the implementation of these algorithms to a wider audience within the CFD community. To this effect, it is shown that all multi-fluid algorithms can be implemented using a two-step procedure, whereby in the first step a multi-fluid pressure equation is derived based either on Volume Conservation [49,63-65] or Mass Conservation [50,63-70]. Then, in the second step, the different segregated single fluid algorithms are applied to the constraint equation, yielding a multi-fluid correction equation that drives the global iterations towards convergence in a manner similar to the pressure correction equation in single-fluid flows.

In what follows, the governing equations for multi-fluid flows are presented and their discretization outlined so as to lay the ground for the derivation of the pressure or pressure-correction equation. Then, using the unified notation, the different multi-fluid algorithms are described and the framework for implementing them explained. For compactness, either the Mass Conservation or the Geometric Conservation form of an algorithm will be given. For the same reason, only the generic forms of the interfacial mass, momentum, and energy transfers are given. Moreover, it should be stressed that the intention of the paper is not to compare the relative performance of the different multi-fluid algorithms, this would be a work in progress; rather, the aim is to unify their formulation.

The Governing Equations

In multi-fluid flows the various components coexist with different concentrations at different locations in the flow domain and move with unequal velocities. Thus, the equations governing multi-fluid flows are the conservation laws of mass, momentum, and energy for each individual fluid in addition to a set of auxiliary relations.

Conservation of mass

The volume fraction $r^{(k)}$, which is the proportion of volumetric space occupied by the k^{th} fluid ($\Omega^{(k)}/\Omega$) along with the k^{th} fluid density, $\rho^{(k)}$, and velocity, $\mathbf{u}^{(k)}$, in order to satisfy the mass-conservation principle, have to obey the differential equation:

$$\frac{\partial\left(r^{(k)}\rho^{(k)}\right)}{\partial t}+\nabla.\left(r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}\right)=r^{(k)}\dot{M}^{(k)} \quad (1)$$

Mass sources are often non-zero, as when one fluid is transformed to another fluid. However, summation over all fluids leads to the following "overall mass-conservation" equation:

$$\sum_k\left(\frac{\partial\left(r^{(k)}\rho^{(k)}\right)}{\partial t}+\nabla.\left(r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}\right)\right)=0 \quad (2)$$

The zero on the right-hand side signifies that the sum of mass sources (generation and loss) is zero.

Conservation of momentum

Denoting the velocity of the k^{th} phase by $\mathbf{u}^{(k)}$, then the momentum equation for the k^{th} phase can be written as:

$$\frac{\partial\left(r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}\right)}{\partial t}+\nabla.\left(r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}\mathbf{u}^{(k)}\right)=\nabla.\left[r^{(k)}\left(\mu^{(k)}+\mu_t^{(k)}\right)\nabla\mathbf{u}^{(k)}\right]+r^{(k)}\left(-\nabla P+\mathbf{B}^{(k)}\right)+\mathbf{I}_M^{(k)} \quad (3)$$

Here P stands for the pressure, which is regarded as being shared by the fluids, $\mathbf{B}^{(k)}$ is the body force per unit volume of phase (k), $\mathbf{I}_M^{(k)}$ is the momentum transfer to phase (k) resulting from interaction with other phases and can be written in the following form

$$\mathbf{I}_M^{(k)}=\sum_{m\neq k}g^{(km)}\left(\mathbf{u}^{(m)}-\mathbf{u}^{(k)}\right) \quad (4)$$

Conservation of energy

Let $T^{(k)}$ be the temperature of the k^{th} phase, the energy equation for the k^{th} phase is then given by:

$$\frac{\partial\left(r^{(k)}\rho^{(k)}T^{(k)}\right)}{\partial t}+\nabla.\left(r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}T^{(k)}\right)=\nabla.\left[r^{(k)}\left(\frac{\mu^{(k)}}{Pr^{(k)}}+\frac{\mu_t^{(k)}}{Pr_t^{(k)}}\right)\nabla T^{(k)}\right] \\ +\frac{r^{(k)}}{c_P^{(k)}}\left\{\beta^{(k)}T^{(k)}\left[\frac{\partial P}{\partial t}+\nabla.\left(P\mathbf{u}^{(k)}\right)-P\nabla.\left(\mathbf{u}^{(k)}\right)\right]+\Phi^{(k)}+\dot{q}^{(k)}\right\}+\frac{I_t^{(k)}}{c_P^{(k)}} \qquad (5)$$

where $\Phi^{(k)}$ is the viscous dissipation function of the k^{th} phase, $\beta^{(k)}$ the thermal expansion coefficient of the k^{th} phase which is equal to $1/T^{(k)}$ for an ideal gas, and $I_t^{(k)}$ is the interfacial energy transfer to phase (k).

Turbulence Modeling

The effect of turbulence on interfacial mass, momentum, and energy transfer is a difficult modeling task and is an active area of research. Similar to single-fluid flow, researchers have used several models to describe turbulence that depend on the flow type. These models vary in complexity from simple algebraic [--] models to state-of-the-art Reynolds-stress [--] models. However, the widely used multi-phase turbulence model, presented next, is the two-equation k-ε model [--] that is based on its single-phase counterpart. Without going into details, the conservation equations governing the turbulence kinetic energy (k) and turbulence dissipation rate (ε) are given by:

$$\frac{\partial\left(r^{(k)}\rho^{(k)}k^{(k)}\right)}{\partial t}+\nabla.\left(r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}k^{(k)}\right)=\nabla.\left(r^{(k)}\frac{\mu_t^{(k)}}{\sigma_k^{(k)}}\nabla k^{(k)}\right)+r^{(k)}\left(G^{(k)}-\rho^{(k)}\varepsilon^{(k)}\right)+I_k^{(k)} \qquad (-)$$

$$\frac{\partial\left(r^{(k)}\rho^{(k)}\varepsilon^{(k)}\right)}{\partial t}+\nabla.\left(r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}\varepsilon^{(k)}\right)=\nabla.\left(r^{(k)}\frac{\mu_t^{(k)}}{\sigma_\varepsilon^{(k)}}\nabla\varepsilon^{(k)}\right)+ \\ r^{(k)}\frac{\varepsilon^{(k)}}{k^{(k)}}\left(c_{1\varepsilon}G^{(k)}-c_{2\varepsilon}\rho^{(k)}\varepsilon^{(k)}\right)+I_\varepsilon^{(k)} \qquad (--)$$

where $I_k^{(k)}$ and $I_\varepsilon^{(k)}$ represent the interfacial turbulence terms. The turbulent viscosity is calculated as:

$$\mu_t^{(k)}=C_\mu\frac{\left[k^{(k)}\right]^2}{\varepsilon^{(k)}} \qquad (--)$$

The General Multi-Fluid Scalar Equation

A review of the above differential equations reveals that they are similar in structure. If a typical representative variable associated with phase (k) is denoted by $\phi^{(k)}$, the general differential equation may be written as:

$$\frac{\partial\left(r^{(k)}\rho^{(k)}\phi^{(k)}\right)}{\partial t}+\nabla.\left(r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}\phi^{(k)}\right)=\nabla.\left(r^{(k)}\Gamma^{(k)}\nabla\phi^{(k)}\right)+r^{(k)}Q^{(k)} \tag{6}$$

where the expression for $\Gamma^{(k)}$ and $Q^{(k)}$ can be deduced from the parent equations.

Auxiliary Relations

The above set of differential equations has to be solved in conjunction with observance of constraints on the values of the variables represented by algebraic relations. These auxiliary relations include the equations of state and the geometric conservation equation.

Physically, the geometric conservation equation is a statement indicating that the sum of volumes occupied by the different fluids within a cell is equal to the volume of the cell containing the fluids.

$$\sum_k r^{(k)}=1 \tag{7}$$

For a compressible multi-fluid flow, auxiliary equations of state relating density to pressure and temperature are needed. For the k^{th} phase, such an equation can be written as:

$$\rho^{(k)}=\rho^{(k)}\left(P,T^{(k)}\right) \tag{8}$$

In order to present a complete mathematical problem, thermodynamic relations may be needed and initial and boundary conditions should supplement the above equations.

Discretization Procedure

In the previous sections the differential equations governing multi-fluid flow phenomena were outlined as well as the associated auxiliary relations. The task now is to present the Finite Volume-based numerical solution algorithm for solving these equations.

Discretization of the General Conservation Equation

The general conservation equation (6) is integrated over a finite volume (Fig. 1) to yield the following expression:

$$\iint_{\Omega} \frac{\partial\left(r^{(k)}\rho^{(k)}\phi^{(k)}\right)}{\partial t} d\Omega + \iint_{\Omega} \nabla.\left(r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}\phi^{(k)}\right) d\Omega = \iint_{\Omega} \nabla.\left(r^{(k)}\Gamma^{(k)}\nabla\phi^{(k)}\right) d\Omega + \iint_{\Omega} r^{(k)}Q^{(k)} d\Omega \tag{9}$$

Where Ω is the volume of the control cell. Using the divergence theorem to transform the volume integral into a surface integral and then replacing the surface integral by a summation of the fluxes over the sides of the control volume, equation (9) is transformed to:

$$\frac{\partial\left(r^{(k)}\rho^{(k)}\phi^{(k)}\Omega\right)}{\partial t} + \sum_{nb=e,w,n,s,t,b}\left(\mathbf{J}_{nb}^{(k)D} + \mathbf{J}_{nb}^{(k)C}\right) = r^{(k)}Q^{(k)}\Omega \tag{10}$$

where $\mathbf{J}_{nb}^{(k)D}$ and $\mathbf{J}_{nb}^{(k)C}$ are the diffusive and convective fluxes, respectively. The discretized form of the diffusive flux along an east face is given by:

$$\mathbf{J}_e^{(k)D} = -r_e^{(k)}\Gamma_e^{(k)}\left[\left(\phi_E^{(k)} - \phi_P^{(k)}\right)\frac{\mathbf{S}_e.\mathbf{S}_e}{\mathbf{S}_e.\mathbf{d}_e} + \left(\overline{\nabla\phi^{(k)}}\right)_e.\kappa_e\right] \tag{11}$$

where the over bar denotes a value obtained by interpolation, κ_e is a space vector defined as,

$$\kappa_{\mathbf{e}} = \left(\hat{\mathbf{n}}_e - \left(\gamma\hat{\mathbf{d}}\right)_e\right)S_e = \kappa_e^x\mathbf{i} + \kappa_e^y\mathbf{j} + \kappa_e^z\mathbf{k} \tag{12}$$

and γ is a scaling factor given by [70],

$$\gamma_e = \frac{1}{\hat{\mathbf{n}}_e.\hat{\mathbf{d}}_e} = \frac{S_e d_e}{\mathbf{S}_e.\mathbf{d}_e} \tag{13}$$

and $\hat{\mathbf{n}}_f$ and $\hat{\mathbf{d}}_f$ are the contravariant and covariant unit vectors respectively. The discretized convective flux along an east side is given by:

$$J_e^{(k)C} = \left(r^{(k)}\rho^{(k)}\mathbf{u}^{(k)}\cdot\mathbf{S}\right)_e\phi_e^{(k)} = \left(r^{(k)}\rho^{(k)}U^{(k)}\right)_e\phi_e^{(k)} = C_e^{(k)}\phi_e^{(k)} \tag{14}$$

where $\mathbf{S}_e$ and C_e are the surface vector and convection flux coefficient at cell face 'e', respectively. After substituting the face values by their functional relationship relating to the node values of ϕ, Eq. (10) is transformed after some algebraic manipulations into the following discretized equation:

$$A_P^{(k)}\phi_P^{(k)} = \sum_{NB} A_{NB}^{(k)}\phi_{NB}^{(k)} + B_P^{(k)} \tag{15}$$

where the coefficients $A_P^{(k)}$ and $\phi_{NB}^{(k)}$ depend on the selected scheme and $B_P^{(k)}$ is the source term of the discretized equation . In compact form, the above equation can be written as

$$\phi^{(k)} = H_P\left[\phi^{(k)}\right] = \frac{\sum_{NB} A_{NB}^{(k)}\phi_{NB}^{(k)} + B_P^{(k)}}{A_P^{(k)}} \tag{16}$$

Discretization of the momentum equation

The discretization procedure for the momentum equation yields an algebraic equation of the form:

$$\mathbf{A}_P^{(k)}\mathbf{u}_P^{(k)} = \sum_{NB(P)} \mathbf{A}_{NB}^{(k)}\mathbf{u}_{NB}^{(k)} + \mathbf{B}_P^{(k)} - r_P^{(k)}\Omega_P\nabla_P(P) + \Omega_P\sum_{m\neq k} g^{(km)}\left(\mathbf{u}_p^{(m)} - \mathbf{u}_p^{(k)}\right) \tag{17}$$

In the above equation, the inter-phase term is written out explicitly to show the strong coupling among the momentum equations of the different fluids. This is in contrast with the *spatial* coupling that exists among the neighboring velocities of the same fluid. One way to improve the overall convergence and robustness of the algorithm is to rewrite the discretized momentum equations for the various phases such that:

$$\mathbf{A}_P^{(k)}\mathbf{u}_P^{(k)} = \sum_{NB} \mathbf{A}_{NB}^{(k)}\mathbf{u}_{NB}^{(k)} + \mathbf{B}_P^{(k)} - r_P^{(k)}\Omega_P\nabla_P(P) + \Omega_P\sum_{m\neq k} g^{(km)}\mathbf{u}_p^{(m)} \tag{18}$$

Where now

$$\mathbf{A}_P^{(k)} \leftarrow \mathbf{A}_P^{(k)} + \Omega_P\sum_{m\neq k}\left(g_P^{(km)}\right) \tag{19}$$

