Diffuse interface models for two-phase flows in artificial compressibility approach

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Abstract. We present an approach to numerical simulation of two-phase flows in the so-called one-fluid formulation, combining the Entropically Damped Artificial Compressibility (EDAC) method for flow solution and a chosen variant of the Phase Field Method (PFM) that belongs to a wider family of the Diffuse Interface (DI) methods of interface capturing. The resulting governing equations express a set of conservation laws and are of the advection–diffusion type, convenient in numerical handling. These equations, rewritten in the semi-discrete form, can be efficiently solved on parallel devices using the method of lines. We applied the conservative finite difference method for the spatial discretisation and a variant of the Runge–Kutta method to advance the solution in time. The results presented in this work contain the analysis of spurious currents in the case of stationary droplet together with the pressure jump across its surface, as well as the deformation of a droplet subjected to the laminar Couette flow. The presented EDAC-DI approach, offering very high computational efficiency, gives results comparable to other well-established methods for the simulations of the interfacial flows.

1. Introduction

The present work aims to assess the potential of the artificial compressibility (AC) approach for simulations of two-phase interfacial flows based on a chosen one-fluid formulation. The AC methods are attractive due to their “elliptic-free” character which matches the advection (possibly advection-diffusion) type of the equations governing the dynamics of fluid interfaces arising in the interface capturing methods like Volume Of Fluid, Level-Set and Phase Field Method (PFM). The systems of equations of the same type are easier in numerical and algorithmic handling and offer a potential of very efficient solution algorithm using the Single Instruction Multiple Threads (SIMT) approach on parallel devices (e.g. Graphics Processing Units, GPU). On the other hand, the explicit integration methods preferred for the time marching problems suffer from the time step size restrictions that in our case stem from the acoustic effects and/or strongly diffusive behaviour.

In the following we first present the chosen model of the two-phase flow and describe the discretisation of the governing equations. Next we show results of the standard benchmark tests – the stationary droplet and deformation of droplet under the Couette flow. Last but not least, we discuss the numerical and computational issues stemming from the chosen modelling approach and its usefulness at particular flow regimes.
2. Two-phase flow model

The flow is modelled by means of the Entropically Damped Artificial Compressibility (EDAC) method introduced by Clausen [3], Eqs. (1) and (2) below, while the dynamics of the fluid-fluid interface is governed by a variant of the Phase Field Method, Eq. (3), proposed by Chiu and Lin [2]:

\[ \partial_t \mathbf{u} = -\nabla \cdot (\mathbf{u} \mathbf{u} + pI - Re^{-1} \nabla \mathbf{u}) + \mathbf{g} + \mathbf{F}_{st}, \]  
\[ \partial_t p = -\nabla \cdot (p \mathbf{u} + M^{-2} \mathbf{u} - Re^{-1} \nabla p), \]  
\[ \partial_t \Phi = -\nabla \cdot (\Phi \mathbf{u} + \gamma \Phi (1 - \Phi) \mathbf{n} - \gamma \epsilon \nabla \Phi). \]  

In the above equations, \( \mathbf{u} = (u, v, w) \) is the velocity field, \( p \) is the pressure, \( \Phi : \Omega \rightarrow [0, 1] \) is the phase indicator function and \( \mathbf{n} = \nabla \Phi / |\nabla \Phi| \) is the unit vector normal to the interface; \( I \) stands for the unit tensor; \( \mathbf{g} \) and \( \mathbf{F}_{st} \) denote the body force and the contribution of the surface tension, respectively. \( M \) and \( Re \) are the Mach and Reynolds numbers, defined by a suitably chosen velocity scale \( U \), length scale \( L \) and the artificial speed of sound \( c_s \).

Let us now take a closer look at Eq. (3). This PFM model is based on the Conservative Level Set (CLS) method of Olsson and Kreiss [8] who proposed to capture the interface by advecting the level set function \( \Phi \) and performing its re-initialisation in artificial time \( \tau \) separately:

\[ \partial_t \Phi = -\nabla \cdot (\Phi \mathbf{u}), \]  
\[ \partial_\tau \Phi = -\nabla \cdot (\Phi (1 - \Phi) \mathbf{n} - \epsilon \nabla \Phi). \]  

Equation (5) can be considered as a modification of the viscous Burgers equation: the first term on the right hand side sharpens the interface profile (creates a “shock”) and bounds \( \Phi \in [0, 1] \); the second term introduces diffusion (therefore the name Diffuse Interface). In the equilibrium state the interface profile (for clarity in one spatial dimension) is given by \( \Phi(x) = \frac{1}{2} (1 + \tanh \frac{x}{\delta}) \). It is clear that the width of the interface is of the order of \( \epsilon \). The constant \( \gamma \) in Eq. (3) controls the “strength” of the interface profile reshaping. The advantage of the considered PFM model over the CLS is mainly algorithmical – all equations are solved simultaneously and there is no need to check the convergence of the integration process in artificial time. A detailed discussion of different one-fluid formulations of multiphase flow models can be found in [6].

