Derivation of two-phase volume averaged conservation equations for volume-of-fluid interface tracking

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Problem and motivation

- **Volume-of-fluid (VOF) computations in literature:**
  finite difference discretization of *local* equations

$$\boxed{\frac{\partial f}{\partial t} + \nabla \cdot f\,\mathbf{v} = 0} \quad (0 \le f \le 1),\ \rho_m = f\rho_1 + (1-f)\rho_2,\ \mu_m = f\mu_1 + (1-f)\mu_2$$

$$\boxed{\frac{\partial \rho_m \mathbf{v}}{\partial t} + \nabla \cdot \rho_m \mathbf{v}\mathbf{v} = -\nabla p + \nabla \cdot \mu_m\left(\nabla \mathbf{v} + \nabla \mathbf{v}^{\mathsf{T}}\right) + \rho_m \mathbf{g} + \sigma\kappa\mathbf{n}\delta_S} \quad \boxed{\nabla \cdot \mathbf{v} = 0}$$

- **Obvious inconsistency:**
  some quantities are averaged f, ρ_m, μ_m
  and some are not $\mathbf{v}, p$

(Problem and motivation)

- Both phases are assumed to move with same velocity, namely the center-of-mass velocity
  $\Rightarrow$ comput. grid must resolve boundary layer at interface
- Which are the additional terms if the boundary layer is <u>not</u> fully resolved, i.e. the phase velocities differ?
- **Goal:** Derive <u>consistent</u> volume-averaged equations for volume-of-fluid computations (VA-VOF eqs. for phases of constant density)

Procedure to derive VA-VOF equations

1. local mass & momentum cons.-eqs. for phase $k=1,2$ valid in $\Omega_k(t)$
2. multiply eqs. by respective phase indicator function $X_k(\mathbf{x},t)$
3. apply to each term VA operator $\overline{\psi_k}^k \equiv \frac{1}{V_k}\int_V \psi_k(\mathbf{x}+\boldsymbol{\eta},t) X_k(\mathbf{x}+\boldsymbol{\eta},t)\, d\mathbf{x}$
4. apply Gauss & Leibnitz rules to obtain eqs. of <u>two-fluid model</u>:

$$\frac{\partial \alpha_k \rho_k}{\partial t} + \nabla \cdot \alpha_k \rho_k \overline{\mathbf{v_k}}^k = 0 \qquad k = 1,2$$

$$\frac{\partial \alpha_k \rho_k \overline{\mathbf{v_k}}^k}{\partial t} + \nabla \cdot \alpha_k \rho_k \left(\overline{\mathbf{v_k}}^k \overline{\mathbf{v_k}}^k + \overline{\mathbf{v}'_\mathbf{k} \mathbf{v}'_\mathbf{k}}^k \right) = -\nabla \alpha_k \overline{p_k}^k + \alpha_k \rho_k \mathbf{g} + \nabla \cdot \alpha_k \overline{\boldsymbol{\tau}_\mathbf{k}}^k + \mathbf{M_k}$$

(Procedure to derive VA-VOF equations)

5. for simplied representation of VA-VOF eqs. we introduce

- liquid volumetric fraction $f \equiv \alpha_1$

- mixture density $\rho_m \equiv \sum_{k=1}^{2} \alpha_k \rho_k = f\rho_1 + (1-f)\rho_2$

- center-of-mass velocity $\mathbf{v_m} \equiv \frac{1}{\rho_m} \sum_{k=1}^{2} \alpha_k \rho_k \overline{\mathbf{v_k}}^k = \frac{f\rho_1 \overline{\mathbf{v}_1}^1 + (1-f)\rho_2 \overline{\mathbf{v}_2}^2}{\rho_m}$

- relative velocity $\mathbf{v_r} = \mathbf{v_{21}} \equiv \overline{\mathbf{v_2}}^2 - \overline{\mathbf{v_1}}^1$

$$\Rightarrow \quad \overline{\mathbf{v_1}}^1 = \mathbf{v_m} - \frac{\alpha_2 \rho_2}{\rho_m} \mathbf{v_r}, \quad \overline{\mathbf{v_2}}^2 = \mathbf{v_m} + \frac{\alpha_1 \rho_1}{\rho_m} \mathbf{v_r}$$

