Numerical Simulation of Two-Phase Flows using a Pressure-based Solver

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   - Application to test cases with experimental data

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Introduction

Motivation

- Industrial need for calculation of thermohydraulic components in nuclear reactors by sophisticated models such as the bi-fluid 6-equation model.

Context of numerical simulation

- Density-based solvers: upwind scheme for all the waves (material and pressure) (e.g. OVAP, component code) on unstructured grids with colocated variables, accurate but present inconsistency problems at low Mach number.

- Pressure-based solvers: on structured grids with staggered variables (e.g. CATHARE, system code), perform well at low Mach number, but not extended over unstructured grids.

1: A structured grid with staggered variables.
Bi-fluid 6-equation model

Mass, momentum and energy equations \((k = v, l)\):

\[
\frac{\partial}{\partial t}(\alpha_k \rho_k) + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) = \Gamma_k, \tag{1}
\]

\[
\alpha_k \rho_k \frac{\partial}{\partial t} \mathbf{u}_k + \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k \otimes \mathbf{u}_k) - \mathbf{u}_k \nabla \cdot (\alpha_k \rho_k \mathbf{u}_k) + \alpha_k \nabla P + (P - P^{int}) \nabla \alpha_k
\]

\[
= \alpha_k \mathbf{g} + \mathbf{M}_{ik} + \Gamma_k \mathbf{u}^i - \Gamma_k \mathbf{u}_k, \tag{2}
\]

\[
\frac{\partial}{\partial t}(\alpha_k \rho_k h_k) + \nabla \cdot (\alpha_k \rho_k e_k \mathbf{u}_k) = \alpha_k \frac{\partial}{\partial t} P - P \nabla \cdot (\alpha_k \mathbf{u}_k) + Q_{ik} + \Gamma_k h_{ik}. \tag{3}
\]

- Interfacial terms: \(\Gamma_k, Q_{ik}, \mathbf{M}_{ik}, h_{ik}, \mathbf{u}^i\).
- Basic model \((P^{int} = P)\) is not hyperbolic.
- Intermediary model\(^1\) for the interfacial pressure default:

\[
P - P^{int} = \delta \frac{\alpha_v \alpha_l \rho_v \rho_l}{\alpha_v \rho_l + \alpha_l \rho_v} |\mathbf{u}_v - \mathbf{u}_l|^2 + \frac{1}{c_v^2} \left(\rho_v - \delta \frac{\alpha_v \alpha_l \rho_v \rho_l}{\alpha_v \rho_l + \alpha_l \rho_v}\right) |\mathbf{u}_v - \mathbf{u}_l|^4.
\]

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Semi-implicit method\(^2\)

\[ f = c_0 \cap c_1 \]

---

The discretized momentum equation for phase $k$:

\[
\begin{aligned}
\frac{(\alpha_k \rho_k)}{c_0} \left( \frac{u_k}{c_0} \right)_{n+1}^{n+1} - (u_k)_{c_0}^n \right) \Delta t &+ \frac{1}{V_{c_0}} \sum_f (\frac{\alpha_k \rho_k u_k}{c_0})_f^n (\Phi_k)_f^n - (\frac{u_k}{c_0})_{c_0}^n \sum_f (\alpha_k \rho_k)_f^n (\Phi_k)_f^n \\
= (\alpha_k \rho_k)_{c_0}^n g - (u_k \Gamma_k)_{c_0}^n + (\Gamma_k u_i)_{c_0}^n - (\alpha_k)_{c_0}^n \nabla P_{c_0}^{n+1} + (M_{ik})_{c_0}^{n+1}.
\end{aligned}
\] (4)

