Flux-Based Level Set Method for Two-Phase Flow

Towards pure finite volume discretization of incompressible two-phase flow using a level set formulation

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ABSTRACT. We describe a pure finite volume method for the problem of incompressible two-phase flow using a level set formulation to track the interface between phases. Similar discrete local balance formulations are used for the approximation of the conservation of all related values — the momentum, the mass and the level set function. Moreover, a possible jump of the pressure at the interface is modeled directly within the method. As result we found very good conservation properties of the method and negligible parasite currents in examples considered here. The presented calculations are performed without any artificial post-processing steps often used in the numerical methods for two-phase flows based on the level set formulation.

KEYWORDS: incompressible two-phase flow, level set method, finite volume method

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1. Introduction

Numerical simulation of incompressible two-phase flows is a challenging problem. Even in a simple situation like a gas bubble fully immersed in the secondary fluid, the additional complexities of the two-phase formulation are substantial, regardless of the difficulties solving the single phase Navier-Stokes equations numerically. First, a sharp interface between the fluids with discontinuities of the material parameters occurs. Second, the interface introduces a non-trivial coupling of the separated phases due to phenomena like the surface tension depending on its curvature. Finally, non-
zero fluid velocity on the interface requires dynamic tracking of the phase separation with possible topological changes like splitting of the bubble.

Many authors treat the two-phase model using some kind of level set methods [SUS 94, TOR 00, Van 05, GRO 06, OLS 07, MAR 07]. The most important advantage of the level set formulation is straightforward calculation of geometric properties of the interface. On the other hand, sometimes undesirable properties are reported for the level set methods when applied to problems of two-phase flows. Often a loss of mass conservation is found, i.e., the fact that the volume of a bubble is not conserved during the calculations, and numerical instabilities in the calculations of the curvature are reported. Typically, such problems are solved by using some post-processing steps (e.g., redistancing of the level set function) or by coupling with other methods (e.g., the volume of fluid or particle tracking method); see an overview in [LOS 06].

Our aim is to derive a pure finite volume discretization of incompressible two-phase flows using the level set formulation that requires no (or a minimum) of post-processing steps for stable behavior and good conservation properties. The idea is to apply analogously discretized local balance formulations for the conservation of momentum, mass and level set function.

This paper reports the first successful results towards implementing the pure finite volume method for two-phase flows problem. In section 2 we introduce the mathematical model, in section 3 the finite volume discretization, in section 4 the flux-based level set method. In section 5, we report some numerical experiments.

2. Mathematical model

Briefly, the Navier-Stokes equations for incompressible two-phase flow will be written in the following form:

\[ \rho_i (\partial_t u_i + u_i \cdot \nabla u_i) = \nabla \cdot T_i + g, \quad (t, x) \in [0, T] \times \Omega_i , \]
\[ \nabla \cdot u_i = 0, \quad (t, x) \in [0, T] \times \Omega_i , \]

where the index \( i \) corresponds to a bubble \( (i = 1) \) or a surrounding fluid \( (i = 2) \). Here, \( T_i = -\rho_i I + \mu_i (\nabla u_i + (\nabla u_i)^T) \) are the stress tensors, and the parameters \( \rho_i, \mu_i \) and \( g \) represent the fluid densities, kinematic viscosities and the gravity force, resp. Unknown functions are the pressures \( p_i \) and the fluid velocities \( u_i \).

System [1]–[2] is considered in a domain \( \Omega \subset \mathbb{R}^d \) and a time interval \([0, T]\). Subdomains \( \Omega_1(t) \cup \Omega_2(t) = \Omega \) can change in time, but the bubble \( \Omega_1(t) \) is supposed to be fully immersed in the secondary fluid \( \Omega_2(t) \), so that \( \partial \Omega_1(t) \cap \partial \Omega = \emptyset \). The common interface \( \Gamma(t) = \partial \Omega_1(t) \) is supposed to be a closed curve if \( d = 2 \) or a closed surface if \( d = 3 \). System [1]–[2] must be accompanied with an initial condition for \( u_i(0, x) \) and some standard boundary conditions on \( \partial \Omega \).
Systems [1]–[2] for \(i = 1\) and \(i = 2\) are coupled with each other by the interface condition describing the surface tension:

\[
\begin{align*}
\mathbf{u}_1 &= \mathbf{u}_2, \quad x \in \Gamma(t), t \in [0, T], \\
(\mathbf{T}_1 - \mathbf{T}_2)\mathbf{n} &= \sigma \kappa \mathbf{n}, \quad x \in \Gamma(t), t \in [0, T],
\end{align*}
\]

where \(\mathbf{n}\) is the unit outward normal vector w.r.t. \(\partial \Omega_1\), \(\kappa\) is the mean curvature of \(\Gamma(t)\), and \(\sigma\) is the surface tension factor. Note that due to [3], a globally continuous velocity function \(\mathbf{u}\) can be defined that coincides with \(\mathbf{u}_i\) in \(\Omega_i(t)\).