For later reference, the value of $\mathbf{A}_P^{(k)}$ before the addition of the inter-phase terms will be denoted by $\tilde{\mathbf{A}}_P^{(k)}$. To this end, the discretized form of the momentum equation can be rewritten as:

$$\mathbf{u}_P^{(k)} = \mathbf{HP}_P\left[\mathbf{u}^{(k)}\right] - r^{(k)}\mathbf{D}_P^{(k)}\nabla_P(P) \tag{20}$$

where the body force and inter-phase terms are absorbed in the $\mathbf{B}_P^{(k)}$ source term within the $\mathbf{HP}_P\left[\mathbf{u}^{(k)}\right]$ term, or as

$$\mathbf{u}_P^{(k)} = \mathbf{HI}_P\left[\mathbf{u}^{(k)}\right] + \mathbf{D}_P^{(k)}\sum_{m\neq k}\left(g^{(km)}\mathbf{u}_P^{(m)}\right) \tag{21}$$

where the body force and pressure gradient terms are absorbed in the $\mathbf{B}_P^{(k)}$ source term within the $\mathbf{HI}_P\left[\mathbf{u}^{(k)}\right]$ term. For later use, modified forms of the $\mathbf{HP}_P\left[\mathbf{u}^{(k)}\right]$ and $\mathbf{D}_P^{(k)}$ operators are defined as:

$$\widetilde{\mathbf{HP}}_P[\mathbf{u}^{(k)}] = \frac{\sum_{NB} \mathbf{A}_{NB}^{(k),u} \mathbf{u}_{NB}^{(k)}}{\mathbf{A}_P^{(k),u}} \qquad \widetilde{\mathbf{D}}_P^{(k)} = \frac{\mathbf{D}_P^{(k)}[\mathbf{u}]}{1 - \widetilde{\mathbf{HP}}_P[1]} \tag{22}$$

Discretization of the Continuity Equation

The mass-conservation principle (Eq. (1)) can be viewed as a volume fraction equation for the k^{th} phase in which case it can be discretized and written in the form

$$r_P^{(k)} = H_P\left[r^{(k)}\right] \tag{23}$$

or as a continuity equation for the k^{th} phase to be used in deriving the pressure correction equation, in which case it is discretized in the following form:

$$\frac{\left(r_P^{(k)}\rho_P^{(k)}\right) - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega - \Delta_P\left[r^{(k)}\mathbf{u}^{(k)}.\mathbf{S}\right] = r^{(k)}\dot{M}^{(k)} \tag{24}$$

where the Δ operator represents the following operation:

$$\Delta_P\left[\Theta\right] = \sum_{f=NB(P)} \Theta_f \tag{25}$$

Discretization of the Energy equation

The discretization of the energy equation follows that of the general multi-fluid scalar equation. The only difference is the one pertaining to the discretization of the additional source terms. Since a control volume approach is followed, the integral of these sources over the control volume appears in the discretized equation. By using the divergence theorem, the volume integral is transformed into a surface integral and the resultant discretized expressions are evaluated explicitly.

Multi-Fluid Solution Algorithms

Before detailing the multi-fluid segregated solution algorithms, it will be shown that these algorithms may be grouped under two categories denoted in this work by the **Geometric Conservation Based Algorithms** and the **Mass Conservation Based Algorithms**. To justify this classification, attention is focussed on the equations and variables involved in a multi-fluid flow situation with n-fluids. In such a case, there will be n momentum equations, n volume fraction (or mass conservation) equations, a geometric conservation equation, and for the case of a compressible flow an additional n auxiliary pressure-density relations. Moreover, the variables involved are the n velocity vectors, the n volume fractions, the pressure field, and for a compressible flow an additional n unknown density fields. It is clear that the n-velocity fields are associated with the n-momentum equations, i.e. the momentum equations can directly be used to calculate the velocity fields. The volume fractions could arguably be calculated from the volume fraction equations, which means that the remaining equation i.e. the geometric conservation equation (the volume fractions sum to 1) has to be used in deriving the pressure equation, or equivalently the pressure correction equation. This results in what is called here the **Geometric Conservation Based Algorithm (GCBA)**.

The equations can be arranged differently, with the n momentum equations used to calculate the n velocity fields, n-1 volume fraction (mass conservation) equations used to calculate n-1 volume fraction fields, and the last volume fraction field calculated using the geometric conservation equation

$$r^{(n)} = 1 - \sum_{k \neq n} r^{(k)} \tag{26}$$

The remaining volume fraction equation can be used to calculate the pressure field. However, instead of using this last volume fraction equation, the global conservation equation can be employed, i.e. the sum of the individual mass conservation equations, to derive a pressure correction equation. The resulting algorithm is denoted in this case by the **Mass Conservation Based Algorithm (MCBA)**.

With this classification, attention will now be directed towards presenting the various MCBA and GCBA in addition to several techniques that were introduced to enhance the performance and accelerate the convergence of these algorithms.

Part I - Mass Conservation Based Algorithms

The sequence of events in the Mass Conservation Based Algorithm (MCBA) is as follows:

- Solve the momentum equations for velocities.
- Solve the pressure correction equation based on global mass conservation.
- Correct velocities, densities, and pressure.
- Solve the individual mass conservation equations for volume fractions.
- Solve the energy equations.

- Return to the first step and repeat until convergence.

The above steps, along with some of the techniques that were developed to improve on them, are detailed next.

Solving for Velocities

In this first step, the following systems of momentum equations are solved to find $\mathbf{u}_P^{(k)*}$ based on guessed or previously calculated volume fraction and pressure fields:

$$\mathbf{u}_P^{(k)} = \mathbf{HI}_P\left[\mathbf{u}^{(k)}\right] + \mathbf{D}_P^{(k)} \sum_{m \neq k} g^{(km)} \mathbf{u}_P^{(m)} \tag{27}$$

From Eq. (27) it is clear that the $\mathbf{HI}_P\left[\mathbf{u}^{(k)}\right]$ term couples $\mathbf{u}_P^{(k)}$ to the neighbouring phase (k) velocities (*geometric or spatial coupling*) while the $\mathbf{D}_P^{(k)} \sum_{m \neq k} g^{(km)} \mathbf{u}_P^{(m)}$ term couples $\mathbf{u}_P^{(k)}$ to the velocity of all other phases at grid point P (*inter-phase coupling*). Therefore, the rate of convergence of the iterative solution procedure used to solve the above system will greatly depend on its capability to resolve both types of coupling. The spatial coupling presents no problem to the well-established iterative techniques since it couples velocities of the same phase. The inter-phase coupling is however problematic since it relates velocities of different phases. An explicit evaluation of this term slows the convergence rate considerably especially when the inter-fluid momentum transfer terms, represented by $g^{(mn)}$, are large. To accelerate convergence, the Partial Elimination Algorithm (PEA) [68] and the SImultaneous solution of Non-linearly Coupled Equations (SINCE) [67] technique were developed.

Improvement #1: The Partial Elimination Algorithm and The SImultaneous solution of Non-linearly Coupled Equations technique

The central idea in the Partial Elimination Algorithm (PEA), applicable to two-fluid flow, is to render the discretized momentum equations more implicit by de-coupling the two sets of equations. This is achieved in a straightforward manner and it results in a modification to the values of $\mathbf{A}_P^{(k)}$ and $\mathbf{B}_P^{(k)}$.

For the case of two-fluid flow, the momentum equations are given by:

$$\mathbf{u}_P^{(1)} = \mathbf{HI}_P\left[\mathbf{u}^{(1)}\right] + \mathbf{D}_P^{(1)} g^{(12)} \mathbf{u}_P^{(2)} \qquad \mathbf{u}_P^{(2)} = \mathbf{HI}_P\left[\mathbf{u}^{(2)}\right] + \mathbf{D}_P^{(2)} g^{(21)} \mathbf{u}_P^{(1)} \tag{28}$$

It is clear that each of the equations (28) contains both variables $\mathbf{u}_P^{(1)}$ and $\mathbf{u}_P^{(2)}$ simultaneously. In order to eliminate the velocity of one of the phases from the other phase momentum equation, and vice versa, these equations may be rewritten using the PEA as

$$\mathbf{u}_P^{(1)} = \frac{\mathbf{HI}_P\left[\mathbf{u}^{(1)}\right] + \mathbf{D}_P^{(1)} g^{(12)} \mathbf{HI}_P\left[\mathbf{u}^{(2)}\right]}{1 - \mathbf{D}_P^{(1)} g^{(12)} \mathbf{D}_P^{(2)} g^{(21)}} \qquad \mathbf{u}_P^{(2)} = \frac{\mathbf{HI}_P\left[\mathbf{u}^{(2)}\right] + \mathbf{D}_P^{(2)} g^{(21)} \mathbf{HI}_P\left[\mathbf{u}^{(1)}\right]}{1 - \mathbf{D}_P^{(1)} g^{(12)} \mathbf{D}_P^{(2)} g^{(21)}} \tag{29}$$

This treatment renders the equations more implicit ($\mathbf{u}_P^{(2)}$ is absent from the $\mathbf{u}_P^{(1)}$ equation and vice versa) and enhances the rate of convergence, which otherwise would have been slowed down by the lagging inter-linkage of the two equations.

The use of the PEA technique with more than two fluids can become cumbersome. The SImultaneous solution of Non-linearly Coupled Equations (SINCE) method [67], is a technique similar to the PEA in its aim, applicable to three or more phases. It is however different than the PEA in that the equations' spatial coupling and inter-phase coupling are accounted for in two distinct steps. In the first step, the inter-phase coupling is resolved by solving the momentum equations on each grid point without accounting for the spatial coupling, i.e. by moving the $\mathbf{HI}_P\left[\mathbf{u}^{(k)}\right]$ terms to the right hand side and treating them as source terms. The system of equations for a k-fluid flow can be re-arranged and written in the following form:

$$\begin{aligned}
\breve{\mathbf{u}}_P^{(1)} &= \mathbf{D}_P^{(1)} \sum_{m \neq 1} g^{(1m)} \breve{\mathbf{u}}_P^{(m)} + \mathbf{HI}_P\left[\mathbf{u}^{(1)}\right] \\
\breve{\mathbf{u}}_P^{(2)} &= \mathbf{D}_P^{(2)} \sum_{m \neq 2} g^{(2m)} \breve{\mathbf{u}}_P^{(m)} + \mathbf{HI}_P\left[\mathbf{u}^{(2)}\right] \\
&\vdots \\
\breve{\mathbf{u}}_P^{(k)} &= \mathbf{D}_P^{(k)} \sum_{m \neq k} g^{(km)} \breve{\mathbf{u}}_P^{(m)} + \mathbf{HI}_P\left[\mathbf{u}^{(k)}\right]
\end{aligned} \tag{30}$$

These equations are solved in a first step for the respective control volumes, and the solution used as a first estimate of the velocity fields $\left(\breve{\mathbf{u}}_P^{(k)}\right)$ in calculating the inter-phase terms. In the second step, the inter-phase friction terms are absorbed into the standard source terms of equation (15) and the full-field solution of the momentum equations is accomplished in a sequential manner using the normal calculation method via the following system of equations:

$$\mathbf{u}_P^{(k)*} = \mathbf{HI}_P\left[\mathbf{u}^{(k)*}\right] + \mathbf{D}_P^{(k)} \sum_{m \neq k} g^{(km)} \breve{\mathbf{u}}_P^{(m)} \tag{31}$$

Solving for Pressure Correction

Before convergence, the velocities calculated from the momentum equations do not satisfy the mass conservation equations. In the segregated approach, the burden of restoring balance rests on the pressure correction equation, which in this case is derived from the overall mass conservation equation. The segregated MCBA can be viewed as extensions to the SIMPLE algorithm and its variants, in which, the pressure correction equation derivation follows the same pattern as in SIMPLE (or any of its variants), and the corrections are applied only to the velocity, pressure, and density fields. No correction is applied to the volume fractions; rather, they are obtained by solving the individual continuity and geometric constraint equations.