The discretized mass and energy equations for phase $k$ (we adopt the notation $\Delta (\cdot) = (\cdot)^{n+1} - (\cdot)^n$):

\[
\begin{aligned}
\frac{(\Delta \alpha_k \rho_k)}{c_0} \Delta t &+ \frac{\sum_f (\alpha_k \rho_k)_f^n (\Phi_k)_f^{n+1}}{V_{c_0}} = (\Gamma_k)_{c_0}^{n+1}, \\
\frac{(\Delta \alpha_k \rho_k h_k)}{c_0} \Delta t &+ \frac{\sum_f (\alpha_k \rho_k e_k)_f^n (\Phi_k)_f^{n+1}}{V_{c_0}} = (\alpha_k)_{c_0}^n \frac{(\Delta P)}{c_0} \Delta t - (P)_{c_0}^n \frac{\sum_f (\alpha_k)_f^n (\Phi_k)_f^{n+1}}{V_{c_0}} \\
&+ (Q_{ik} + \Gamma_k h_{ik})_{c_0}^{n+1}.
\end{aligned}
\] (5)

(6)

\(^2\text{D. R. Liles and Wm. H. Reed. A semi-implicit method for two-phase fluid dynamics. Journal of Computational Physics, 1978.}\)
Semi-implicit method

The discretized momentum equation for phase $k$:

$$
\frac{(\alpha_k \rho_k)^n_{c_0}}{\Delta t} \frac{(u_k)^{n+1}_{c_0} - (u_k)^n_{c_0}}{\Delta t} + \frac{1}{V_{c_0}} \sum_f (\alpha_k \rho_k u_k)_f^n (\Phi_k)_f^n - \frac{(u_k)^n_{c_0}}{V_{c_0}} \sum_f (\alpha_k \rho_k)_f^n (\Phi_k)_f^n \\
= (\alpha_k \rho_k)^n_{c_0} g - (u_k \Gamma_k)^n_{c_0} + (\Gamma_k u^i)^n_{c_0} - (\alpha_k)^n_{c_0} \nabla P_{c_0}^{n+1} + (M_{ik})^{n+1}_{c_0}.
\tag{4}
$$

The discretized mass and energy equations for phase $k$ (we adopt the notation $\Delta(\cdot) = (\cdot)^{n+1} - (\cdot)^n$):

$$
\frac{(\Delta \alpha_k \rho_k)_{c_0}}{\Delta t} + \frac{\sum_f (\alpha_k \rho_k)_f^n (\Phi_k)_f^{n+1}}{V_{c_0}} = (\Gamma_k)^{n+1}_{c_0},
\tag{5}
$$

$$
\frac{(\Delta \alpha_k \rho_k h_k)_{c_0}}{\Delta t} + \frac{\sum_f (\alpha_k \rho_k e_k)_f^n (\Phi_k)_f^{n+1}}{V_{c_0}} = (\alpha_k)^n_{c_0} \frac{(\Delta P)_{c_0}}{\Delta t} - (P)^n_{c_0} \frac{\sum_f (\alpha_k)_f^n (\Phi_k)_f^{n+1}}{V_{c_0}} \\
+ (Q_{ik} + \Gamma_k h)_{c_0}^{n+1}.
\tag{6}
$$

---

The discretized momentum equation for phase $k$:

\[
\begin{align*}
\frac{(\alpha_k \rho_k)^n}{c_0} & \frac{(u_k)^{n+1} - (u_k)^n}{\Delta t} + \frac{1}{V_{c_0}} \sum_f (\alpha_k \rho_k u_k)^n (\Phi_k)^n_f - \frac{(u_k)^n}{c_0 V_{c_0}} \sum_f (\alpha_k \rho_k)^n (\Phi_k)^n_f \\
&= (\alpha_k \rho_k)^n_{c_0} g - (u_k \Gamma_k)^n_{c_0} + (\Gamma_k u^i)^n_{c_0} - (\alpha_k)^n_{c_0} \nabla P_{c_0}^{n+1} + (M_{ik})_{c_0}^{n+1}.
\end{align*}
\] (4)