In general, \(\rho_1 \neq \rho_2\) and \(\mu_1 \neq \mu_2\) for \(x \in \Gamma(t)\). If a special case with \(\mu_1 = \mu_2 = \mu\) at \(\Gamma(t)\) is considered (or some artificial smoothing of the jump \(\mu_2 - \mu_1\) is introduced in the model), we can show that [4] attains a simpler form,

\[
(p_2 - p_1)\mathbf{n} = \sigma \kappa \mathbf{n}, \quad x \in \Gamma(t), t \in [0, T].
\]

The interface \(\Gamma(t)\) will be described implicitly using a level set function \(\phi(t, x)\),

\[
\phi(t, x) = 0, \quad x \in \Gamma(t), t \in [0, T].
\]

Moreover, each subdomain will be identified by a sign of \(\phi(t, x)\), namely, \(\phi(t, x) < 0\) for \(x \in \Omega_1(t)\) and \(\phi(t, x) > 0\) for \(x \in \Omega_2(t)\). We can easily show that if \(\phi(0, x)\) is chosen with such properties, e.g., the signed distance function to \(\Gamma(0)\), then the level set function \(\phi(t, x)\) with the desired properties can be obtained by solving the advective level set equation,

\[
\partial_t \phi + \mathbf{u} \cdot \nabla \phi = 0.
\]

3. Finite volume discretization

All equations involved in our mathematical model will be discretized using a vertex-centred finite volume method. The method is closely related to finite element method and is often called “control volume method” or “finite volume element method”. The basic idea is to construct a dual mesh (in our case the so called barycentred based) of finite volumes with respect to the primary finite element mesh. We restrict the level of detail to what is necessary to introduce the notation. For references about this method see [NÄG 07] and [FRO 07c].

Let \(\partial \Omega\) be piecewise linear. We consider a triangulation \(\mathcal{T}_h\) of \(\Omega\) that resolves \(\partial \Omega\), and we assume that all elements \(E \in \mathcal{T}_h\) are triangles (in 2D) or tetrahedra (in 3D). We denote the vertices of \(\mathcal{T}_h\), i.e. the corners of the elements, by \(x_j, j = 1, 2, \ldots, J\). With each vertex \(x_j\), a control volume \(B_j\) from the dual finite volume mesh is associated. Typically, \(\partial B_j\) is polygonal (or polyhedral in 3D), and with each side \(\Gamma_{ip}\) of \(\partial B_j\), we associate an integration point \(\gamma_{ip}\) (the barycentre of \(\Gamma_{ip}\)) to apply numerical quadrature of integrals over this side.
To approximate a solution of [1]–[2] numerically, we associate the standard finite element approximations \( u_h^k, p_{1,h}^k, p_{2,h}^k \) and \( \phi_h^k \) that are continuous and piecewise linear functions on \( \Omega \) with \( T_h \) at each discrete time \( t^k \in (0, T] \). Discrete pressures \( p_{1,h}^k \) and \( p_{2,h}^k \) are defined only in elements \( E \subset \Omega_{1,h}^{k-1} := \{ x \in \Omega : \phi_h^{k-1}(x) \leq 0 \} \) and \( E \subset \Omega_{2,h}^{k-1} := \{ x \in \Omega : \phi_h^{k-1}(x) > 0 \} \), resp. All these functions are uniquely defined by their nodal values in grid points \( x_j \) with particular values \( u_{j}^k := u_h^k(x_j) \), and \( \phi_j^k := \phi_h^k(x_j) \) given directly from the initial conditions.

To derive a finite volume method (FVM) for the model, each PDE is integrated over \((t^{k-1}, t^k) \times B_j \). Once such an analytic integral form of the equations is formulated, we can derive a discrete form by applying some quadrature rules to approximate integrals. Details of the vertex-centered finite volume method for single-phase Navier-Stokes model can be found in [NÄG 07]. For instance, applying this approach directly to the left part of [2] using the global velocity \( u \) at \( t = t^k \), we obtain

\[
\int_{\Omega_j} \nabla \cdot u(t^k, x) = \int_{\partial \Omega_j} \mathbf{n}_j(\gamma) \cdot u(t^k, \gamma) \approx \sum_{ip} |\Gamma_{ip}| \mathbf{n}_{j,ip} \cdot \mathbf{u}_{ip}^k,
\]

where \( \mathbf{n}_{j,ip} := \mathbf{n}_j(\gamma_{ip}) \) and \( \mathbf{u}_{ip}^k := \mathbf{u}_h^k(\gamma_{ip}) \). Note that a discretization analogous to [8] will be used in the approximation of the level set equation in section 4.