The term \( \mathbf{F}_{st} \) couples the interfacial effects and the momentum of the system and is defined according to the classical Continuum Surface Force (CSF) model of Brackbill et al. [1], which consists in smoothing the surface tension across the interfacial region:

\[ \mathbf{F}_{st} = -We^{-1} \kappa \mathbf{n} \delta \approx -We^{-1} \kappa \nabla \Phi, \]  

where \( We = \rho U^2 L / \sigma \) is the Weber number (\( \sigma \) being the surface tension coefficient) and \( \rho \) is the reference density. The interface curvature \( \kappa = \nabla \cdot \mathbf{n} \). Clearly, the CSF utilises the fact that \( |\nabla \Phi| \approx \delta \), where \( \delta \) is the surface Dirac delta function.

The boundary conditions (BC) for the solid walls (oriented parallely to the \( x - z \) plane) are as follows:

\[ \mathbf{u} = 0, \quad \partial_y p = Re^{-1} \partial_y w, \quad \partial_y \Phi = 0, \]  

i.e. the velocity vanishes on the solid walls, the pressure is computed from the momentum equation, there is no flux of the phase indicator function through the walls and the contact angle (when relevant) is 90 degrees.

We emphasize here that the presented model is expressed as a set of conservation laws, in contrast to standard Level Set method and some variants of the PFM (see e.g. [9]). On the other hand, the CSF approach can not be rewritten in the divergence form and therefore minor imperfections in the momentum conservation can be expected. This disadvantage can
be overcome by the application of the Continuum Surface Stress (CSS) model of the surface tension effects, see [12]. However, for the preliminary tests we decided to use CSF since the CSS implementation is more complicated.

Another important feature of the presented model is the purely parabolic type of the equations. Application of an explicit time integration method eliminates the need of solving linear algebraic system, which is an inherent part of modelling the truly incompressible flows due to the divergence-free velocity field restriction which in turn is no longer valid in the EDAC approach. The diffusive terms present in the EDAC equations as well as the considered PFM equation allow for the use of central finite difference schemes in spatial discretisation. In our recent work we have shown that the above features allow for easy, effective and efficient implementation of the single-phase EDAC flow solver on parallel devices [4]. We have also discussed there the incompressible flow limit with the EDAC model.

3. Discretisation

As mentioned earlier, we use the method of lines to numerically solve Eqs. (1)–(3) by rewriting the system in semi-discrete form (the indices i, j, k number the grid nodes in the x, y, z directions, respectively):

$$\frac{d}{dt} u_{i,j,k} = - \frac{(F_{i+\frac{1}{2},j,k} - F_{i-\frac{1}{2},j,k})}{\Delta x} - \frac{(G_{i,j+\frac{1}{2},k} - G_{i,j-\frac{1}{2},k})}{\Delta y} - \frac{(H_{i,j,k+\frac{1}{2}} - H_{i,j,k-\frac{1}{2}})}{\Delta z},$$  

(8)

where $U = (u, v, w, p, \Phi)$ is the vector of the dependent variables and $F, G, H$ are the discrete fluxes. Using parallel devices the solution is advanced in time at each node by a separate thread centered FD schemes. For example the $x$ flux component we have (other fluxes are defined by analogy):

$$F_{i+1/2,j,k} = \begin{bmatrix}
C(pu) + M^{-2}D(u) - Re^{-1}L(p) \\
C(uu) + D(p) - Re^{-1}L(u) \\
C(u\Phi) - Re^{-1}L(\Phi) \\
C(\Phi) + \gamma D(\Phi(1-\Phi)n_x) - \gamma \epsilon L(\Phi)
\end{bmatrix}_{i+1/2,j,k},$$  

(9)

where (for brevity, we omit the $j,k$ indices from the notation):

$$C(u^\alpha u^\beta)_{i+1/2} = \frac{1}{4}(u^\alpha_i + u^\alpha_{i+1})(u^\beta_i + u^\beta_{i+1}),$$  

(10)

$$D(f)_{i+1/2} = (f_i + f_{i+1})/2,$$  

(11)

$$L(f)_{i+1/2} = (f_{i+1} - f_i)/\Delta x.$$  

(12)

The normal vectors $\mathbf{n}$ and the interface curvature $\kappa$ are also computed with 2nd order centered FD schemes. For example the $x$ - component of $\mathbf{n}$ is given by:

$$n_{x,i} = \frac{(\Phi_{i+1} - \Phi_{i-1})}{2\Delta x} \frac{1}{|\nabla \Phi|},$$  

(13)

and for the curvature we have

$$\kappa_i = \frac{(n_{x,i+1} - n_{x,i-1})}{2\Delta x} + \frac{(n_{y,i+1} - n_{y,i-1})}{2\Delta y} + \frac{(n_{z,i+1} - n_{z,i-1})}{2\Delta z}. $$  

(14)
We use the ghost node technique to impose the boundary conditions in the conservative manner. Let the wall be placed in the middle between the nodes indexed by \( j = 0 \) and \( j = 1 \).