VA-VOF mass conservation equations

- two-fluid model mass conservation equations for $k=1,2$:

$$\frac{\partial f \rho_1}{\partial t} + \nabla \cdot f \rho_1 \mathbf{v_m} = \nabla \cdot f(1-f)\frac{\rho_1 \rho_2}{\rho_m}\mathbf{v_r} \qquad (1)$$

$$\frac{\partial (1-f)\rho_2}{\partial t} + \nabla \cdot (1-f)\rho_2 \mathbf{v_m} = -\nabla \cdot f(1-f)\frac{\rho_1 \rho_2}{\rho_m}\mathbf{v_r} \qquad (2)$$

- rearrange to yield:

$$\boxed{\begin{aligned} &\frac{\partial f}{\partial t} + \nabla \cdot f \mathbf{v_m} = \nabla \cdot f(1-f)\frac{\rho_2}{\rho_m}\mathbf{v_r} \\ &\nabla \cdot \mathbf{v_m} = -\nabla \cdot f(1-f)\frac{\rho_1 - \rho_2}{\rho_m}\mathbf{v_r} \end{aligned}} \qquad \begin{aligned} &(1)/\rho_1 \\ &(1)/\rho_1 + (2)/\rho_2 \end{aligned}$$

VA single-field momentum equation

- sum of the momentum equations of the two-fluid model for phase 1 and 2 within averaging volume V

$$\frac{\partial}{\partial t}\sum_{k=1}^{2}\alpha_k\rho_k\overline{\mathbf{v_k}}^k+\nabla\cdot\sum_{k=1}^{2}\alpha_k\rho_k\overline{\mathbf{v_k}}^k\,\overline{\mathbf{v_k}}^k=$$

$$-\nabla\sum_{k=1}^{2}\alpha_k\overline{p_k}^k+\sum_{k=1}^{2}\alpha_k\rho_k\mathbf{g}+\nabla\cdot\sum_{k=1}^{2}\alpha_k\left(\overline{\underline{\boldsymbol{\tau}}_\mathbf{k}}^k+\underline{\boldsymbol{\tau}}_\mathbf{sgs}^\mathbf{k}\right)+\mathbf{M_1}+\mathbf{M_2}$$

where $\underline{\boldsymbol{\tau}}_\mathbf{sgs}=-\sum_{k=1}^{2}\alpha_k\rho_k\overline{\mathbf{v}_\mathbf{k}'\mathbf{v}_\mathbf{k}'}^k$

(VA single-field momentum equation)

- sum of momentum transfer terms (jump condition)

$$\mathbf{M_1} + \mathbf{M_2} = \frac{\sigma}{V}\int_{S_i(\mathbf{x},t)} \kappa\,\mathbf{n}\,dS \cong \sigma\,\overline{\kappa}^V\,\overline{\mathbf{n}}^V\,\frac{1}{V}\int_{S_i(\mathbf{x},t)} dS = \sigma\,\overline{\kappa}^V\,\overline{\mathbf{n}}^V a_{int}$$

interfacial area concentration

- sum of convective terms

$$\sum_{k=1}^{2} \alpha_k \rho_k \overline{\mathbf{v_k}}^k\,\overline{\mathbf{v_k}}^k = \rho_m \mathbf{v_m}\mathbf{v_m} + \underline{\mathbf{D}}_{\mathbf{int}},$$

where $\underline{\mathbf{D}}_{\mathbf{int}} \equiv \alpha_1\alpha_2 \frac{\rho_1\rho_2}{\rho_m}\mathbf{v_r}\mathbf{v_r} \quad = \quad$ "momentum drift flux term"

(VA single-field momentum equation)