The straightforward application of [8] to approximate continuity equation [2] leads to an unstable discretization. To obtain a stable vertex-centered FVM, we extend the discrete continuity equation with additional terms [NÄG 07]. This has the important consequence that the numerical velocity field in our discretization is not divergence free, but its divergence tends to zero as the grid is refined.

System [1]–[7] is fully coupled. To solve it, we apply the usual splitting method by solving [1]–[5] with the solution of [6]–[7] being fixed on values from the previous time step, and vice versa.

The discretization of Navier-Stokes equations [1]–[2] on the whole grid is defined as a sum of the contributions of local discretizations in every \( E \in T_h \) (cf. [NÄG 07]). To generalize it to the two-phase case, we distinguish between the elements \( E \subset \Omega_{1,h}^{k-1} \), \( E \subset \Omega_{2,h}^{k-1} \) and the elements intersected by \( \Gamma_h^{k-1} := \{ x \in \Omega : \phi_h^{k-1}(x) = 0 \} \).

For \( E \subset \Omega_{i,h}^{k-1} \), \( i = 1, 2 \) we use the unchanged version of the scheme as described in [NÄG 07]. The resulting local discretization is formulated in terms of \( u_h^k \) and \( p_{i,h}^k \) which are well-defined in \( E \).

In elements \( E \) intersected by \( \Gamma_h^{k-1} \), neither \( p_{1,h}^k \) nor \( p_{2,h}^k \) are defined on the whole element. In each such \( E \), we approximate the mean curvature of \( \Gamma(t^{k-1}) \) by a constant \( \kappa_E^{k-1} \) and define \( p_{i,h}^k(x_j) \) for \( x_j \in \Omega_{i,h}^{k-1} \) using the following discretization of [5]:

\[
p_{i,h}^k(x_j) := p_{2,h}^k(x_j) - \sigma \kappa_E^{k-1}.
\]

These nodal values of \( p_{i,h}^k(x_j) \) are interpolated over \( E \) linearly, and the usual scheme with this pressure from [NÄG 07] is applied. This approach is similar to the so called ghost fluid method [FED 99] or extended pressure finite element space [GRO 07].
Finally, we define $\kappa^k_E$ for all $E \in T_h$ intersected by $\Gamma^k_h$. For that purpose, [7] is solved not on $T_h$, but on a uniformly refined triangulation $T_h/2$. For instance, in the 2D case, $T_h/2$ is obtained by splitting each triangle $E \in T_h$ regularly into four subtriangles. The velocity $u^k_{h/2}$ used in the calculation of $\phi^k_{h/2}$ is obtained by the linear interpolation of $u^k_{h}$. The nodal values of $\phi^k_{h/2}$ are then used to construct a quadratic approximation of $\phi$ on $E \in T_h$ to be used with the relation $\kappa(t, x) = \nabla \cdot \frac{\nabla \phi(t, x)}{|\nabla \phi(t, x)|}$ (cf., e.g., [OSH 03]) to compute $\kappa^k_E$.

4. Finite volume discretization of level set equation

To approximate [7] for $t \in (t^k, t^{k+1})$, we apply the so called high-resolution flux-based level set method [FRO 07c]. This is the vertex-centred finite volume method applied to an equivalent formulation of [7] in the form of conservation laws with a source term [FRO 07b],

$$\phi_t = -\nabla \cdot (v \phi) + \phi \nabla \cdot v.$$  \hspace{1cm} [9]

In our two-phase flow application, we have $v(x) := u^k_{h/2}(x)$.