The discretized mass and energy equations for phase $k$ (we adopt the notation $\Delta(\cdot) = (\cdot)^{n+1} - (\cdot)^n$):

\[
\begin{align*}
\frac{(\Delta \alpha_k \rho_k)^n}{c_0} + \frac{\sum_f (\alpha_k \rho_k)^n (\Phi_k)^n_f}{V_{c_0}} &= (\Gamma_k)^{n+1}_{c_0}, \\
\frac{(\Delta \alpha_k \rho_k h_k)^n}{c_0} + \frac{\sum_f (\alpha_k \rho_k e_k)^n (\Phi_k)^n_f}{V_{c_0}} &= (\alpha_k)^n_{c_0} \frac{(\Delta P)^n}{c_0} - (P)^n_{c_0} \frac{\sum_f (\alpha_k)^n (\Phi_k)^n_f}{V_{c_0}} \\
&+ (Q_{ik} + \Gamma_k h_{ik})^{n+1}_{c_0}.
\end{align*}
\] (5, 6)

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Volumetric flow:

\[(\Phi_k)^m_f = (u_k)^m_f \cdot S_f, \text{ where } m \in \{n, n+1\}.\]
Semi-implicit method

Phasic velocity at cell center

Linearisation of the implicit term: $M_{ik}^{n+1} = M_{ik}^n + \left( \frac{\partial M_{ik}}{\partial u_k} \right)^n \cdot (u_{k}^{n+1} - u_{k}^n)$. The velocity at cell center in compact form:

$$(u_k)_{c0}^{n+1} = (\gamma_k)_{c0}^n - (\beta_k)_{c0}^n \nabla P_{c0}^{n+1}. \quad (7)$$
Semi-implicit method

Phasic velocity at cell center

Linearisation of the implicit term: $M_{ik}^{n+1} = M_{ik}^n + \left( \frac{\partial M_{ik}}{\partial u_k} \right)^n \cdot (u_{k}^{n+1} - u_{k}^n)$. The velocity at cell center in compact form:

$$(u_k)^{n+1} = (\gamma_k)^n_c - (\beta_k)^n_c \nabla P_{c0}^{n+1}.$$ (7)

Phasic velocity at cell face

Centered scheme: $$(u_k)_f^{n+1} = \frac{1}{2} (u_k)^{n+1}_c + \frac{1}{2} (u_k)^{n+1}_c.$$ 

2: A structured grid with colocated variables (checker-board problem).
Semi-implicit method

**Phasic velocity at cell center**

Linearisation of the implicit term: $M_{ik}^{n+1} = M_{ik}^n + \left( \frac{\partial M_{ik}}{\partial u_k} \right)_n \cdot (u_k^{n+1} - u_k^n)$. The velocity at cell center in compact form:

$$
(u_k)^{n+1}_{c0} = (\gamma_k)^n_{c0} - (\beta_k)^n_{c0} \nabla P^{n+1}_{c0}.
$$

(7)

**Phasic velocity at cell face**

Rhie and Chow’s interpolation to calculate the velocity at cell face

- Adding a dissipation term

$$
(u_k)^{n+1}_f = \frac{1}{2} (u_k)^{n+1}_{c0} + \frac{1}{2} (u_k)^{n+1}_{c1} - (\beta_k)^n_f \frac{P_{c1}^{n+1} - P_{c0}^{n+1}}{|\text{dr}_{01}|} n_f + \frac{1}{2} (\beta_k)^n_{c0} \nabla P^{n+1}_{c0} + \frac{1}{2} (\beta_k)^n_{c1} \nabla P^{n+1}_{c1}.
$$

(8)

- Analogy to the calculation of the velocity at cell center

$$
(u_k)^{n+1}_f = (\gamma_k)^n_f - (\beta_k)^n_f \nabla P^{n+1}_f = \frac{1}{2} \left[ (\gamma_k)^n_{c0} + (\gamma_k)^n_{c1} \right] - (\beta_k)^n_f \frac{P_{c1}^{n+1} - P_{c0}^{n+1}}{|\text{dr}_{01}|} n_f.
$$

(9)

These two formulations (8) and (9) are equivalent considering the formula (7).