- sum of diffusive terms

$$\sum_{k=1}^{2} \alpha_k \overline{\underline{\boldsymbol{\tau}}_{\mathbf{k}}}^{k} = \sum_{k=1}^{2} \alpha_k \mu_k \left(\nabla \overline{\mathbf{v}_{\mathbf{k}}}^{k} + (\nabla \overline{\mathbf{v}_{\mathbf{k}}}^{k})^{\mathrm{T}} \right) \equiv \underline{\boldsymbol{\tau}}_{\mathbf{m}} + \underline{\boldsymbol{\tau}}_{\mathbf{int}}$$

$$\text{where} \quad \underline{\boldsymbol{\tau}}_{\mathbf{m}} \equiv \mu_m \left(\nabla \mathbf{v}_{\mathbf{m}} + (\nabla \mathbf{v}_{\mathbf{m}})^{\mathrm{T}} \right), \quad \mu_m \equiv f \mu_1 + (1-f)\mu_2$$

$$\Rightarrow \underline{\boldsymbol{\tau}}_{\mathbf{int}} = \alpha_2 \mu_2 \left(\nabla \frac{\alpha_1 \rho_1}{\rho_m} \mathbf{v}_{\mathbf{r}} + \left(\nabla \frac{\alpha_1 \rho_1}{\rho_m} \mathbf{v}_{\mathbf{r}} \right)^{\mathrm{T}} \right) - \alpha_1 \mu_1 \left(\nabla \frac{\alpha_2 \rho_2}{\rho_m} \mathbf{v}_{\mathbf{r}} + \left(\nabla \frac{\alpha_2 \rho_2}{\rho_m} \mathbf{v}_{\mathbf{r}} \right)^{\mathrm{T}} \right)$$

$$\underline{\boldsymbol{\tau}}_{\mathbf{int}} = \text{"interfacial friction term"}$$

Set of VA-VOF equations

$$\frac{\partial f}{\partial t} + \nabla \cdot f \mathbf{v_m} = \nabla \cdot f(1-f)\frac{\rho_2}{\rho_m}\mathbf{v_r}$$

$$\nabla \cdot \mathbf{v_m} = -\nabla \cdot f(1-f)\frac{\rho_1 - \rho_2}{\rho_m}\mathbf{v_r}$$

$$\frac{\partial \rho_m \mathbf{v_m}}{\partial t} + \nabla \cdot \left(\rho_m \mathbf{v_m}\mathbf{v_m} + \underline{\mathbf{D}}_{\mathbf{int}}\right) = -\nabla \sum_{k=1}^{2} \alpha_k \overline{p_k}^k + \rho_m \mathbf{g} + \sigma \overline{\kappa}^V \overline{\mathbf{n}}^V a_{int}$$

$$+ \nabla \cdot \mu_m \left(\nabla \mathbf{v_m} + (\nabla \mathbf{v_m})^{\mathrm{T}}\right) + \nabla \cdot \left(\underline{\boldsymbol{\tau}}_{\mathbf{int}} + \underline{\boldsymbol{\tau}}_{\mathbf{sgs}}\right)$$

(Set of VA-VOF equations)

limit $V \Rightarrow 0 \;\Rightarrow \mathbf{v_r} = 0$
$\Rightarrow$ local VOF equations

$$\frac{\partial f}{\partial t} + \nabla \cdot f \mathbf{v_m} = \cancel{\nabla \cdot f(1-f)\frac{\rho_2}{\rho_m}\mathbf{v_r}} = 0$$

$$\nabla \cdot \mathbf{v_m} = \cancel{-\nabla \cdot f(1-f)\frac{\rho_1 - \rho_2}{\rho_m}\mathbf{v_r}} = 0$$

$$\frac{\partial \rho_m \mathbf{v_m}}{\partial t} + \nabla \cdot \left(\rho_m \mathbf{v_m} \mathbf{v_m} + \cancel{\underline{\mathbf{D}}_{\mathbf{int}}}\right) = -\nabla \sum_{k=1}^{2} \alpha_k \overline{p_k}^{k} + \rho_m \mathbf{g} + \sigma \overline{\kappa}^V \overline{\mathbf{n}}^V a_{int}$$

$$+ \nabla \cdot \mu_m \left(\nabla \mathbf{v_m} + (\nabla \mathbf{v_m})^{\mathrm{T}}\right) + \nabla \cdot \left(\cancel{\underline{\boldsymbol{\tau}}_{\mathbf{int}}} + \cancel{\underline{\boldsymbol{\tau}}_{\mathbf{sgs}}}\right)$$