The flux-based integral formulation of [9] is obtained by integrating this equation over $B_j \times (t^k, t^{k+1})$ and using integration by parts where possible:

$$\int_{B_j} \phi(t^{k+1}, x) = \int_{B_j} \phi(t^k, x) - \int_{t^k}^{t^{k+1}} \int_{\partial B_j} (n_j \cdot v)(\gamma) \phi(t, \gamma) + \int_{t^k}^{t^{k+1}} \int_{B_j} \phi(t, x) \nabla \cdot v(x).$$  \hspace{1cm} [10]

Replacing in [10] the integrals by quadrature formulas, we derive

$$\phi^{k+1}_j = \phi^k_j - \Delta t^k \sum_{\Gamma_{ip}} |\Gamma_{ip}| n_{ip,j} \cdot v_{ip} \left( \phi^{k+1/2}_{ip} - \phi^{k-1/2}_{ip} \right).$$  \hspace{1cm} [11]

Note that an important step in the method is the application of [8] for the approximation of $\nabla \cdot v$ in the last integral of [10], see [FRO 07c, FRO 08] for more details.

Now, we explain some important details of the high-resolution flux-based level set method [11]. The initial conditions are exploited by using $\phi^0_j = \phi(0, x_j)$. Note that opposite to the classical finite volume approach, the values $\phi^0_j$ are not defined as cell averages $\phi^0_j = |B_j|^{-1} \int_{B_j} \phi(0, x)$.

To apply a second order accurate method, we have to associate each grid point $x_j$ not only with the value $\phi^k_j$, but also with some approximative gradient $\nabla \phi^k_j \approx \nabla \phi(t^k, x_j)$. To do so, we can use any averaging procedure using constant gradients $\nabla \phi^k_E := \nabla \phi^k_h(x), x \in E$ on elements $E$ with $x_j$ being their corner, e.g.,

$$\nabla \phi^k_j := \left( \sum_E |E| \right)^{-1} \sum_E |E| \nabla \phi^k_E.$$  \hspace{1cm} [12]
Now we are ready to define the flux values $\phi_{k+1/2}^{ip}$ in [11] by using, e.g., finite Taylor series and standard upwind arguments [FRO 08]:

$$
\phi_{k+1/2}^{ip} := \begin{cases} 
\phi_j^k + \left( \gamma_{ip} - x_j - \frac{\Delta t}{2} \mathbf{v}(x_j) \right) \cdot \nabla \phi_j^k, & n_j \cdot \mathbf{v}_{ip} > 0, \\
\phi_j^k + \left( \gamma_{ip} - x_j' - \frac{\Delta t}{2} \mathbf{v}(x_j') \right) \cdot \nabla \phi_j^k, & n_j \cdot \mathbf{v}_{ip} < 0.
\end{cases}
$$

Note that $\Gamma_{ip} \subset \partial B_j \cap \partial B_j'$, and that [7] was used in [13] to replace the time derivatives of $\phi$ in the Taylor series. If $n_j \cdot \mathbf{v}_{ip} < 0$ and $\Gamma_{ip} \subset \partial \Omega$, we have to use some inflow boundary conditions to define $\phi_{k+1/2}^{ip}$.

Finally we define the approximation $\phi_{k+1/2}^{j,s} \approx \phi(t_{k+1/2}, x_j)$ that is used in numerical integration of the “source” term in [10]. Following [FRO 07c], we use the arithmetic average of “inflow” and “outflow” values,

$$
\phi_{j,s}^{k+1/2} = \frac{1}{2} \left( \sum_{ip} [n_{j,ip} \cdot \mathbf{v}_{ip}]^{+} \phi_{ip}^{k+1/2} + \sum_{ip} [-n_{j,ip} \cdot \mathbf{v}_{ip}]^{+} \phi_{ip}^{k+1/2} \right),
$$

where $[a]^+ = \max \{0, a\}$. For a degenerate case when one of the denominators in [14] vanishes, the first order accurate approximation $\phi_{j,s}^{k+1/2} := \phi_j^k$ can be used.

5. Numerical experiments

In this section, we present two numerical experiments in 2D space obtained with the discretization method described above. More details on calculational methods (e.g. the solvers) can be found in [FRO 07a] where also 3D calculations are presented.

In experiments, the following values of the parameters are used [GRO 06]:

$$
\rho_1 = 995 \frac{kg}{m^3}, \quad \mu_1 = 10.4 \cdot 10^{-3} \frac{Ns}{m^2}, \quad \rho_2 = 1.107 \frac{kg}{m^3}, \quad \mu_2 = 4.8 \cdot 10^{-3} \frac{Ns}{m^2}, \quad \sigma = 2 \cdot 10^{-3} \frac{N}{m}, \quad g = (0, 9.8) \frac{m}{s^2}.
$$

In the first experiment, we simulate a rising bubble in a counter flow. The domain $\Omega$ is a rectangle $5 \times 10^{-3} \text{m} \times 10^{-2} \text{m}$. On the left and the right side of $\Omega$, the condition $u = 0$ is imposed. A parabolic inflow profile of $u$ is defined on the upper boundary. On the lower side the zero-stress outflow boundary conditions for $u$ and $p$ are used. The initial condition is a parabolic velocity profile from the upper side spread along the height of the domain. The bubble is described initially by a signed distance function to a circle with the diameter $3.5 \times 10^{-3} \text{m}$.