To derive the pressure-correction equation, the mass conservation equations of the various phases are added to yield the overall mass conservation equation given by:

$$\sum_k \left\{ \frac{\left(r_P^{(k)}\rho_P^{(k)}\right) - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega + \Delta_P\left(r^{(k)}\rho_P^{(k)}\mathbf{u}^{(k)}.\mathbf{S}\right)\right\} = \sum_k r^{(k)}\dot{M}^{(k)} = 0 \qquad (32)$$

In the predictor stage a guessed or estimated pressure field from the previous iteration denoted by P^{o}, is substituted into the momentum equations. The resulting velocity fields denoted by $\mathbf{u}^{(k)*}$ which now satisfy the momentum equations will not, in general, satisfy the mass conservation equations. Thus, corrections are needed in order to yield velocity and pressure fields that satisfy both equations. Denoting the corrections for pressure, velocity, and density by P', $\mathbf{u}^{(k)'}$, and $\rho^{(k)'}$ respectively, the corrected fields are written as:

$$P = P^{o} + P', \mathbf{u}^{(k)} = \mathbf{u}^{(k)^*} + \mathbf{u}^{(k)'}, \rho^{(k)} = \rho^{(k)^o} + \rho^{(k)'} \qquad (33)$$

Thus, before the pressure field is known, the velocities obtained from the momentum equations are actually $\mathbf{u}^{(k)*}$ rather than $\mathbf{u}^{(k)}$. Hence the equations solved in the predictor stage are:

$$\mathbf{u}_P^{(k)*} = \mathbf{HP}_P[\mathbf{u}^{(k)*}] - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P^{o} \qquad (34)$$

While the final solutions satisfy

$$\mathbf{u}_P^{(k)} = \mathbf{HP}_P[\mathbf{u}^{(k)}] - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P \qquad (35)$$

Subtracting the two sets of equation (35) and (34) from each other yields the following equation involving the correction terms:

$$\mathbf{u}_P^{(k)'} = \mathbf{HP}_P[\mathbf{u}^{(k)'}] - r^{(k)^o}\mathbf{D}_P^{(k)}\nabla_P P' \quad (36)$$

The velocity and density fields are corrected to satisfy mass conservation. Therefore, the new density and velocity fields, $\rho^{(k)}$ and $\mathbf{u}^{(k)}$, will satisfy the overall mass conservation equation if:

$$\sum_k \left\{ \frac{\left(r_P^{(k)o}\rho_P^{(k)}\right) - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega + \Delta_P\left[r^{(k)o}\rho^{(k)}\mathbf{u}^{(k)}.\mathbf{S}\right] \right\} = 0 \quad (37)$$

Linearizing the $(\rho^{(k)}\mathbf{u}^{(k)})$ term, one gets

$$\left(\rho^{(k)*} + \rho^{(k)'}\right)\left(\mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}\right) = \rho^{(k)*}\mathbf{u}^{(k)*} + \rho^{(k)*}\mathbf{u}^{(k)'} + \rho^{(k)'}\mathbf{u}^{(k)*} + \rho^{(k)'}\mathbf{u}^{(k)'} \quad (38)$$

Substituting equations (38) and (36) into equation (37), rearranging and replacing density correction by pressure correction, the final form of the pressure-correction equation is written as:

$$\begin{aligned}\sum_k \left\{ \frac{\Omega}{\delta t} r_P^{(k)o}C_\rho^{(k)}P_P' + \Delta_P\left[r^{(k)o}U^{(k)*}C_\rho^{(k)}P'\right] - \Delta_P\left[r^{(k)^o}\rho^{(k)*}\left(r^{(k)^o}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right] \right\} \\ = -\sum_k \left\{ \begin{aligned} &\frac{r_P^{(k)o}\rho_P^{(k)*} - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega + \Delta_P\left[r^{(k)o}\rho^{(k)*}U^{(k)*}\right] \\ &+ \Delta_P\left[r^{(k)^o}\rho^{(k)*}\left(\mathbf{HP}\left[\mathbf{u}^{(k)'}\right]\right).\mathbf{S}\right] + \Delta_P\left[r^{(k)o}\rho^{(k)'}\mathbf{u}^{(k)'}.\mathbf{S}\right] \end{aligned} \right\}\end{aligned} \quad (39)$$

The second order correction term $\rho^{(k)'}\mathbf{u}^{(k)'}$ is usually neglected. Moreover, if the $\mathbf{HP}\left[\mathbf{u}^{(k)'}\right]$ term in the above equation is retained, there will result a pressure correction equation relating the pressure correction value at a point to all values in the domain. To facilitate implementation and reduce cost, simplifying assumptions related to this term have been introduced. Depending on these assumptions, different algorithms are obtained. These algorithms were originally developed for incompressible single-fluid flow and most of them have not yet been extended to compressible multi-fluid flow. It is an objective of this work to perform this extension.

Extending the Segregated class of single-fluid flow algorithms to multi-fluid flow situations

Moukalled and Darwish [21] have recently unified the formulation of the segregated class of algorithms for single-fluid flow and detailed the philosophies behind them. Therefore, it is sufficient here to present the symbolic form of the multi-fluid version of these algorithms. For additional discussion related to their development the reader is referred to [21].

In the derivations to follow, the superscripts "old" and "o" denote values from the previous time step and previous iteration, respectively. Moreover, the superscripts *, **, ***, and **** represent the first, second, third, and fourth updated values at the current iteration, respectively.

The MCBA following SIMPLE (MCBA-SIMPLE): Symbolic Form

Predictor:

$$\mathbf{u}_P^{(k)*} = \mathbf{HP}_P[\mathbf{u}^{(k)*}] - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P^o \tag{40}$$

Corrector:

$$\left(\mathbf{u}^{(k)'}, P', \rho^{(k)'}\right)\left(\mathbf{u}^{(k)**} = \mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}, P^* = P^o + P', \rho^{(k)*} = \rho^{(k)o} + \rho^{(k)'}\right) \tag{41}$$

$$\mathbf{u}_P^{(k)**} = \mathbf{HP}_P[\mathbf{u}^{(k)**}] - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P^* = \mathbf{HP}_P[\mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}] - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P\left(P^o + P'\right) \tag{42}$$

$$\therefore \begin{cases} \mathbf{u}_P^{(k)'} = \mathbf{HP}_P[\mathbf{u}^{(k)'}] - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P' \\ \rho^{(k)'} = C_\rho^{(k)} P' \end{cases} \tag{43}$$

Condition:

$$\begin{aligned} &\sum_k \left\{ \frac{\Omega}{\delta t} r_P^{(k)o} C_\rho^{(k)} P_P' + \Delta_P\left[r^{(k)o} C_\rho^{(k)} U^{(k)*} P'\right] - \Delta_P\left[r^{(k)^o}\rho^{(k)o}\left(r^{(k)^o}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right\} \\ &\qquad = -\sum_k \left\{ \begin{aligned} &\frac{r_P^{(k)o}\rho_P^{(k)o} - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega + \Delta_P\left[r^{(k)o}\rho^{(k)o}U^{(k)*}\right] \\ &+ \Delta_P\left[r^{(k)^o}\rho^{(k)o}\left(\mathbf{HP}\left[\mathbf{u}^{(k)'}\right]\right).\mathbf{S}\right] + \Delta_P\left[r^{(k)o}\rho^{(k)'}\mathbf{u}^{(k)'}.\mathbf{S}\right] \end{aligned} \right\} \end{aligned} \tag{44}$$

Approximation:

$$\text{Neglect: } \mathbf{HP}\left[\mathbf{u}^{(k)'}\right],\ \Delta_P\left[r^{(k)o}\rho^{(k)'}\mathbf{u}^{(k)'}.\mathbf{S}\right] \quad \Rightarrow \quad \mathbf{u}_P^{(k)'} = -r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P' \tag{45}$$

Approximate Equation:

$$\begin{aligned} &\sum_k \left\{ \frac{\Omega}{\delta t} r_P^{(k)o} C_\rho^{(k)} P_P' + \Delta_P\left[r^{(k)o} C_\rho^{(k)} U^{(k)*} P'\right] - \Delta_P\left[r^{(k)^o}\rho^{(k)o}\left(r^{(k)^o}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right\} \\ &\qquad = -\sum_k \left\{ \frac{r_P^{(k)o}\rho_P^{(k)o} - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega + \Delta_P\left[r^{(k)o}\rho^{(k)o}U^{(k)*}\right] \right\} \end{aligned} \tag{46}$$

A Global MCBA-SIMPLE Iteration

- *Solve implicitly for* $\mathbf{u}^{(k)}$*, using the old pressure and density fields.*
- *Calculate the* $\mathbf{D}^{(k)}$ *fields.*
- *Solve the pressure correction equation and correct* $\mathbf{u}^{(k)}$, P *and* $\rho^{(k)}$*.*
- *Solve implicitly for* $r^{(k)}$*.*
- *Solve implicitly the energy equations and update the density fields.*
- *Return to the first step and iterate until convergence.*

The MCBA following SIMPLEST (MCBA-SIMPLEST): Symbolic Form

Predictor:

$$\mathbf{u}_P^{(k)*} = \mathbf{HP}_P^D\left[\mathbf{u}^{(k)*}\right] + \mathbf{HP}_P^C\left[\mathbf{u}^{(k)o}\right] - r^{(k)o}\mathbf{D}_P^{(k)*}\nabla_P P^o \tag{47}$$

Corrector:

$$\left(\mathbf{u}^{(k)'}, P', \rho^{(k)'}\right)\left(\mathbf{u}^{(k)**} = \mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}, P^* = P^o + P', \rho^{(k)*} = \rho^{(k)o} + \rho^{(k)'}\right) \tag{48}$$

$$\therefore \begin{aligned} \mathbf{u}_P^{(k)**} &= \mathbf{HP}_P^D\left[\mathbf{u}^{(k)*}\right] + \mathbf{HP}_P^D\left[\mathbf{u}^{(k)'}\right] + \mathbf{HP}_P^C\left[\mathbf{u}^{(k)*}\right] + \mathbf{HP}_P^C\left[\mathbf{u}^{(k)'}\right] \\ &- r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P^o - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P' \end{aligned} \tag{49}$$

$$\therefore \begin{cases} \mathbf{u}_P^{(k)'} = \mathbf{HP}_P[\mathbf{u}^{(k)'}] + \mathbf{HP}_P^C[\mathbf{u}^{(k)*} - \mathbf{u}^{(k)o}] - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P' \\ \rho^{(k)'} = C_\rho^{(k)} P' \end{cases} \tag{50}$$

Condition:

$$\begin{aligned} &\sum_k \left\{ \frac{\Omega}{\delta t} r_P^{(k)o} C_\rho^{(k)} P_P' + \Delta_P\left[r^{(k)o} C_\rho^{(k)} U^{(k)*} P'\right] - \Delta_P\left[r^{(k)^o}\rho^{(k)o}\left(r^{(k)^o}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right\} \\ &= -\sum_k \left\{ \begin{aligned} &\frac{r_P^{(k)o}\rho_P^{(k)o} - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega + \Delta_P\left[r^{(k)o}\rho^{(k)o}U^{(k)*}\right] \\ &+ \Delta_P\left[r^{(k)^o}\rho^{(k)o}\left(\mathbf{HP}^C\left[\mathbf{u}^{(k)*} - \mathbf{u}^{(k)o}\right] + \mathbf{HP}\left[\mathbf{u}^{(k)'}\right]\right).\mathbf{S}\right] + \Delta_P\left[r^{(k)o}\rho^{(k)'}\mathbf{u}^{(k)'}.\mathbf{S}\right] \end{aligned} \right\} \end{aligned} \tag{51}$$

Approximation:

$$\text{Neglect: } \mathbf{HP}^C\left[\mathbf{u}^{(k)*} - \mathbf{u}^{(k)o}\right],\ \mathbf{HP}\left[\mathbf{u}^{(k)'}\right],\ \Delta_P\left[r^{(k)o}\rho^{(k)'}\mathbf{u}^{(k)'}.\mathbf{S}\right] \Rightarrow \mathbf{u}_P^{(k)'} = -r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P' \tag{52}$$

Approximate Equation:

$$\begin{aligned} &\sum_k \left\{ \frac{\Omega}{\delta t} r_P^{(k)o} C_\rho^{(k)} P_P' + \Delta_P\left[r^{(k)o} C_\rho^{(k)} U^{(k)*} P'\right] - \Delta_P\left[r^{(k)^o}\rho^{(k)o}\left(r^{(k)^o}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right\} \\ &= -\sum_k \left\{ \frac{r_P^{(k)o}\rho_P^{(k)o} - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega + \Delta_P\left[r^{(k)o}\rho^{(k)o}U^{(k)*}\right]\right\} \end{aligned} \tag{53}$$

A Global MCBA-SIMPLEST Iteration

- *Solve for* $\mathbf{u}^{(k)}$*, treating* $\mathbf{HP}^D\left[\mathbf{u}^{(k)}\right]$ *implicitly and* $\mathbf{HP}^C\left[\mathbf{u}^{(k)}\right]$ *explicitly.*
- *Calculate the* $\mathbf{D}^{(k)}$ *fields.*
- *Solve the pressure correction equation and correct* $\mathbf{u}^{(k)}$*,* P *and* $\rho^{(k)}$*.*
- *Solve implicitly for* $r^{(k)}$*.*
- *Solve implicitly the energy equations and update the density fields.*
- *Return to the first step and iterate until convergence.*

The MCBA following PISO (MCBA-PISO): Symbolic Form

First Predictor:

$$\mathbf{u}_P^{(k)*} = \mathbf{HP}_P[\mathbf{u}^{(k)*}] - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P^o \tag{54}$$

First Corrector:

$$\left(\mathbf{u}^{(k)'}, P', \rho^{(k)'}\right)\left(\mathbf{u}^{(k)**} = \mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}, P^* = P^o + P', \rho^{(k)*} = \rho^{(k)o} + \rho^{(k)'}\right) \tag{55}$$

$$\therefore \mathbf{u}_P^{(k)**} = \mathbf{HP}_P[\mathbf{u}^{(k)**}] - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P^* = \mathbf{HP}_P[\mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}] - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P\left(P^o + P'\right) \tag{56}$$

$$\therefore \begin{cases} \mathbf{u}_P^{(k)'} = \mathbf{HP}_P[\mathbf{u}^{(k)'}] - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P' \\ \rho^{(k)'} = C_\rho^{(k)} P' \end{cases} \tag{57}$$

Condition:

$$\sum_k \left\{ \frac{\Omega}{\delta t} r_P^{(k)o} C_\rho^{(k)} P'_P + \Delta_P\left[r^{(k)o} C_\rho^{(k)} U^{(k)*} P'\right] - \Delta_P\left[r^{(k)^o}\rho^{(k)o}\left(r^{(k)^o}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right\} = -\sum_k \left\{ \begin{aligned} &\frac{r_P^{(k)o}\rho_P^{(k)o} - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega + \Delta_P\left[r^{(k)o}\rho^{(k)o}U^{(k)*}\right] \\ &+ \Delta_P\left[r^{(k)^o}\rho^{(k)o}\left(\mathbf{HP}\left[\mathbf{u}^{(k)'}\right]\right).\mathbf{S}\right] + \Delta_P\left[r^{(k)o}\rho^{(k)'}\mathbf{u}^{(k)'}.\mathbf{S}\right] \end{aligned} \right\} \tag{58}$$