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Semi-implicit method (discretization of the scalar equations)

The discretized mass and energy equations for phase $k$ ($\Delta(\cdot) = (\cdot)^{n+1} - (\cdot)^n$):

$$
\frac{(\Delta \alpha_k \rho_k)_{c0}}{\Delta t} + \frac{\sum_f (\alpha_k \rho_k)^n_f (\Phi_k)_f^{n+1}}{V_{c0}} = (\Gamma_k)_{c0}^{n+1}, \tag{10}
$$

$$
\frac{(\Delta \alpha_k \rho_k h_k)_{c0}}{\Delta t} + \frac{\sum_f (\alpha_k \rho_k e_k)^n_f (\Phi_k)_f^{n+1}}{V_{c0}} = (\alpha_k)_{c0}^n \frac{(\Delta P)_{c0}}{\Delta t} - (P)_{c0}^n \frac{\sum_f (\alpha_k)^n_f (\Phi_k)_f^{n+1}}{V_{c0}} + (Q_{ik} + \Gamma_k h_{ik})_{c0}^{n+1}. \tag{11}
$$

Linearisations:

- Product terms: $\Delta(\alpha_k \rho_k) = (\rho_k)^n_{c0} (\Delta \alpha_k)_{c0} + (\alpha_k)^n_{c0} (\Delta \rho_k)$,
  $\Delta(\alpha_k \rho_k h_k) = (\rho_k)^n_{c0} (h_k)^n_{c0} (\Delta \alpha_k)_{c0} + (\alpha_k)^n_{c0} (\rho_k)^n_{c0} (\Delta h_k)_{c0} + (\alpha_k)^n_{c0} (h_k)^n (\Delta \rho_k)_{c0}$

- Density: $\Delta \rho_k = \left( \frac{\partial \rho_k}{\partial P} \right)^n \Delta P + \left( \frac{\partial \rho_k}{\partial h_k} \right)^n \Delta h_k$.

- Source terms: $(q_k)^{n+1} - (q_k)^n = \left( \frac{\partial q_k}{\partial P} \right)^n \Delta P + \left( \frac{\partial q_k}{\partial h_v} \right)^n \Delta h_v + \left( \frac{\partial q_k}{\partial h_l} \right)^n \Delta h_l$, where $q_k \in \{\Gamma_k, Q_{ik} + \Gamma_k h_{ik}\}$. 
Discretization of the scalar equations

The discretized scalar equations in matrix form:

$$\mathcal{A}_c x_c = (s)_{c0}^n - \sum_f (g)_{f}^n (\Phi_v)_{f}^{n+1} - \sum_f (l)_{f}^n (\Phi_I)_{f}^{n+1},$$  \hspace{1cm} (12)

where $x$ is the vector of unknowns, $x = (\Delta h_v, \Delta h_I, \Delta \alpha_v, \Delta P)^T$. By inverting the system of scalar equations we obtain

$$x = A^{-1}(s)_{c0}^n - A^{-1} \sum_f (g)_{f}^n (\Phi_v)_{f}^{n+1} - A^{-1} \sum_f (l)_{f}^n (\Phi_I)_{f}^{n+1}.$$  \hspace{1cm} (13)
Discretization of the scalar equations

The discretized scalar equations in matrix form:

$$\mathcal{A}_{c_0} \mathbf{x}_{c_0} = (s)_{c_0}^n - \sum_f (g)_f^n (\Phi_v)_f^{n+1} - \sum_f (l)_f^n (\Phi_l)_f^{n+1},$$  \hspace{1cm} (12)

where $\mathbf{x}$ is the vector of unknowns, $\mathbf{x} = (\Delta h_v, \Delta h_l, \Delta \alpha_v, \Delta P)^T$. By inverting the system of scalar equations we obtain

$$\mathbf{x} = \mathcal{A}^{-1} (s)_{c_0}^n - \mathcal{A}^{-1} \sum_f (g)_f^n (\Phi_v)_f^{n+1} - \mathcal{A}^{-1} \sum_f (l)_f^n (\Phi_l)_f^{n+1}. $$ \hspace{1cm} (13)