Due to gravitation, the bubble is pressed upwards, but the incoming fluid hinders the bubble to move up. The results of the calculation on a regular grid of triangles with $129 \times 193$ nodes (that can be considered almost “grid independent”) are presented in Figure 1. The time step used was $\Delta t = 1.25 \cdot 10^{-4}$ that corresponds to maximal
Courant number about 0.89 for the advective level set equation. Although the velocity field was not exactly divergence free (cf. section 3), the error in the volume of the bubble was about 0.05% after 600 time steps.

In the second experiment, we investigate the dependence of parasite currents on the grid. Opposite to previous settings of the example, the condition $u = 0$ is imposed on the whole boundary $\partial \Omega$ and $g = 0$. Furthermore, following the Laplace law, we set initially $u = 0$ and

$$p|_{t=0} = p^0(x) := \begin{cases} 0, & x \in \Omega_1, \\ \frac{\sigma}{R}, & x \in \Omega_2. \end{cases}$$

In the analytical solution, $u$, $p$ and $\phi$ do not depend on time and are equal to these initial conditions. Due to inexact calculations of the curvature, this is not the case in the numerical solution; see Figure 1 for an illustration of resulting parasite currents. In Table 5, the norms of numerically calculated $u_h$ and $p_h$ at time $t = 0.0025$ for 4

<table>
<thead>
<tr>
<th>$\Omega_h$</th>
<th>$\Delta t$</th>
<th>Time steps</th>
<th>$|u_h|_0$</th>
<th>$|u_h|_2$</th>
<th>$|e_p|_{2,FV}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$33 \times 49$</td>
<td>0.00025</td>
<td>10</td>
<td>$2.230 \cdot 10^{-4}$</td>
<td>$3.618 \cdot 10^{-4}$</td>
<td>$5.56 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>$65 \times 97$</td>
<td>0.000125</td>
<td>20</td>
<td>$1.052 \cdot 10^{-4}$</td>
<td>$1.463 \cdot 10^{-5}$</td>
<td>$2.08 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>$129 \times 193$</td>
<td>0.0000625</td>
<td>40</td>
<td>$0.519 \cdot 10^{-4}$</td>
<td>$0.447 \cdot 10^{-7}$</td>
<td>$0.762 \cdot 10^{-5}$</td>
</tr>
<tr>
<td>$257 \times 385$</td>
<td>0.00003125</td>
<td>80</td>
<td>$0.199 \cdot 10^{-4}$</td>
<td>$0.087 \cdot 10^{-7}$</td>
<td>$0.239 \cdot 10^{-5}$</td>
</tr>
</tbody>
</table>

Table 1. Norms of the parasite currents and errors in the pressure on different grids.
successively refined (in space as well as in time) grids are compared. The technical
details for definitions of used norms can be found in [FRO 07a].

6. References

Approach to Interfaces in Multimaterial Flows (The Ghost Fluid Method)

[FRO 07a] FROLKOVIĆ P., LOGASHENKO D., WITTUM G., “Towards Finite Volume Dis-
cretization of Two-Phase Flow Using Level-Set Formulation”, SiT-Report (SiT, University
of Heidelberg), 15/12/2007.

p. 436-454.

[FRO 07c] FROLKOVIĆ P., MIKULA K., “High-resolution flux-based level set method”, SIAM

[FRO 08] FROLKOVIĆ P., WEHNER C., “Flux-based level set method on rectangular grids and
computation of first arrival time functions”, Comput. Vis. Sci, DOI: 10.1007/s00791-008-
0115-z, 2008.

[GRO 06] GROSS S., REICHELT V., REUSKEN A., “A Finite Element Based Level Set Method

p. 40-58.


finite element method using a discontinuous level set approach for the computation of


[OSH 03] OSHER S., FEDKIW R., Level Set Methods and Dynamic Implicit Surfaces,


[TOR 00] TORNBERG A.-K., ENGQUIST B., “A finite element based level set method for
multiphase flow applications”, Computing and Visualization in Science, vol. 3, 2000,

[Van 05] VAN DER PIJL S. P., SEGAL A., VUIK C., WESSELING P., “A mass-conserving