Closure of VA-VOF equations

- 3 equations: f-equation = liquid mass conservation eq.
  divergence condition = gas mass conserv. eq.
  mixture momentum equation
- 5 unknows $f\,,\mathbf{v_m}\,,\mathbf{v_r}\,,\overline{p_1}^{1}\,,\overline{p_2}^{2}$

- 1st assumption: both phases share same pressure field
- 2nd closure relation: constitutive equation for $\mathbf{v_r}$
  - trivial closure: “homogenous model” $\mathbf{v_r} = \mathbf{0}$

Relevance of modelling $\mathbf{v_r}$

- estimate for thickness of boundary layer

$$\delta \approx \frac{d_b/2}{\sqrt{\mathrm{Re_b}}}, \quad \text{where} \quad \mathrm{Re_b} = \frac{d_b U_\infty}{\upsilon_l}$$

- resolve boundary layer by 3 mesh cells

$$\Rightarrow \quad \frac{d_b}{\Delta x} = 6\sqrt{\mathrm{Re_b}}$$

$\mathrm{Re_b}$	10	100	1,000
$d_b / \Delta x$	19	60	189

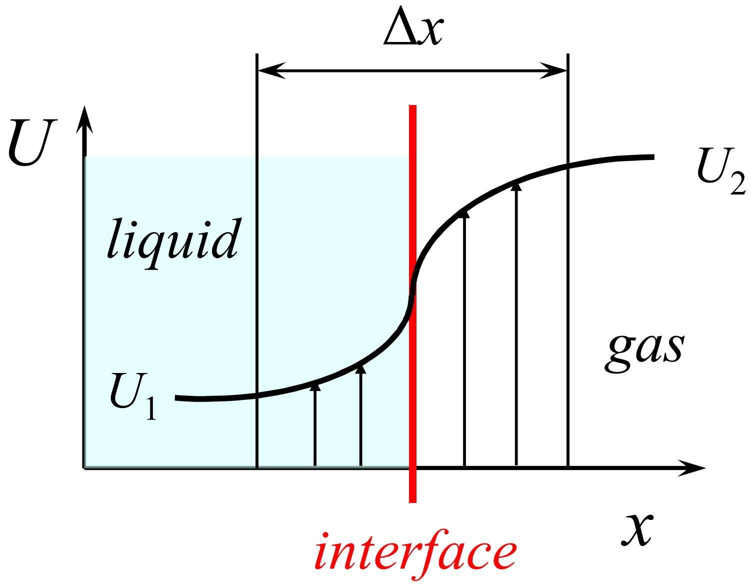
- current 3D VOF computations: $\mathrm{Re_b} \leq O(100)$, $d_b/\Delta x \leq 50$

Order of magnitude estimation

- momentum drift flux term

$$\frac{D_{int}}{\rho_m U_m U_m} = q\left(f, \rho_1, \rho_2, U_1, U_2\right)$$

$$\frac{f}{1-f} = \frac{\rho_1}{\rho_2} \Rightarrow q = q_{max} \cong \frac{1}{2}\frac{U_2 - U_1}{U_1 + U_2}$$



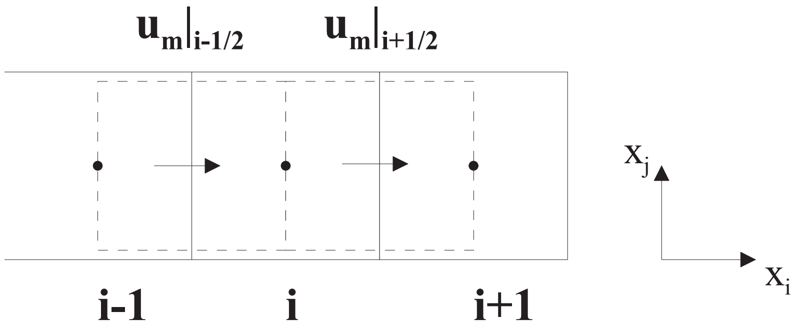
- interfacial friction term

$$\rho_1 = \rho_2, \mu_1 = \mu_2 \Rightarrow \frac{\tau_{int}}{\tau_m} \propto \frac{\left(U_2 - U_1\right)\frac{\partial f}{\partial x}}{\frac{\partial U_m}{\partial x}} \cong \frac{\left(U_2 - U_1\right)\frac{1-0}{\Delta x}}{\frac{U_2 - U_1}{\Delta x}} = 1$$