A relation between $P_{c_0}^{n+1}$ and $(\Phi_k)_f^{n+1}$ resulting from the fourth equation of the preceding system:

$$P_{c_0}^{n+1} = P_{c_0}^n + \mathbf{A}_4 \cdot \left[ (s)_{c_0}^n - \sum_f (g)_f^n (\Phi_v)_f^{n+1} - \sum_f (l)_f^n (\Phi_l)_f^{n+1} \right], $$ \hspace{1cm} (14)

where $\mathbf{A}_4$ is the fourth row of the matrix $\mathcal{A}^{-1}$. 

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Discretization of the scalar equations

The discretized scalar equations in matrix form:

\[ \mathcal{A}_c \mathbf{x}_c = (s)^n_{c0} - \sum_f (g)^n_f (\Phi_v)^{n+1}_f - \sum_f (l)^n_f (\Phi_l)^{n+1}_f, \quad (12) \]

where \( \mathbf{x} \) is the vector of unknowns, \( \mathbf{x} = (\Delta h_v, \Delta h_l, \Delta \alpha_v, \Delta P)^T \). By inverting the system of scalar equations we obtain

\[ \mathbf{x} = \mathcal{A}^{-1}(s)^n_{c0} - \mathcal{A}^{-1} \sum_f (g)^n_f (\Phi_v)^{n+1}_f - \mathcal{A}^{-1} \sum_f (l)^n_f (\Phi_l)^{n+1}_f. \quad (13) \]

- A relation between \( P^{n+1}_{c0} \) and \( (\Phi_k)^{n+1}_f \) resulting from the fourth equation of the preceding system:

\[ P^{n+1}_{c0} = P^n_{c0} + A_4 \cdot \left[ (s)^n_{c0} - \sum_f (g)^n_f (\Phi_v)^{n+1}_f - \sum_f (l)^n_f (\Phi_l)^{n+1}_f \right], \quad (14) \]

where \( A_4 \) is the fourth row of the matrix \( \mathcal{A}^{-1} \).

- Another relation between the volumetric flow and the pressure resulting from the discretization of the momentum equation:

\[ (\Phi_k)^{n+1}_f = (u_k)^{n+1}_f \cdot \mathbf{S}_f = \frac{1}{2} \left[ (\gamma_k)^n_{c0} + (\gamma_k)^n_{c1} \right] \cdot \mathbf{S}_f - (\beta_k)^n_f \frac{P^n_{c1} - P^n_{c0}}{\left| \mathbf{d}r_{01} \right|} |\mathbf{S}_f|. \quad (15) \]
The combination of the equations (14) and (15) leads to an equation in which the pressure at time \(n+1\) is the only unknown:

\[
\left(1 + A_4 \cdot \sum_f C_f\right) P_{c0}^{n+1} - A_4 \cdot \sum_f C_f P_{c1}^{n+1} = P_c^n + A_4 \cdot \left\{ (s)_{c0}^n - \frac{1}{2} \sum_f (g)_{f}^n \left[(\gamma_v)_{c0}^n + (\gamma_v)_{c1}^n\right] \cdot S_f - \frac{1}{2} \sum_f (l)_{f}^n \left[(\gamma_l)_{c0}^n + (\gamma_l)_{c1}^n\right] \cdot S_f \right\},
\]

(16)

where \(C_f = \frac{|S_f|}{|dr_{01}|} \left[ (g)_{f}^n (\beta_v)_f^n + (l)_{f}^n (\beta_l)_f^n \right] > 0.\)
Why the semi-implicit method is not conservative (e.g. Euler’s equations)

- Use of non-conservative variables the velocity and enthalpy in the discretization of momentum and energy equations respectively.
- Linearization of the density using equations of state.