Approximation:

$$\text{Neglect: } \mathbf{HP}\left[\mathbf{u}^{(k)'}\right],\ \Delta_P\left[r^{(k)o}\rho^{(k)'}\mathbf{u}^{(k)'}.\mathbf{S}\right] \quad \Rightarrow \quad \mathbf{u}_P^{(k)'} = -r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P' \tag{59}$$

Approximate Equation:

$$\sum_k \left\{ \frac{\Omega}{\delta t} r_P^{(k)o} C_\rho^{(k)} P'_P + \Delta_P\left[r^{(k)o} C_\rho^{(k)} U^{(k)*} P'\right] - \Delta_P\left[r^{(k)^o}\rho^{(k)o}\left(r^{(k)^o}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right\} = -\sum_k \left\{ \frac{r_P^{(k)o}\rho_P^{(k)o} - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega + \Delta_P\left[r^{(k)o}\rho^{(k)o}U^{(k)*}\right] \right\} \tag{60}$$

Second Corrector:

$$\left(\mathbf{u}^{(k)''}, P'', \rho^{(k)''}\right)\left(\mathbf{u}^{(k)****} = \mathbf{u}^{(k)***} + \mathbf{u}^{(k)''}, P^{**} = P^* + P'', \rho^{(k)**} = \rho^{(k)*} + \rho^{(k)''}\right) \tag{61}$$

$$\therefore \mathbf{u}_P^{(k)****} = \mathbf{HP}_P^{**}[\mathbf{u}^{(k)****}] - r^{(k)o}\mathbf{D}_P^{(k)**}\nabla_P\left(P^* + P''\right) \tag{62}$$

$$\mathbf{u}_P^{(k)***} = \mathbf{HP}_P^{**}[\mathbf{u}^{(k)**}] - r^{(k)o}\mathbf{D}_P^{(k)**}\nabla_P P^* \tag{63}$$

$$\therefore \begin{cases} \mathbf{u}_P^{(k)''} = \mathbf{HP}_P^{**}[\mathbf{u}^{(k)***} - \mathbf{u}^{(k)**} + \mathbf{u}^{(k)''}] - r^{(k)o}\mathbf{D}_P^{(k)**}\nabla_P P'' \\ \rho^{(k)''} = C_\rho^{(k)} P'' \end{cases} \tag{64}$$

Condition:

$$\sum_k \left\{ \frac{\Omega}{\delta t} r_P^{(k)o} C_\rho^{(k)} P''_P + \Delta_P\left[r^{(k)o} C_\rho^{(k)} U^{(k)***} P''\right] - \Delta_P\left[r^{(k)^o}\rho^{(k)*}\left(r^{(k)^o}\mathbf{D}^{(k)**}\nabla P''\right).\mathbf{S}\right]\right\} = -\sum_k \left\{ \begin{aligned} &\frac{r_P^{(k)o}\rho_P^{(k)*} - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega + \Delta_P\left[r^{(k)o}\rho^{(k)*}U^{(k)***}\right] \\ &+ \Delta_P\left[r^{(k)^o}\rho^{(k)*}\left(\mathbf{HP}^{**}\left[\mathbf{u}^{(k)***} - \mathbf{u}^{(k)**} + \mathbf{u}^{(k)''}\right]\right).\mathbf{S}\right] + \Delta_P\left[r^{(k)o}\rho^{(k)''}\mathbf{u}^{(k)''}.\mathbf{S}\right] \end{aligned} \right\} \tag{65}$$

Approximation:

$$\text{Neglect: } \mathbf{HP}^{**}\left[\mathbf{u}^{(k)***} - \mathbf{u}^{(k)**} + \mathbf{u}^{(k)''}\right],\ \Delta_P\left[r^{(k)o}\rho^{(k)''}\mathbf{u}^{(k)''}.\mathbf{S}\right] \Rightarrow \mathbf{u}_P^{(k)''} = -r^{(k)o}\mathbf{D}_P^{(k)**}\nabla_P P'' \tag{66}$$

Approximate Equation:

$$\sum_k \left\{ \frac{\Omega}{\delta t} r_P^{(k)o} C_\rho^{(k)} P_P'' + \Delta_P \left[r^{(k)o} C_\rho^{(k)} U^{(k)***} P'' \right] - \Delta_P \left[r^{(k)^o} \rho^{(k)*} \left(r^{(k)^o} \mathbf{D}^{(k)**} \nabla P'' \right) . \mathbf{S} \right] \right\}$$
$$= -\sum_k \left\{ \frac{r_P^{(k)o} \rho_P^{(k)*} - \left(r_P^{(k)} \rho_P^{(k)} \right)^{Old}}{\delta t} \Omega + \Delta_P \left[r^{(k)o} \rho^{(k)*} U^{(k)***} \right] \right\} \quad (67)$$

A Global MCBA-PISO Iteration

- *Solve implicitly for* $\mathbf{u}^{(k)}$ *using the old pressure and density fields.*
- *Calculate the* $\mathbf{D}^{(k)}$ *fields.*
- *Solve the pressure correction equation and correct* $\mathbf{u}^{(k)}$, P, *and* $\rho^{(k)}$.
- *Solve implicitly for* $r^{(k)}$.
- *Solve implicitly the energy equation and update the density fields.*
- *Solve the momentum equations explicitly and calculate the* $\mathbf{D}^{(k)}$ *fields.*
- *Solve the pressure correction equation and correct* $\mathbf{u}^{(k)}$, P, *and* $\rho^{(k)}$.
- *Return to step one and iterate until convergence*

The MCBA following SIMPLEX (MCBA-SIMPLEX): Symbolic Form

Predictor:

$$\mathbf{u}_P^{(k)*} = \mathbf{HP}_P[\mathbf{u}^{(k)*}] - r^{(k)o} \mathbf{D}_P^{(k)} \nabla_P P^o \quad (68)$$

Corrector:

$$\left(\mathbf{u}^{(k)'}, P', \rho^{(k)'} \right) \left(\mathbf{u}^{(k)**} = \mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}, P^* = P^o + P', \rho^{(k)*} = \rho^{(k)o} + \rho^{(k)'} \right) \quad (69)$$

$$\therefore \mathbf{u}_P^{(k)**} = \mathbf{HP}_P[\mathbf{u}^{(k)**}] - r^{(k)o} \mathbf{D}_P^{(k)} \nabla_P P^* = \mathbf{HP}_P[\mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}] - r^{(k)o} \mathbf{D}_P^{(k)} \nabla_P \left(P^o + P' \right) \quad (70)$$

$$\therefore \begin{cases} \mathbf{u}_P^{(k)'} = \mathbf{HP}_P[\mathbf{u}^{(k)'}] - r^{(k)o} \mathbf{D}_P^{(k)} \nabla_P P' \\ \rho^{(k)'} = C_\rho^{(k)} P' \end{cases} \quad (71)$$

Condition:

$$\sum_k \left\{ \begin{array}{l} \dfrac{r_P^{(k)o} \left(\rho_P^{(k)o} + \rho_P^{(k)'} \right) - \left(r_P^{(k)} \rho_P^{(k)} \right)^{Old}}{\delta t} \Omega \\ + \Delta_P \left[r^{(k)o} \rho^{(k)'} \mathbf{u}^{(k)*} . \mathbf{S} \right] + \Delta_P \left[r^{(k)o} \rho^{(k)o} \mathbf{u}^{(k)'} . \mathbf{S} \right] \end{array} \right\} = -\sum_k \left\{ \begin{array}{l} \Delta_P \left[r^{(k)o} \rho^{(k)o} \mathbf{u}^{(k)*} . \mathbf{S} \right] \\ + \Delta_P \left[r^{(k)o} \rho^{(k)'} \mathbf{u}^{(k)'} . \mathbf{S} \right] \end{array} \right\} \quad (72)$$

Approximation:

Neglect: $\Delta_P \left[r^{(k)o} \rho^{(k)'} \mathbf{u}^{(k)'} . \mathbf{S} \right]$ and let

$$\mathbf{u}_P^{(k)'} = \mathbf{HP}_P[\mathbf{u}^{(k)'}] - r_P^{(k)o} \mathbf{D}_P^{(k)} \nabla_P P' = -r_P^{(k)o} \mathbf{D}_P^{(k)SX} \nabla_P P' \quad (73)$$

$$\Rightarrow - r_P^{(k)o} \mathbf{D}_P^{(k)SX} \nabla_P P' = \mathbf{HP}_P[-r^{(k)o} \mathbf{D}^{(k)SX} \nabla_P P'] - r_P^{(k)o} \mathbf{D}_P^{(k)} \nabla_P P' \quad (74)$$

Assume that the pressure difference local to the velocity is representative of all pressure differences i.e. $\mathbf{HP}_P[-r^{(k)o} \mathbf{D}^{(k)SX} \nabla_P P'] = -\left(\nabla_P P' \right) \mathbf{HP}_P[r^{(k)o} \mathbf{D}^{(k)SX}]$, thus:

$$r_P^{(k)o} \mathbf{D}_P^{(k)SX} = \mathbf{HP}_P[r^{(k)o} \mathbf{D}^{(k)SX}] + r_P^{(k)o} \mathbf{D}_P^{(k)} \quad (75)$$

Approximate Equation:

$$\sum_k \left\{ \frac{\Omega}{\delta t} r_P^{(k)o} C_\rho^{(k)} P'_P + \Delta_P \left[r^{(k)o} C_\rho^{(k)} U^{(k)*} P' \right] - \Delta_P \left[r^{(k)^o} \rho^{(k)o} \left(r^{(k)^o} \mathbf{D}^{(k)SX} \nabla P' \right) . \mathbf{S} \right] \right\} = -\sum_k \left\{ \frac{r_P^{(k)o} \rho_P^{(k)o} - \left(r_P^{(k)} \rho_P^{(k)} \right)^{Old}}{\delta t} \Omega + \Delta_P \left[r^{(k)o} \rho^{(k)o} U^{(k)*} \right] \right\} \tag{76}$$

A Global MCBA-SIMPLEX Iteration

- *Solve implicitly for* $\mathbf{u}^{(k)}$*, using the old pressure and density fields.*
- *Calculate the* $\mathbf{D}^{(k)}$ *fields.*
- *Solve implicitly for the* $\mathbf{D}^{(k)SX}$ *fields.*
- *Solve the pressure correction equation using these* $\mathbf{D}^{(k)SX}$ *fields.*
- *Correct* $\mathbf{u}^{(k)}$, P *and* $\rho^{(k)}$.
- *Solve implicitly for* $r^{(k)}$.
- *Solve implicitly the energy equations and update the density fields.*
- *Return to the first step and iterate until convergence.*

The Expanded Form of the Pressure-Correction Equation

It is obvious by now that the various simplified pressure-correction equations are similar and may be written as:

$$\sum_k \left\{ \frac{\Omega}{\delta t} r_P^{(k)o} C_\rho^{(k)} P'_P + \Delta_P \left[r^{(k)o} C_\rho^{(k)} U^{(k)} P' \right] - \Delta_P \left[r^{(k)^o} \rho^{(k)} \left(r^{(k)^o} \mathbf{D}^{(k)} \nabla P' \right) . \mathbf{S} \right] \right\} = -\sum_k \left\{ \frac{r_P^{(k)o} \rho_P^{(k)} - \left(r_P^{(k)} \rho_P^{(k)} \right)^{Old}}{\delta t} \Omega + \Delta_P \left[r^{(k)o} \rho^{(k)} U^{(k)} \right] \right\} \tag{77}$$

Where, depending on the algorithm used, $U^{(k)}$ and $\rho^{(k)}$ represent values from the previous iteration or from a previous corrector step. The second term on the left hand side is similar to a convection term and may be discretized using any convective scheme (the upwind scheme is employed here). The term $\Delta_P \left[r^{(k)^o} \rho^{(k)} \left(r^{(k)^o} \mathbf{D}^{(k)} \nabla P' \right) . \mathbf{S} \right]$ is discretized following the same procedure used in discretizing the diffusion flux. Substituting the various terms in Eq. (77) by their equivalent expressions and neglecting the non-orthogonal terms, the final form of the pressure-correction equation is written as:

$$A_P^{P'} P'_P = A_E^{P'} P'_E + A_W^{P'} P'_W + A_N^{P'} P'_N + A_S^{P'} P'_S + A_T^{P'} P'_T + A_B^{P'} P'_B + B_P^{P'} \tag{78}$$

where

$$A_F^{P'} = \sum_k \left(\Gamma_f^{(k)} + \left(r^{(k)o} C_\rho^{(k)} \right)_f \left\| -U_f^{(k)}, 0 \right\| \right) \tag{79}$$

$$A_P^{P'} = \sum_{NB} A_F^{P'} + \sum_k \left(\frac{\left(r^{(k)o} C_\rho^{(k)} \right)_P \Omega_P}{\delta t} + \sum_{nb} \left(r^{(k)o} C_\rho^{(k)} \right)_f U_f^{(k)} \right) \tag{80}$$

$$B_P^{P'} = -\sum_k \left\{ \frac{\left(r_P^{(k)o}\rho_P^{(k)} - r_P^{(k)old}\rho_P^{(k)old} \right)}{\delta t}\Omega_P + \sum_{nb} r_f^{(k)}\rho_f^{(k)}U_f^{(k)} \right\}$$

$$\Gamma_f = r_f^{(k)\circ} r_f^{(k)\circ} \rho_f^{(k)} \frac{\sum_{i=1}^{3} \overline{D}_f^{(k)}[u_i]\left(S_f^{x_i}\right)^2}{\mathbf{S}_f \cdot \mathbf{d}_f} \tag{81}$$

The corrections are then applied to the velocity, pressure, and density fields using the following equations:

$$\mathbf{u}_P^{(k)*} = \mathbf{u}_P^{(k)o} - r^{(k)o}\mathbf{D}_P^{(k)}\nabla_P P',\; P^* = P^o + P',\; \rho^{(k)*} = \rho^{(k)o} + C_\rho^{(k)}P' \tag{82}$$

Improvement #2: Weighted Pressure Correction

Numerical experiments [72] using the above approach to simulate air-water flows have shown poor conservation of the lighter fluid. To understand this behavior, the residual error of the continuity equation of the kth phase, after any global iteration, that arises because the velocity, density, and volume fraction fields do not yet satisfy the continuity equation is denoted by RESC$^{(k)}$. The pressure correction equation being derived from the global conservation equation, the intention is to correct the velocity fields so as to drive the global residual error, which is equal to the sum of the local residuals, to zero i.e. RESC$^{(1)}$+ RESC$^{(2)}$ + .. + RESC$^{(n)}$ $\rightarrow$0.