A first model proposal for $\mathbf{v_r}$

- local algebraic model for $\mathbf{v_r} = (u_r, v_r, w_r)^{\mathrm{T}}$
- for conservative discretization of $\underline{\mathrm{D}}_{\mathrm{int}}$ on staggered grid $\mathbf{v_r}$ must be formulated cell-centered, e.g. $u_{r;i} = u_{2;i} - u_{1;i}$
- 2 equations from definitions:

$$u_{m;i\pm1/2} = \frac{f_{i\pm1/2}\rho_1 u_{1;i\pm1/2} + \left(1 - f_{i\pm1/2}\right)\rho_2 u_{2;i\pm1/2}}{\rho_{m;i\pm1/2}}$$



- 6 unknowns:

$$u_{1;i+1/2},\quad u_{1;i-1/2},\quad u_{1;i},\quad u_{2;i+1/2},\quad u_{2;i-1/2},\quad u_{2;i}$$

(A first model proposal for v_r)

- assumption: $u_{1;i+1/2} = u_{1;i-1/2} = u_{1;i}\ ,\quad u_{2;i+1/2} = u_{2;i-1/2} = u_{2;i}$

  Local **U**niform **R**elative **V**elocity model (LURV)

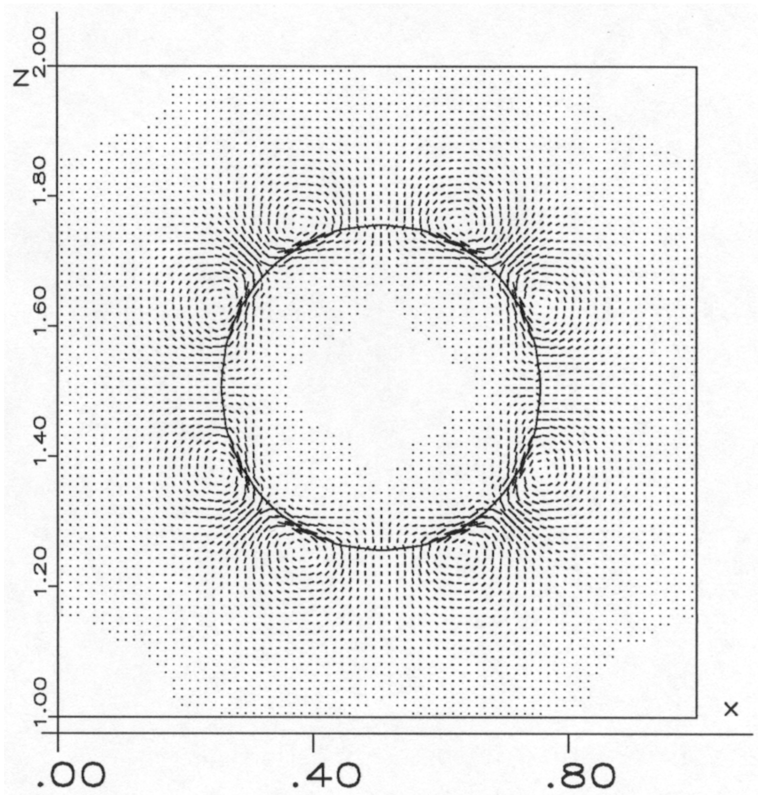
- after some algebraic manipulations we obtain:

$$u_{r;i} = -\left(1 + \frac{\rho_1 - \rho_2}{\rho_2} f_{i-1/2}\right)\left(1 + \frac{\rho_1 - \rho_2}{\rho_2} f_{i+1/2}\right)\frac{\rho_2}{\rho_1}\frac{u_{m;i+1/2} - u_{m;i-1/2}}{f_{i+1/2} - f_{i-1/2}}$$