Semi-implicit method for Euler equations

\[
\frac{(\Delta \rho)_{c_0}}{\Delta t} + \sum_f (\rho)^n_f (\Phi)^{n+1}_f = 0, \tag{17}
\]

\[
\rho^n_{c_0} \frac{u^{n+1}_{c_0} - u^n_{c_0}}{\Delta t} = \frac{u^n_{c_0}}{V_{c_0}} \sum_f (\rho)^n_f (\Phi)^n_f - \frac{1}{V_{c_0}} \sum_f (\rho u)^n_f (\Phi)^n_f - \nabla P^{n+1}_{c_0} + \rho^n_{c_0} g, \tag{18}
\]

\[
\frac{\rho^n_{c_0} (\Delta h)_{c_0} + h^n_{c_0} (\Delta \rho)_{c_0}}{\Delta t} + \sum_f (\rho e)^n_f (\Phi)^{n+1}_f = \frac{(\Delta P)_{c_0}}{\Delta t} - \frac{P^n_{c_0}}{V_{c_0}} \sum_f (\Phi)^{n+1}_f, \tag{19}
\]

where

\[
\Delta \rho = \left( \frac{\partial \rho}{\partial P} \right)^n \Delta P + \left( \frac{\partial \rho}{\partial h} \right)^n \Delta h. \tag{20}
\]
Conservative semi-implicit method

\[
\frac{(\alpha_k \rho_k)^{n+1}_c - (\alpha_k \rho_k)^n_c}{\Delta t} + \left( \sum_f \frac{\alpha_k \rho_k u_k^n_f (\Phi_k)^{n+1}_f}{V_{c_0}} \right) \frac{1}{V_{c_0}} = 0,
\]

\[
\text{where } P_f^* \text{ and } (\alpha_k)^*_c \text{ are obtained by the non-conservative semi-implicit method.}
\]

Advantages of a conservative method

- Exact shock capture in single-phase flows.
- Exact conservation of mass, momentum and total energy of the mixture in two-phase flows.
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Sod’s shock tube

- Riemann problem (ideal gas for the fluid).
- Exact shock capture by the conservative semi-implicit method.

2: Density comparison at $t = 0.2s$.

3: Velocity comparison at $t = 0.2s$. 
Ransom’s faucet

- Capture of a void fraction front.
- Convergence study with an interfacial pressure default model.

4 : Ransom’s water faucet at $t = 0$, $0 < t < t_{\text{converge}}$ and $t = t_{\text{converge}}$ (the time to reach the steady state).

5 : Ransom’s faucet : void fraction at $t = 0.6s$. 
Sedimentation

- Phase separation by gravity.
- Cover the full range of void fraction from 0 to 1.

6: Illustration of the sedimentation test case.

7: Sedimentation: void fraction profile at different time instants.
Tee junction

- Dynamic separation of gas and liquid due to geometry.
- Unstructured 2D grid.

8: Geometry of Tee junction test case, dimension in [m].

Water hammer

- Propagation of a pressure wave in a pipe.
- Simulation of the water hammer phenomenon for the safety study of an industrial installation.
- Validation by experimental data.

10: Illustration of the water hammer problem.

11: Single-phase water hammer: pressure at the valve as a function of time.

Notation: $c$ is the sound speed, $L$ is the length of the pipe.
Water hammer

(a) Pressure at the valve $P(t)$.

(b) Void fraction at the valve $\alpha_v(t)$.

12 : Two-phase water hammer.
Rapid depressurization

- Study of the accidental scenario of a pipe breach in the primary circuit of a nuclear reactor.
- Comparison with experimental data and numerical results of a density-based solver (VFFC\textsuperscript{4}).

13 : Geometry of the rapid depressurization test case, all dimensions in [mm].

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General conclusions:

- Development of a pressure solver on non-structured grids with colocated variables for the bi-fluid six-equation model.
- Development of a conservative semi-implicit method.
- A battery of test cases to validate the numerical methods and to evaluate their behavior at different physical configurations.

Perspectives:

- Development of a 2nd order discretization in time and in space.
- Inclusion of more realistic interfacial terms and consideration of other physical phenomena (e.g. diffusion, turbulent effects) to have a code for industrial use.
- Improvement of code performance.
- ...