In the presence of a relatively very high density fluid such that $\rho^{(n)} >> \rho^{(k)}$ for $k \neq n$, the residual error of the nth fluid will be of a magnitude commensurate with the respective phase density, i.e. RESC$^{(n)}$ is expected to be much larger than RESC$^{(k)}$ for $k \neq n$. In this case, only the residual of the high-density fluid will be significant while that of the low-density fluid will be relatively negligible, and hence the pressure correction will tend to drive the high-density fluid to conservation.

This problem can be considerably alleviated by normalizing the individual continuity equations, and hence the global mass conservation equation, by means of a weighting factor such as a reference density $\underline{\rho}^{(k)}$ (which is fluid dependent) to give a conservation equation of the form:

$$\sum_k \left\{ \frac{\left(r_P^{(k)}\rho_P^{(k)}/\underline{\rho}^{(k)} \right) - \left(r_P^{(k)}\rho_P^{(k)}/\underline{\rho}^{(k)} \right)^{Old}}{\delta t}\Omega_P + \Delta_P\left[r^{(k)}\left(\frac{\rho^{(k)}}{\underline{\rho}^{(k)}} \right)\mathbf{u}^{(k)}\cdot\mathbf{S} \right] \right\} = 0 \tag{83}$$

In this case the pressure correction equation is obtained by simply replacing $\rho^{(k)}$ by $\rho^{(k)}/\underline{\rho}^{(k)}$.

Solving for volume fractions

The volume fractions can be obtained by solving the fluid continuity equations (Eq. (23)). However, if all volume fractions are obtained by solving the continuity equations, the geometric constraint will not be enforced unless the appropriate velocity field is available, which is not the case until convergence. One remedy is to solve for n-1 volume fractions using the fluid mass conservation equations, and then to employ the geometric conservation equation to find the last volume fraction field. Thus, for fluids k=1 to n-1, solve

$$r_P^{(k)*} = H_P\left[r^{(k)*}\right] \text{ and for k=n use } r_P^{(n)*} = 1 - \sum_{k \neq n} r_P^{(k)*} \tag{84}$$

A drawback of this procedure is that the volume fraction field of any phase will not be influenced by the volume fraction fields of other phases except when calculating the n^{th} phase. This can affect the convergence rate negatively. Better solutions are presented below.

Improvement #3: Mutual influence of Volume Fractions

An improvement on the above procedure, is to solve all continuity equations to obtain all volume fractions and then enforce the geometric conservation constraint on the resulting volume fraction values using the following equation:

$$r^{(k)} = \frac{r^{(k)*}}{\sum_m r^{(m)*}} = \frac{H_P\left[r^{(k)*}\right]}{\sum_m r^{(m)*}} \quad \text{for all k} \tag{85}$$

The summation is carried out for all phases, and $r^{(k)}$ is the value of the volume fraction for fluid (k) which is carried into subsequent calculations. These $r^{(k)}$ of course, do sum to unity, and the values of every phase are affected by all other phases.

Improvement #4: Implicit Volume Fraction Equations

The solution of the volume fraction equations can be improved by implicitly accounting for the influence of the volume fractions of the different phases on each other. The details of the procedure will be presented for a two-fluid flow and then generalized to n-fluid flow situations. For that purpose, the following simplified form of the volume fraction equation is considered:

$$r_P^{(k)*} = H\left[r^{(k)*}\right] = \frac{\sum_{NB} A_{NB}^{(k)} r_{NB}^{(k)*} + B_P^{`(k)}}{A_P^{(k)}} \tag{86}$$

For the case of a two-fluid flow, the sum to 1 rule can be written in the following form

$$r_P^{(1)*} + r_P^{(2)*} = 1 = \frac{\sum_{NB} A_{NB}^{(1)} r_{NB}^{(1)*} + B_P^{`(1)}}{A_P^{(1)}} + \frac{\sum_{NB} A_{NB}^{(2)} r_{NB}^{(2)*} + B_P^{`(2)}}{A_P^{(2)}} \tag{87}$$

Based on this equation, the volume fraction equation for fluid (1) or (2) can be written as

$$r_P^{(1or2)*} = \frac{\left(\sum_{NB} A_{NB}^{(1or2)} r_{NB}^{(1or2)*} + B_P^{`(1or2)}\right)}{A_P^{(1or2)}\left(1 - \frac{RESR^{(1)}}{A_P^{(1)}} - \frac{RESR^{(2)}}{A_P^{(2)}}\right)} \tag{88}$$

For the case of n fluids, the kth volume fraction equation can be easily deduced from the above equation and is given by,

$$r_P^{(k)*} = \frac{\left(\sum_{NB} A_{NB}^{(k)} r_{NB}^{(k)*} + B_P^{`(k)}\right)}{A_P^{(k)}\left(1 - \sum_m \frac{RESR^{(m)}}{A_P^{(m)}}\right)} \tag{89}$$

Improvement #5: Bounding the Volume Fractions

While the above technique can be used to solve the volume fraction equations, it does not guarantee that the volume fraction values are bounded (i.e. between 0 and 1). This is a feature of iterative methods, which are known to return intermediate values that violate the set bounds. While these restrictions can be explicitly enforced after obtaining the solution from the discretized equations, a number of techniques were developed that lead to the implicit enforcing of these constraints.

The procedure developed by Carver [73] is an example of such methods based on a modification to the under-relaxation practice of Patankar [16]. In this approach, instead of solving the volume fraction equation directly for $r^{(k)}$ to yield $r^{(k)imp}$, under-relaxation is used to yield a value $r^{(k)C}=\beta\, r^{(k)imp} +(1-\beta)\, r^{(k)\circ}$, where β is between [0,1] and $r^{(k)\circ}$ is the solution from the previous iteration. Equation (15) is thus rewritten as:

$$\frac{A_P}{\beta} r_P^{(k)C} = \sum_{NB} A_{NB} r_{NB}^{(k)C} + B_P + \frac{(1-\beta)}{\beta} A_P r_P^{(k)o} \tag{90}$$

In the Carver procedure, the value of $r_P^{(k)C}$ over each control volume is monitored by explicitly calculating an intermediate value $r_P^{(k)\,int}$ as:

$$r_P^{(k)int} = \frac{\sum_{NB} A_{NB} r_{NB}^{(k)o} + B_P + \frac{(1-\beta)}{\beta} A_P r_P^{(k)o}}{\frac{A_P}{\beta}} \tag{91}$$

If $r_P^{(k)int} > (1-\varepsilon)$ then the under-relaxation factor is modified to the form $\beta = MAX(1 - r_P^{(k)o}, \gamma)$. The parameters ε and γ are small; Carver suggests values of 0.05 and 10^{-10}. The system of equations for each volume fraction is then solved implicitly using, for every control volume, the individually assigned relaxation parameter.

Solving the energy equations

The solutions of the energy equations follow that of the general multi-fluid scalar equation. As such, nothing new needs to be added in that regard (though in many cases coupling of the energy equation with the momentum and continuity equations is beneficial).

Part II - Geometric Conservation Based Algorithms

The sequence of events in the Geometric Conservation Based Algorithm (GCBA) is as follows:

- Solve the individual mass conservation equations for volume fractions.
- Solve the momentum equations for velocities.
- Solve the pressure correction equation.
- Correct velocity, volume fraction, density, and pressure fields.
- Solve the individual energy equations.
- Return to the first step and repeat until convergence.

As in the MCBA, the GCBA uses the momentum equations for a first estimate of velocities. However, the volume fractions are calculated without enforcing the geometric conservation equation. Hence, the mass conservation equations of all fluids are used to calculate the volume fractions. The pressure correction equation is based on the geometric conservation equation and is used to restore the imbalance of volume fractions. The errors in the calculated volume fractions are expressed in terms of pressure correction (P'), which is also used to adjust the velocity and density fields. An example of a GCBA is the original IPSA, developed by Spalding [74], which introduces a stronger coupling between the pressure and the volume fractions than the MCBA.

For compactness, the techniques introduced earlier that are also applicable here, will not be repeated. Rather, attention will be directed towards the derivation of the pressure correction equation and the introduction of the various GCBA. This is followed by a comparison between the two families.

Solving for Pressure Correction

After solving the continuity equations for the volume fraction fields and the momentum equations for the velocity fields, the next step is to correct the various fields such that the volume fraction fields satisfy the compatibility equation and the velocity and pressure fields satisfy the continuity equations. For that purpose, an approach similar to the one used with the MCBA is adopted. The difference between the two approaches lies in the constraint equation employed in deriving the pressure or pressure correction equation. In the MCBA, the overall mass conservation equation was utilized. In the GCBA, the pressure correction equation is derived from the geometric conservation equation.

To start the derivation, it is noticed that initially the volume fraction fields denoted by $r^{(k)*}$, do not satisfy the compatibility equation and a discrepancy exists i.e.

$$RESG_P = 1 - \sum_k r_P^{(k)*} \tag{92}$$

A change to $r^{(k)*}$ is sought that would restore the balance. The corrected r value, denoted by $r^{(k)}$ $\left(r^{(k)} = r^{(k)*} + r^{(k)'}\right)$, is such that

$$\sum_k \left(r^{(k)'}\right) = 1 - \sum_k \left(r^{(k)*}\right) = RESG_P \tag{93}$$

Correction to the volume fraction, $r^{(k)'}$, will be associated with a correction to the velocity, density, and pressure fields, $\mathbf{u}^{(k)'}$, $\rho^{(k)'}$, and P' respectively. Thus, the corrected fields are given as:

$$r^{(k)} = r^{(k)^*} + r^{(k)'}, P = P^{o} + P', \mathbf{u}^{(k)} = \mathbf{u}^{(k)^*} + \mathbf{u}^{(k)'}, \rho^{(k)} = \rho^{(k)^o} + \rho^{(k)'} \tag{94}$$

The discretized form of the corrected continuity equation of phase (k) can be written as

$$\begin{aligned} &\frac{\left(r_P^{(k)*} + r_P^{(k)'}\right)\left(\rho_P^{(k)\circ} + \rho_P^{(k)'}\right) - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P \\ &\quad + \Delta_P\left(\left(r^{(k)*} + r^{(k)'}\right)\left(\rho^{(k)\circ} + \rho^{(k)'}\right)\left(\mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}\right).\mathbf{S}\right) = \dot{M}_P^{(k)}\left(r_P^{(k)*} + r_P^{(k)'}\right)\Omega_P \end{aligned} \tag{95}$$

Neglecting second and third order terms (i.e. $r_P^{(k)'}\rho_P^{(k)'}$, $\rho_P^{(k)'}\mathbf{u}^{(k)'}$, $r_P^{(k)'}\mathbf{u}^{(k)'}$, and $r_P^{(k)'}\rho_P^{(k)'}\mathbf{u}^{(k)'}$), its expanded form reduces to:

$$\begin{aligned}&\frac{\left(r_P^{(k)*}\rho_P^{(k)'}+r_P^{(k)'}\rho_P^{(k)\circ}\right)}{\delta t}\Omega_P+\Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}\mathbf{u}^{(k)'}.\mathbf{S}+r^{(k)*}U^{(k)*}\rho_P^{(k)'}+\rho^{(k)\circ}U^{(k)*}r^{(k)'}\right)\right]\\&-\dot{M}_P^{(k)}r_P^{(k)'}\Omega_P=-\frac{\left(r_P^{(k)*}\rho_P^{(k)\circ}\right)-\left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P-\Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}U^{(k)*}\right)\right]+\dot{M}_P^{(k)}r_P^{(k)*}\Omega_P\end{aligned} \tag{96}$$

Writing $\mathbf{u}^{(k)'}$ as a function of P', similar to what is usually done in a SIMPLE-like algorithm, the correction momentum equations become

$$\mathbf{u}^{(k)'}=\mathbf{HP}[\mathbf{u}^{(k)'}]-r^{(k)*}\mathbf{D}^{(k)}\nabla P'-r^{(k)'}\mathbf{D}^{(k)}\nabla P^{\circ}-r^{(k)'}\mathbf{D}^{(k)}\nabla P' \tag{97}$$

Substituting Eq. (97) into Eq. (96), rearranging, and discretizing one gets

$$\begin{aligned}&r_P^{(k)'}-H_P\left[r^{(k)'}\right]=\\&-R_P^{(k)}\left(\begin{array}{l}\dfrac{r_P^{(k)*}\Omega_P}{\delta t}\rho_P^{(k)'}+\Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(\begin{array}{l}\mathbf{HP}[\mathbf{u}^{(k)'}]-r^{(k)*}\mathbf{D}^{(k)}\nabla P'\\-r^{(k)'}\mathbf{D}^{(k)}\nabla P'\end{array}\right).\mathbf{S}+r^{(k)*}U^{(k)*}\rho^{(k)'}\right]\\+\dfrac{\left(r_P^{(k)*}\rho_P^{(k)\circ}\right)-\left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P+\Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}U^{(k)*}\right)\right]-\dot{M}_P^{(k)}r_P^{(k)*}\Omega_P\end{array}\right)\end{aligned} \tag{98}$$

where $R_P^{(k)}=1/A_P^{(k)}$.