(valid only for $f_{i+1/2} \neq f_{i-1/2}$)

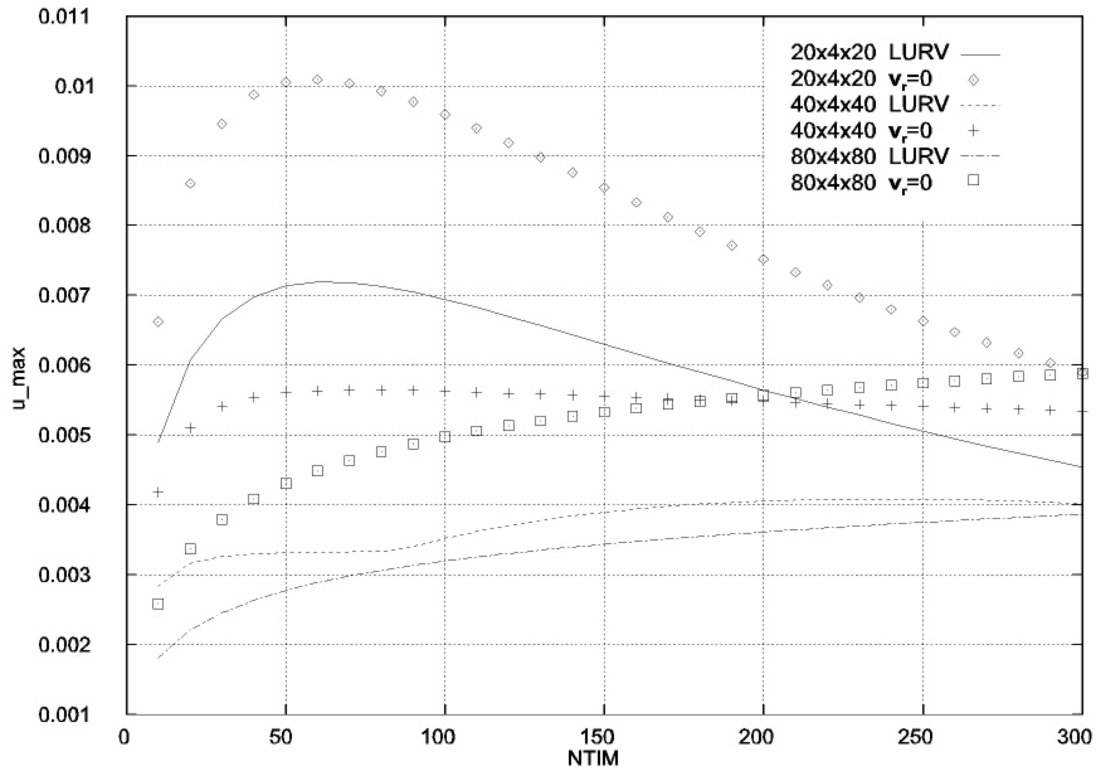
Preliminary results

- LURV model only
  in momentum equation
- “homogeneous model” in
  f-equation and in
  divergence equation
- static 2D interface $\Rightarrow$
  pressure jump correctly computed
  but unphysical “spurious currents”



(Preliminary results)

- amplitude of *unphysical* “spurious currents” may be slightly reduced or slightly increased
  - ⇒ LURV model will be tested for *physical* flow fields



Conclusions and outlook

- Derivation of volume-averaged VOF equations
  - phase velocities may differ from center-of-mass velocity
    $\Rightarrow$ additional terms in interface cells as compared to local VOF eqs.
  - closure assumption for relative phase velocity $\mathbf{v}_\mathbf{r}$ is required
    $\Rightarrow$ suitable models for $\mathbf{v}_\mathbf{r}$ must be developed and tested
  - perspective of "low bubble resolution" VOF simulations for high Re_b
  - VA momentum eq. applies also to level-set and front-tracking method
- Two-phase "large-eddy simulation" with interface tracking
  - SGS model for unresolved velocity fluctuations in single phase cells
  - model for $\mathbf{v}_\mathbf{r}$ to account for unresolved boundary layer