Neglecting the correction to neighboring cells, equation (98) reduces to:

$$r_P^{(k)'}=-R_P^{(k)}\left(\begin{array}{l}\dfrac{r_P^{(k)*}\Omega_P}{\delta t}\rho_P^{(k)'}+\Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(\begin{array}{l}\mathbf{HP}[\mathbf{u}^{(k)'}]-r^{(k)*}\mathbf{D}^{(k)}\nabla P'\\-r^{(k)'}\mathbf{D}^{(k)}\nabla P'\end{array}\right).\mathbf{S}+r^{(k)*}U^{(k)*}\rho^{(k)'}\right]\\+\dfrac{\left(r_P^{(k)*}\rho_P^{(k)\circ}\right)-\left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P+\Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}U^{(k)*}\right)\right]-\dot{M}_P^{(k)}r_P^{(k)*}\Omega_P\end{array}\right) \tag{99}$$

Substituting this equation into the geometric conservation equation and replacing density correction in terms of pressure correction (i.e. $\rho^{(k)'}=C_\rho^{(k)}P'$), the pressure correction equation is obtained as

$$\sum_k\left\{-R_P^{(k)}\left(\begin{array}{l}\dfrac{r_P^{(k)*}\Omega_P C_\rho^{(k)}}{\delta t}P_P'+\Delta_P\left[r^{(k)*}U^{(k)*}C_\rho^{(k)}P'\right]+\\\Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(\mathbf{HP}[\mathbf{u}^{(k)'}]-r^{(k)*}\mathbf{D}^{(k)}\nabla P'-r^{(k)'}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\\+\dfrac{\left(r_P^{(k)*}\rho_P^{(k)\circ}\right)-\left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P+\Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}U^{(k)*}\right)\right]\end{array}\right)\right\}=RESG_P \tag{100}$$

As detailed next, the above equation can be expanded using any simple-like algorithm to yield the new GCBA family of multi-fluid flow algorithms (GCBA-SIMPLE, GCBA-SIMPLEC, GCBA-PISO,…).

The GCBA following SIMPLEC (GCBA-SIMPLEC): Symbolic Form

Predictor:

$$r_P^{(k)*} = H_P[r^{(k)*}] \tag{101}$$

$$\mathbf{u}_P^{(k)*} = \mathbf{HP}_P[\mathbf{u}^{(k)*}] - r_P^{(k)*}\mathbf{D}_P^{(k)}\nabla_P P^o \tag{102}$$

Corrector:

$$\left(\mathbf{u}^{(k)'}, P', \rho^{(k)'}, r^{(k)'}\right)\begin{pmatrix} \mathbf{u}^{(k)**} = \mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}, P^* = P^o + P', \\ \rho^{(k)*} = \rho^{(k)o} + \rho^{(k)'}, r^{(k)**} = r^{(k)*} + r^{(k)'} \end{pmatrix} \tag{103}$$

$$\therefore \mathbf{u}_P^{(k)**} = \mathbf{HP}_P[\mathbf{u}^{(k)**}] - r_P^{(k)**}\mathbf{D}_P^{(k)}\nabla_P P^* = \mathbf{HP}_P[\mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}] - \left(r_P^{(k)*} + r_P^{(k)'}\right)\mathbf{D}_P^{(k)}\nabla_P\left(P^o + P'\right) \tag{104}$$

$$\therefore \mathbf{u}_P^{(k)'} = \mathbf{HP}_P[\mathbf{u}^{(k)'}] - r_P^{(k)*}\mathbf{D}_P^{(k)}\nabla_P P' - r_P^{(k)'}\mathbf{D}_P^{(k)}\nabla_P P^o - r_P^{(k)'}\mathbf{D}_P^{(k)}\nabla_P P' \tag{105}$$

Subtracting $\widetilde{\mathbf{HP}}_P[1]\mathbf{u}_P^{(k)'}$ from both sides, one gets

$$\mathbf{u}_P^{(k)'} = \begin{bmatrix} \dfrac{\mathbf{HP}_P[\mathbf{u}^{(k)'} - \mathbf{u}_P^{(k)'}]}{\left(1 - \widetilde{\mathbf{HP}}_P[1]\right)} - r_P^{(k)*}\dfrac{\mathbf{D}_P^{(k)}}{\left(1 - \widetilde{\mathbf{HP}}_P[1]\right)}\nabla_P P' \\ - r_P^{(k)'}\dfrac{\mathbf{D}_P^{(k)}}{\left(1 - \widetilde{\mathbf{HP}}_P[1]\right)}\nabla_P P^o - r_P^{(k)'}\dfrac{\mathbf{D}_P^{(k)}}{\left(1 - \widetilde{\mathbf{HP}}_P[1]\right)}\nabla_P P' \end{bmatrix} \tag{106}$$

$$\therefore \begin{cases} \mathbf{u}_P^{(k)'} = \dfrac{\mathbf{HP}_P[\mathbf{u}^{(k)'} - \mathbf{u}_P^{(k)'}]}{\left(1 - \widetilde{\mathbf{HP}}_P[1]\right)} - r_P^{(k)*}\widetilde{\mathbf{D}}_P^{(k)}\nabla_P P' - r_P^{(k)'}\widetilde{\mathbf{D}}_P^{(k)}\nabla_P P^o - r_P^{(k)'}\widetilde{\mathbf{D}}_P^{(k)}\nabla_P P' \\ \rho^{(k)'} = C_\rho^{(k)} P' \\ r_P^{(k)'} = -R_P^{(k)}\left(\dfrac{r_P^{(k)*}\Omega_P}{\delta t}\rho_P^{(k)'} + \Delta_P\left[\left(r^{(k)*}\rho^{(k)o}\mathbf{u}^{(k)'}\right).\mathbf{S} + r^{(k)*}U^{(k)*}\rho^{(k)'}\right]\right) \end{cases} \tag{107}$$

Condition:

$$\sum_k\left\{R_P^{(k)}\left(\frac{r_P^{(k)*}\Omega_P C_\rho^{(k)}}{\delta t}P'_P + \Delta_P\left[r^{(k)*}U^{(k)*}C_\rho^{(k)}P'\right] - \Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(r^{(k)*}\widetilde{\mathbf{D}}^{(k)}\nabla P'\right).\mathbf{S}\right]\right)\right\} =$$

$$-\sum_k\left\{R_P^{(k)}\begin{pmatrix} \dfrac{\left(r_P^{(k)*}\rho_P^{(k)\circ}\right) - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P + \Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}U^{(k)*}\right)\right] + \\ \Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(\mathbf{HP}[\mathbf{u}^{(k)'} - \mathbf{u}_P^{(k)'}] - r^{(k)'}\widetilde{\mathbf{D}}^{(k)}\nabla P'\right).\mathbf{S}\right] \end{pmatrix}\right\} - RESG_P \tag{108}$$

Approximation:

$$\text{Neglect: } \mathbf{HP}[\mathbf{u}^{(k)'} - \mathbf{u}_P^{(k)'}],\, r^{(k)'}\tilde{\mathbf{D}}^{(k)}\nabla P' \quad \Rightarrow \quad \mathbf{u}_P^{(k)'} = -r_P^{(k)*}\mathbf{D}_P^{(k)}\nabla_P P' \tag{109}$$

Approximate Equation:

$$\sum_k \left\{ R_P^{(k)} \left(\frac{r_P^{(k)*}\Omega_P C_\rho^{(k)}}{\delta t} P_P' + \Delta_P\left[r^{(k)*}U^{(k)*}C_\rho^{(k)}P'\right] - \Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(r^{(k)*}\tilde{\mathbf{D}}^{(k)}\nabla P'\right).\mathbf{S}\right]\right)\right\} = -\sum_k \left\{ R_P^{(k)} \left(\frac{\left(r_P^{(k)*}\rho_P^{(k)\circ}\right) - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P + \Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}U^{(k)*}\right)\right]\right)\right\} - RESG_P \tag{110}$$

A Global GCBA-SIMPLEC Iteration

- *Solve implicitly for the volume fraction fields.*
- *Solve implicitly for* $\mathbf{u}^{(k)}$*, using the old pressure, density, and volume fraction fields.*
- *Calculate the* $\tilde{\mathbf{D}}^{(k)}$ *fields.*
- *Solve the pressure correction equation and correct* $\mathbf{u}^{(k)}$, P, $r^{(k)}$ *and* $\rho^{(k)}$.
- *Solve implicitly the energy equations and update the density fields.*
- *Return to the first step and iterate until convergence.*

The GCBA following PRIME (GCBA-PRIME): Symbolic Form

Predictor:

$$r_P^{(k)*} = H_P[r^{(k)o}] \tag{111}$$

$$\mathbf{u}_P^{(k)*} = \mathbf{HP}_P[\mathbf{u}^{(k)o}] - r_P^{(k)*}\mathbf{D}_P^{(k)}\nabla_P P^o \tag{112}$$

Corrector:

$$\left(\mathbf{u}^{(k)'}, P', \rho^{(k)'}, r^{(k)'}\right) \begin{pmatrix} \mathbf{u}^{(k)**} = \mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}, P^* = P^o + P', \\ \rho^{(k)*} = \rho^{(k)o} + \rho^{(k)'}, r^{(k)**} = r^{(k)*} + r^{(k)'} \end{pmatrix} \tag{113}$$

$$\therefore \mathbf{u}_P^{(k)**} = \mathbf{HP}_P[\mathbf{u}^{(k)**}] - r_P^{(k)**}\mathbf{D}_P^{(k)}\nabla_P P^* = \mathbf{HP}_P[\mathbf{u}^{(k)*} + \mathbf{u}^{(k)'}] - \left(r_P^{(k)*} + r_P^{(k)'}\right)\mathbf{D}_P^{(k)}\nabla_P\left(P^o + P'\right) \tag{114}$$

$$\therefore \begin{cases} \mathbf{u}_P^{(k)'} = \mathbf{HP}_P[\mathbf{u}^{(k)*} - \mathbf{u}^{(k)o}] + \mathbf{HP}_P[\mathbf{u}^{(k)'}] - r_P^{(k)*}\mathbf{D}_P^{(k)}\nabla_P P' - r_P^{(k)'}\mathbf{D}_P^{(k)}\nabla_P P^o - r_P^{(k)'}\mathbf{D}_P^{(k)}\nabla_P P' \\ \rho^{(k)'} = C_\rho^{(k)}P' \\ r_P^{(k)'} = -R_P^{(k)}\left(\frac{r_P^{(k)*}\Omega_P}{\delta t}\rho_P^{(k)'} + \Delta_P\left[\left(r^{(k)*}\rho^{(k)o}\mathbf{u}^{(k)'}\right).\mathbf{S} + r^{(k)*}U^{(k)*}\rho^{(k)'}\right]\right) \end{cases} \tag{115}$$

Condition:

$$\sum_k \left\{ R_P^{(k)} \left(\frac{r_P^{(k)*}\Omega_P C_\rho^{(k)}}{\delta t} P_P' + \Delta_P\left[r^{(k)*}U^{(k)*}C_\rho^{(k)}P'\right] - \Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(r^{(k)*}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right)\right\} = -\sum_k \left\{ R_P^{(k)} \left(\begin{array}{l} \frac{\left(r_P^{(k)*}\rho_P^{(k)\circ}\right) - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P + \Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}U^{(k)*}\right)\right] + \\ \Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(\mathbf{HP}[\mathbf{u}^{(k)*} - \mathbf{u}^{(k)o}] + \mathbf{HP}[\mathbf{u}^{(k)'}] - r^{(k)'}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right] \end{array}\right)\right\} - RESG_P \tag{116}$$

Approximation:

Neglect: $\mathbf{HP}[\mathbf{u}^{(k)*}-\mathbf{u}^{(k)o}], \mathbf{HP}[\mathbf{u}^{(k)'}], r^{(k)'}\mathbf{D}^{(k)}\nabla P'$

$$\Rightarrow \mathbf{u}_P^{(k)'} = -r_P^{(k)*}\mathbf{D}_P^{(k)}\nabla_P P' \tag{117}$$

Approximate Equation:

$$\begin{aligned}\sum_k \left\{ R_P^{(k)} \left(\frac{r_P^{(k)*}\Omega_P C_\rho^{(k)}}{\delta t} P'_P + \Delta_P\left[r^{(k)*}U^{(k)*}C_\rho^{(k)}P'\right] - \Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(r^{(k)*}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right)\right\} = \\ -\sum_k \left\{ R_P^{(k)} \left(\frac{\left(r_P^{(k)*}\rho_P^{(k)\circ}\right) - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P + \Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}U^{(k)*}\right)\right]\right)\right\} - RESG_P\end{aligned} \tag{118}$$

A Global GCBA-PRIME Iteration

- *Solve explicitly for the volume fraction fields.*
- *Solve explicitly for $\mathbf{u}^{(k)}$, using the old pressure and density fields.*
- *Calculate the $\mathbf{D}^{(k)}$ fields.*
- *Solve the pressure correction equation and correct $\mathbf{u}^{(k)}$, P, $r^{(k)}$ and $\rho^{(k)}$.*
- *Solve implicitly the energy equations and update the density fields.*
- *Return to the first step and iterate until convergence.*

The GCBA following SIMPLER (GCBA-SIMPLER): Symbolic Form

First Predictor:

$$r_P^{(k)*} = H_P[r^{(k)*}] \tag{119}$$

Calculate the coefficients of the momentum equations.

First Corrector:

$$\left(\mathbf{u}^{(k)'}, P', \rho^{(k)'}, r^{(k)'}\right)\begin{pmatrix}\mathbf{u}^{(k)*} = \mathbf{u}^{(k)o} + \mathbf{u}^{(k)'}, P^* = P^o + P', \\ \rho^{(k)*} = \rho^{(k)o} + \rho^{(k)'}, r^{(k)**} = r^{(k)*} + r^{(k)'}\end{pmatrix} \tag{120}$$

$$\therefore \mathbf{u}_P^{(k)*} = \mathbf{HP}_P[\mathbf{u}^{(k)*}] - r_P^{(k)**}\mathbf{D}_P^{(k)}\nabla_P P^* = \mathbf{HP}_P[\mathbf{u}^{(k)o} + \mathbf{u}^{(k)'}] - \left(r_P^{(k)*} + r_P^{(k)'}\right)\mathbf{D}_P^{(k)}\nabla_P\left(P^o + P'\right) \tag{121}$$

$$\mathbf{u}_P^{(k)o} = \mathbf{HP}_P\left[\mathbf{u}^{(k)o}\right] - r_P^{(k)*}\mathbf{D}_P^{(k)}\nabla_P P^o \tag{122}$$

$$\therefore \begin{cases}\mathbf{u}_P^{(k)'} = \mathbf{HP}_P[\mathbf{u}^{(k)'}] - r_P^{(k)*}\mathbf{D}_P^{(k)}\nabla_P P' - r_P^{(k)'}\mathbf{D}_P^{(k)}\nabla_P P^o - r_P^{(k)'}\mathbf{D}_P^{(k)}\nabla_P P' \\ \rho^{(k)'} = C_\rho^{(k)}P' \\ r_P^{(k)'} = -R_P^{(k)}\left(\frac{r_P^{(k)*}\Omega_P}{\delta t}\rho_P^{(k)'} + \Delta_P\left[\left(r^{(k)*}\rho^{(k)o}\mathbf{u}^{(k)'}\right).\mathbf{S} + r^{(k)*}U^{(k)o}\rho^{(k)'}\right]\right)\end{cases} \tag{123}$$

Condition:

$$\sum_k \left\{ R_P^{(k)} \left(\frac{r_P^{(k)*}\Omega_P C_\rho^{(k)}}{\delta t} P'_P + \Delta_P\left[r^{(k)*}U^{(k)o}C_\rho^{(k)}P'\right] - \Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(r^{(k)*}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right)\right\} =$$
$$-\sum_k \left\{ R_P^{(k)} \left(\begin{array}{l} \dfrac{\left(r_P^{(k)*}\rho_P^{(k)\circ}\right)-\left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P + \Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}U^{(k)o}\right)\right] + \\ \Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(\mathbf{HP}[\mathbf{u}^{(k)'}] - r^{(k)'}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right] \end{array}\right)\right\} - RESG_P \tag{124}$$

Approximation:

$$\text{Neglect: } \mathbf{HP}[\mathbf{u}^{(k)'}],\, r^{(k)'}\mathbf{D}^{(k)}\nabla P' \quad \Rightarrow \quad \mathbf{u}_P^{(k)'} = -r_P^{(k)*}\mathbf{D}_P^{(k)}\nabla_P P' \tag{125}$$

Approximate Equation:

$$\sum_k \left\{ R_P^{(k)} \left(\frac{r_P^{(k)*}\Omega_P C_\rho^{(k)}}{\delta t} P'_P + \Delta_P\left[r^{(k)*}U^{(k)o}C_\rho^{(k)}P'\right] - \Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(r^{(k)*}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right)\right\} =$$
$$-\sum_k \left\{ R_P^{(k)} \left(\frac{\left(r_P^{(k)*}\rho_P^{(k)\circ}\right)-\left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P + \Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}U^{(k)o}\right)\right]\right)\right\} - RESG_P \tag{126}$$

Apply correction to pressure, density, and volume fraction fields.

Second Predictor:

$$\mathbf{u}_P^{(k)*} = \mathbf{HP}_P[\mathbf{u}^{(k)*}] - r_P^{(k)**}\mathbf{D}_P^{(k)}\nabla_P P^* \tag{127}$$

Second Corrector:

$$\left(\mathbf{u}^{(k)''}, P'', \rho^{(k)''}, r^{(k)''}\right)\left(\begin{array}{l} \mathbf{u}^{(k)**} = \mathbf{u}^{(k)*} + \mathbf{u}^{(k)''},\, P^{**} = P^* + P'', \\ \rho^{(k)**} = \rho^{(k)*} + \rho^{(k)''},\, r^{(k)***} = r^{(k)**} + r^{(k)''} \end{array}\right) \tag{128}$$

$$\therefore \begin{array}{l} \mathbf{u}_P^{(k)**} = \mathbf{HP}_P\left[\mathbf{u}^{(k)**}\right] - r_P^{(k)***}\mathbf{D}_P^{(k)}\nabla_P P^{**} \\ \qquad = \mathbf{HP}_P\left[\mathbf{u}^{(k)*} + \mathbf{u}^{(k)''}\right] - \left(r_P^{(k)**} + r_P^{(k)''}\right)\mathbf{D}_P^{(k)}\nabla_P\left(P^* + P''\right) \end{array} \tag{129}$$

$$\therefore \left\{ \begin{array}{l} \mathbf{u}_P^{(k)''} = \mathbf{HP}_P[\mathbf{u}^{(k)''}] - r_P^{(k)**}\mathbf{D}_P^{(k)}\nabla_P P'' - r_P^{(k)''}\mathbf{D}_P^{(k)}\nabla_P P^* - r_P^{(k)''}\mathbf{D}_P^{(k)}\nabla_P P'' \\ \rho^{(k)''} = C_\rho^{(k)} P'' \\ r_P^{(k)''} = -R_P^{(k)}\left(\dfrac{r_P^{(k)**}\Omega_P}{\delta t}\rho_P^{(k)''} + \Delta_P\left[\left(r^{(k)**}\rho^{(k)*}\mathbf{u}^{(k)''}\right).\mathbf{S} + r^{(k)**}U^{(k)*}\rho^{(k)''}\right]\right) \end{array}\right. \tag{130}$$

Condition:

$$\sum_k \left\{ R_P^{(k)} \left(\frac{r_P^{(k)**}\Omega_P C_\rho^{(k)}}{\delta t} P''_P + \Delta_P\left[r^{(k)**}U^{(k)*}C_\rho^{(k)}P''\right] - \Delta_P\left[r^{(k)**}\rho^{(k)*}\left(r^{(k)**}\mathbf{D}^{(k)}\nabla P''\right).\mathbf{S}\right]\right)\right\} =$$
$$-\sum_k \left\{ R_P^{(k)} \left(\begin{array}{l} \frac{\left(r_P^{(k)**}\rho_P^{(k)*}\right) - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P + \Delta_P\left[\left(r^{(k)**}\rho^{(k)*}U^{(k)*}\right)\right] + \\ \Delta_P\left[r^{(k)**}\rho^{(k)*}\left(\mathbf{HP}[\mathbf{u}^{(k)''}] - r^{(k)''}\mathbf{D}^{(k)}\nabla P''\right).\mathbf{S}\right] \end{array}\right)\right\} - RESG_P \tag{131}$$

Approximation:

Neglect: $\mathbf{HP}[\mathbf{u}^{(k)''}], r^{(k)''}\mathbf{D}^{(k)}\nabla P'' \quad \Rightarrow \quad \mathbf{u}_P^{(k)''} = -r_P^{(k)**}\mathbf{D}_P^{(k)}\nabla_P P''$ (132)

Approximate Equation:

$$\sum_k \left\{ R_P^{(k)} \left(\frac{r_P^{(k)**}\Omega_P C_\rho^{(k)}}{\delta t} P''_P + \Delta_P\left[r^{(k)**}U^{(k)*}C_\rho^{(k)}P''\right] - \Delta_P\left[r^{(k)**}\rho^{(k)*}\left(r^{(k)**}\mathbf{D}^{(k)}\nabla P''\right).\mathbf{S}\right]\right)\right\} =$$
$$-\sum_k \left\{ R_P^{(k)} \left(\frac{\left(r_P^{(k)**}\rho_P^{(k)*}\right) - \left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P + \Delta_P\left[\left(r^{(k)**}\rho^{(k)*}U^{(k)*}\right)\right]\right)\right\} - RESG_P \tag{133}$$

Apply correction to velocity fields.

A Global GCBA-SIMPLER Iteration

- *Solve implicitly for $r^{(k)}$.*
- *Calculate the $\mathbf{D}^{(k)}$ fields.*
- *Solve the pressure correction equation and update the pressure, density, and volume fraction fields.*
- *Solve implicitly for $\mathbf{u}^{(k)}$ using the new pressure, density, and volume fraction fields*
- *Solve the pressure correction equation using the new velocity fields and correct $\mathbf{u}^{(k)}$.*
- *Solve implicitly the energy equations and update the density fields.*
- *Return to the first step and iterate until convergence.*

The GCBA following SIMPLEM (GCBA-SIMPLEM): Symbolic Form

First Predictor:

$$r_P^{(k)*} = H_P[r^{(k)*}] \tag{134}$$

Calculate the coefficients of the momentum equations.

First Corrector:

$$\left(\mathbf{u}^{(k)'}, P', \rho^{(k)'}, r^{(k)'}\right)\left(\begin{array}{l} \mathbf{u}^{(k)*} = \mathbf{u}^{(k)o} + \mathbf{u}^{(k)'}, P^* = P^o + P', \\ \rho^{(k)*} = \rho^{(k)o} + \rho^{(k)'}, r^{(k)**} = r^{(k)*} + r^{(k)'} \end{array}\right) \tag{135}$$

$$\therefore \mathbf{u}_P^{(k)*} = \mathbf{HP}_P[\mathbf{u}^{(k)*}] - r_P^{(k)**}\mathbf{D}_P^{(k)}\nabla_P P^* = \mathbf{HP}_P[\mathbf{u}^{(k)o} + \mathbf{u}^{(k)'}] - \left(r_P^{(k)*} + r_P^{(k)'}\right)\mathbf{D}_P^{(k)}\nabla_P\left(P^o + P'\right) \tag{136}$$

$$\mathbf{u}_P^{(k)o} = \mathbf{HP}_P\left[\mathbf{u}^{(k)o}\right] - r_P^{(k)*}\mathbf{D}_P^{(k)}\nabla_P P^o \tag{137}$$

$$\therefore \begin{cases} \mathbf{u}_P^{(k)'} = \mathbf{HP}_P[\mathbf{u}^{(k)'}] - r_P^{(k)*}\mathbf{D}_P^{(k)}\nabla_P P' - r_P^{(k)'}\mathbf{D}_P^{(k)}\nabla_P P^o - r_P^{(k)'}\mathbf{D}_P^{(k)}\nabla_P P' \\ \rho^{(k)'} = C_\rho^{(k)} P' \\ r_P^{(k)'} = -R_P^{(k)}\left(\dfrac{r_P^{(k)*}\Omega_P}{\delta t}\rho_P^{(k)'} + \Delta_P\left[\left(r^{(k)*}\rho^{(k)o}\mathbf{u}^{(k)'}\right).\mathbf{S} + r^{(k)*}U^{(k)o}\rho^{(k)'}\right]\right) \end{cases} \tag{138}$$

Condition:

$$\sum_k\left\{R_P^{(k)}\left(\frac{r_P^{(k)*}\Omega_P C_\rho^{(k)}}{\delta t}P'_P + \Delta_P\left[r^{(k)*}U^{(k)o}C_\rho^{(k)}P'\right] - \Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(r^{(k)*}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right)\right\} =$$
$$-\sum_k\left\{R_P^{(k)}\left(\begin{array}{l}\dfrac{\left(r_P^{(k)*}\rho_P^{(k)\circ}\right)-\left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P + \Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}U^{(k)o}\right)\right] + \\ \Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(\mathbf{HP}[\mathbf{u}^{(k)'}] - r^{(k)'}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\end{array}\right)\right\} - RESG_P \tag{139}$$

Approximation:

Neglect: $\mathbf{HP}[\mathbf{u}^{(k)'}], r^{(k)'}\mathbf{D}^{(k)}\nabla P'$

$$\Rightarrow \mathbf{u}_P^{(k)'} = -r_P^{(k)*}\mathbf{D}_P^{(k)}\nabla_P P' \tag{140}$$

Approximate Equation:

$$\sum_k\left\{R_P^{(k)}\left(\frac{r_P^{(k)*}\Omega_P C_\rho^{(k)}}{\delta t}P'_P + \Delta_P\left[r^{(k)*}U^{(k)o}C_\rho^{(k)}P'\right] - \Delta_P\left[r^{(k)*}\rho^{(k)\circ}\left(r^{(k)*}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S}\right]\right)\right\} =$$
$$-\sum_k\left\{R_P^{(k)}\left(\frac{\left(r_P^{(k)*}\rho_P^{(k)\circ}\right)-\left(r_P^{(k)}\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P + \Delta_P\left[\left(r^{(k)*}\rho^{(k)\circ}U^{(k)o}\right)\right]\right)\right\} - RESG_P \tag{141}$$

Second Predictor:

$$\mathbf{u}_P^{(k)**} = \mathbf{HP}_P[\mathbf{u}^{(k)**}] - r_P^{(k)**}\mathbf{D}_P^{(k)*}\nabla_P P^* \tag{142}$$

Second Corrector: No corrector stage.

A Global GCBA-SIMPLEM Iteration

- *Solve implicitly for $r^{(k)}$.*
- *Calculate the $\mathbf{D}^{(k)}$ fields based on values from the previous iteration.*
- *Solve the pressure correction equation.*
- *Correct $\mathbf{u}^{(k)}$, P, $r^{(k)}$, and $\rho^{(k)}$.*
- *Calculate new $\mathbf{HP}^{(k)}$ and $\mathbf{D}^{(k)}$ fields.*
- *Solve implicitly for $\mathbf{u}^{(k)}$ using the new fields.*
- *Solve implicitly the energy equations and update the density fields.*
- *Return to the first step and iterate until convergence.*

The Expanded Form of the Pressure-Correction Equation

The expanded form of the pressure correction equation, applicable to all algorithms, will be presented. For that purpose, let $r^{(k)}$, $U^{(k)}$ and $\rho^{(k)}$ denote values from the previous iteration or from a previous corrector step, then, the pressure correction equation becomes

$$\sum_k \left\{ R_P^{(k)} \left(\frac{r_P^{(k)} C_\rho^{(k)} \Omega_P}{\delta t} P'_P + \Delta_P \left[r^{(k)} U^{(k)} C_\rho^{(k)} P' \right] - \Delta_P \left[r^{(k)} \rho^{(k)} \left(r^{(k)} \mathbf{D}^{(k)} \nabla (P') \right) . \mathbf{S} \right] \right) \right\} =$$
$$- \sum_{k=1}^{nphase} \left\{ R_P^{(k)} \left(\frac{\left(r_P^{(k)} \rho_P^{(k)} \right) - \left(r_P^{(k)} \rho_P^{(k)} \right)^{Old}}{\delta t} \Omega_P + \Delta_P \left[\left(r^{(k)} \rho^{(k)} U^{(k)} \right) \right] \right) \right\} - RESG_P \tag{143}$$

In this form, the resemblance between this equation and the MCBA pressure correction equation is obvious. The discretization of the above equation yields

$$A_P^{P'} P'_P = A_E^{P'} P'_E + A_W^{P'} P'_W + A_N^{P'} P'_N + A_S^{P'} P'_S + A_T^{P'} P'_T + A_B^{P'} P'_B + B_P^{P'} \tag{144}$$

where

$$A_F^{P'} = \sum_k R_P^{(k)} \left[\Gamma_f^{(k)} + \left(r^{(k)} C_\rho^{(k)} \right)_f \left\| - U_f^{(k)}, 0 \right\| \right] \tag{145}$$

$$A_P^{P'} = \sum_{NB} A_F^{P'} + \sum_k R_P^{(k)} \left(\frac{r_P^{(k)} K_P^{(k)} \Omega_P}{\delta t} + \sum_{nb} \left(r^{(k)} C_\rho^{(k)} \right)_f U_f^{(k)} \right) \tag{146}$$

$$B_P^{P'} = - \sum_k R_P^{(k)} \left\{ \frac{\left(r_P^{(k)} \rho_P^{(k)} - r_P^{(k)old} \rho_P^{(k)old} \right)}{\delta t} \Omega_P + \sum_{nb} r_f^k \rho_f^{(k)} U_f^{(k)} \right\} - RESG_P \tag{147}$$

Following the calculation of the pressure correction field, $\mathbf{u}_P^{(k)'}, \rho_P^{(k)'}, \text{and } r_P^{(k)'}$ are obtained using the following equations

$$\mathbf{u}_P^{(k)'} = -r^{(k)} \mathbf{D}_P^{(k)} \nabla_P (P') \qquad \rho^{(k)'} = C_\rho^{(k)} P'$$
$$\therefore \; r_P^{(k)'} = -R_P^{(k)} \left(\frac{r_P^{(k)} \Omega_P}{\delta t} \rho_P^{(k)'} + \Delta_P \left[\left(r^{(k)} \rho^{(k)} \mathbf{u}^{(k)'} \right) . \mathbf{S} + r^{(k)} U^{(k)} \rho^{(k)'} \right] \right) \tag{148}$$

Improvement #6 A Newly Suggested GCBAC Family

The pressure correction equation was derived in the previous section by neglecting the $H_P \left[r^{(k)'} \right]$ term. Following the SIMPLEC methodology, a better approximation could be achieved by adding and subtracting $H_P [1] r_P^{(k)'}$ from the left-hand side of equation (98), which results in neglecting a smaller term $\left(H_P \left[r^{(k)'} - r_P^{(k)'} \right] \right)$. With this approximation, Eq. (98) becomes:

$$r_P^{(k)'} = -\widetilde{R}_P^{(k)} \left(\begin{array}{l} \dfrac{r_P^{(k)*} \Omega_P}{\delta t} \rho_P^{(k)'} + \Delta_P \left[\begin{array}{l} r^{(k)*} \rho^{(k)\circ} \left(\mathbf{HP}[\mathbf{u}^{(k)'}] - r^{(k)*} \mathbf{D}^{(k)} \nabla P' - r^{(k)'} \mathbf{D}^{(k)} \nabla P' \right) . \mathbf{S} \\ + r^{(k)*} U^{(k)*} \rho^{(k)'} \end{array} \right] \\ + \dfrac{\left(r_P^{(k)*} \rho_P^{(k)\circ} \right) - \left(r_P^{(k)} \rho_P^{(k)} \right)^{Old}}{\delta t} \Omega_P + \Delta_P \left[\left(r^{(k)*} \rho^{(k)\circ} U^{(k)*} \right) \right] + \dot{M}_P^{(k)} r_P^{(k)*} \Omega_P \end{array} \right) \tag{149}$$

Where

$$\tilde{R}_P^{(k)} = \frac{R_P^{(k)}}{\left(1 - H_P[1]\right)} \tag{150}$$

The pressure correction equation is obtained by substituting Eq. (149) into the geometric conservation equation. The expanded form of the resulting pressure correction equation is easily obtained from Eqs. (144) and (145) by simply substituting $\tilde{R}_P^{(k)}$ for $R_P^{(k)}$. Furthermore, depending on the approximation made to the $\mathbf{HP}\left[\mathbf{u}^{(k)'}\right]$ term, a new family of GCBA, similar to the one detailed above, can be obtained. Since this family is obtained by using ideas similar to the ones employed in SIMPLEC, the letter C is appended to its acronym and is denoted by the GCBAC family.

Comparing the GCBA and MCBA Formulations

Scaling GCBA to Single-Fluid Flow Simulations

Since the MCBA are derived through direct extension of the single fluid algorithms, they scale down automatically to handle single-fluid flow simulations. On the other hand, because the GCBA algorithms are based on geometric conservation their scaling to single-fluid flow simulations is not obvious. Such a property is useful in the sense that coding for single and multi-fluid models would follow the same structure. To show how multi-fluid GCBA algorithms scale down to single-fluid flow simulations, attention is directed towards Eq. (99). For the case of one fluid flow $r_P^{(k)}$ =1=Cte, thus $r_P^{(k)'}$ =0, removing $r_P^{(k)'}$ from that equation and setting $r_P^{(k)*}$ to 1 yields:

$$0 = -R_P^{(k)}\left(\begin{aligned}&\frac{\Omega_P}{\delta t}\rho_P^{(k)'} + \Delta_P\left[\rho^{(k)\circ}\left(\mathbf{HP}[\mathbf{u}^{(k)'}] - r^{(k)*}\mathbf{D}^{(k)}\nabla P' - r^{(k)'}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S} + U^{(k)*}\rho^{(k)'}\right]\\&+\frac{\left(\rho_P^{(k)\circ}\right) - \left(\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P + \Delta_P\left[\left(\rho^{(k)\circ}U^{(k)*}\right)\right] - \dot{M}_P^{(k)}\Omega_P\end{aligned}\right) \tag{151}$$

Removing $R_P^{(k)}$ and rearranging, the pressure correction equation transforms to

$$\begin{aligned}&\frac{\Omega_P}{\delta t}\rho_P^{(k)'} + \Delta_P\left[\rho^{(k)\circ}\left(\mathbf{HP}[\mathbf{u}^{(k)'}] - r^{(k)*}\mathbf{D}^{(k)}\nabla P' - r^{(k)'}\mathbf{D}^{(k)}\nabla P'\right).\mathbf{S} + U^{(k)*}\rho^{(k)'}\right]\\&\qquad = -\frac{\left(\rho_P^{(k)\circ}\right) - \left(\rho_P^{(k)}\right)^{Old}}{\delta t}\Omega_P - \Delta_P\left[\left(\rho^{(k)\circ}U^{(k)*}\right)\right] + \dot{M}_P^{(k)}\Omega_P\end{aligned} \tag{152}$$

The expansion of the above equation is straightforward and leads to the pressure-correction equation of a single-fluid flow.

The Relation Between the GCBA and MCBA

While the derivations of the GCBA and MCBA are based on different paradigms, it is shown in this section that the GCBA formulation leads to a weighted pressure correction equation that has close similarity with the MCBA formulation to which improvement #2 has been applied.

The respective GCBA and MCBA (with improvement #2) pressure correction equations, as derived earlier, are respectively given by:

$$\sum_k \left\{ R_P^{(k)} \left(\frac{r_P^{(k)} C_\rho^{(k)} \Omega_P}{\delta t} P'_P + \Delta_P \left[r^{(k)} U^{(k)} C_\rho^{(k)} P' \right] - \Delta_P \left[r^{(k)} \rho^{(k)} \left(r^{(k)} \mathbf{D}^{(k)} \nabla (P') \right) . \mathbf{S} \right] \right) \right\} = \\ - \sum_{k=1}^{nphase} \left\{ R_P^{(k)} \left(\frac{\left(r_P^{(k)} \rho_P^{(k)} \right) - \left(r_P^{(k)} \rho_P^{(k)} \right)^{Old}}{\delta t} \Omega_P + \Delta_P \left[\left(r^{(k)} \rho^{(k)} U^{(k)} \right) \right] \right) \right\} - RESG_P \tag{153}$$

$$\sum_k \left\{ \frac{\Omega}{\delta t \underline{\rho}^{(k)}} r_P^{(k)o} C_\rho^{(k)} P'_P + \Delta_P \left[\frac{r^{(k)o} C_\rho^{(k)} U^{(k)} P'}{\underline{\rho}^{(k)}} \right] - \Delta_P \left[r^{(k)^o} \frac{\rho^{(k)}}{\underline{\rho}^{(k)}} \left(r^{(k)^o} \mathbf{D}^{(k)} \nabla P' \right) . \mathbf{S} \right] \right\} \\ = -\sum_k \left\{ \frac{r_P^{(k)o} \left(\rho_P^{(k)} / \underline{\rho}^{(k)} \right) - \left[r_P^{(k)} \left(\rho_P^{(k)} / \underline{\rho}^{(k)} \right) \right]^{Old}}{\delta t} \Omega + \Delta_P \left[r^{(k)o} \frac{\rho^{(k)}}{\underline{\rho}^{(k)}} U^{(k)} \right] \right\} \tag{154}$$

Upon comparing the two equations it is clear that the $R_P^{(k)}$ term plays the role of the reference density, i.e. a weighing factor for the mass conservation equation of the respective phase. As such, the GCBA pressure correction equation is very similar to a weighted MCBA pressure correction equation. The weighting procedure (normalization) is done automatically based on the local strength of the inflow to the control volume (since $R_P^{(k)} = 1/A_P^{(k)}$ of the volume fraction equation) thus, as $r_P^{(1)} >> r_P^{(2)}$ one gets $R_P^{(1)} << R_P^{(2)}$. This treatment yields a more robust behavior since large fluid density differences will not mean that conservation for the lighter fluid is lost due to numerical errors.

The above equations also differ slightly in the source term, where an additional entry ($RESG_P$) is included in equation (143) to account for residuals of the geometric conservation equation. Hence, the MCBA family can be viewed as a subset of the GCBA family, and could be recovered by setting the volume fraction corrections to zero ($r_P^{(k)'} = 0$). As such, codes based on the GCBA can easily cater for the MCBA and vice versa. The main advantage of the GCBA over the MCBA is in its attempt to correct both the velocity and volume fraction fields.

Closing Remarks

The segregated class of single-fluid flow algorithms was extended to predict multi-fluid flow at all speeds. The formulation was done using a unified, compact, and easy to understand notation. Depending on the constraint equation used to derive the pressure correction equation, the extended algorithms were shown to fall under two categories that were denoted by the Mass Conservation Based Algorithms (MCBA) and the Geometric Conservation Based Algorithms (GCBA). The differences and similarities between the two categories were explained. In addition, several techniques developed to promote and accelerate the convergence of these algorithms were also discussed.

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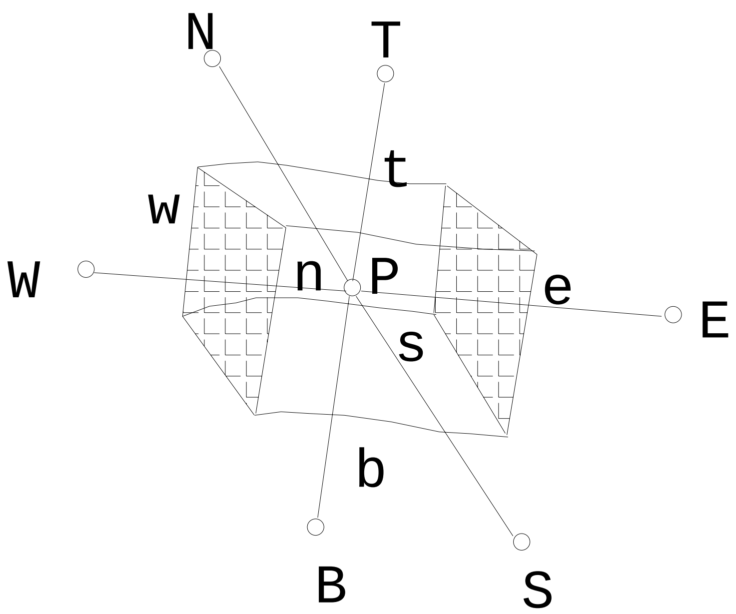

Fig. 1 Control volume.

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