The BCs are discretised as follows:

\[
\begin{align*}
    u_{i,0,k} &= -u_{i,1,k} & v_{i,0,k} &= -v_{i,1,k} & w_{i,0,k} &= -w_{i,1,k}, \\
    p_{i,0,k} &= p_{i,1,k} - \text{Re}^{-1} \frac{d^2}{dy^2} \left[ L_v \left( \frac{y_0 + y_1}{2} \right) \right] \Delta y,
\end{align*}
\]

where \( L_v(y) \) is the Lagrange interpolation polynomial based on the values \( v_{i,0,k}, v_{i,1,k}, v_{i,2,k}, v_{i,3,k} \) at \( y_0, y_1, y_2, y_3 \) and

\[
\Phi_{i,0,k} = \Phi_{i,1,k}.
\]

The normal vectors and curvature at the ghost nodes are computed using one–sided FD stencils.

To advance the solution in time we use the explicit 3-rd order Runge-Kutta method in the low-storage variant proposed by Williamson [10]. The low-storage property is important since we are going to execute the EDAC-DI solver on GPUs. For the details of implementation and issues according to execution on the GPUs we refer the reader to our paper [4]. In 3-dimensional case, the time step size constraints arising from the acoustic effects (CFL condition), viscous terms, surface tension and the diffusion of the interface are (\( \Delta \) is the minimal grid spacing):

\[
\Delta t_{\text{CFL}} \leq 1.6 \frac{\Delta}{u_{\text{max}}(1 + M^{-1})}, \quad \Delta t_v \leq \frac{2.78 \Delta^2}{12 \text{Re}^{-1}}, \quad \Delta t_{\text{sf}} \leq \sqrt{\frac{\Delta^3}{8 \pi \text{We}^{-1}}}, \quad \Delta t_{\text{PFM}} \leq \frac{2.78 \Delta^2}{12 \gamma \epsilon}.
\]

The time step is chosen according to the most severe of the four restrictions above. Many flows in physics and engineering are convection dominated and therefore the CFL condition is the most restrictive. However, in the next section we present also the diffusion dominated case. Fortunately, the constraints resulting from the PFM are usually weaker (or of similar order) than the CFL condition and in AC methods it is commonly accepted to set \( M \leq 0.1 \). For reasonable Weber numbers, the constraint stemming from the surface tension is usually the least restrictive.

4. Tests
All the test have been performed on uniform grids in 3D. The coefficients in the PFM equation were set according to the work of Mirjalili et al. [7]: we take \( \gamma = 1.5 \) and \( \epsilon = 5 \Delta / 6 \). This setting allows to avoid over- and undershoots of \( \Phi \) which can occur when central FD schemes are used and the interface is resolved using a few grid nodes. In all the cases we assume the density ratio of the fluids of either side of the interface equal 1; the same assumption is made on the viscosity.

4.1. Stationary droplet
As a first test we performed the simulation of the stationary (initially spherical) droplet in a cubic domain. Since there is no velocity scale \( U \) (physically, the fluid is at rest), to stay in the non-dimensional setup we treat the Reynolds number as a free parameter that determines the diffusion of the momentum. The domain size is \( 2 \times 2 \times 2 \) and the droplet diameter \( D = 1 \).

The spatial resolution was \( 128^3 \). The aim of this test is to check the agreement of the pressure drop through the interface with the analytical result (Young-Laplace law) \( \Delta p = 4 / \text{We} \). We also quantify the numerical artifacts, the so-called parasitic (or spurious) currents. The phenomenon is fully described by one nondimensional parameter – the Laplace number \( \text{La} = \text{Re}^2 / \text{We} \). The measurements of parasitic currents for different values of \( \text{La} \) are gathered in Table 1 (left panel). They are expressed in terms of the capillary number \( \text{Ca} = U / \text{We} / \text{Re} \), where \( U \) is the maximum observed velocity magnitude in the quasi-steady state. The results are in good agreement with other reports, see e.g. [12]. We emphasize that we observed only minor sensitivity of results to \( M \) for a wide range of the Mach numbers (based on \( U \)) tested, from 0.1 to 0.001.
Figure 1. Stationary droplet at \( We=1 \) and \( La=3 \times 10^5 \). Left: parasitic currents, circle marks the interface \( \Phi = 0.5 \). Right: the pressure profile; the Young-Laplace law predicts \( \Delta p = 4 \).

In the left panel of Fig. 1 the domain cross-section in \( x - y \) plane is shown and the grayscale map denotes the magnitude of the velocity at \( La=3 \times 10^5 \). A pattern similar to other reports is visible. In the right panel of Fig. 1 the pressure profile across the droplet is shown. The pressure jump agrees well with the theoretical prediction.

4.2. Droplet deformation in Couette flow

In this case we placed the droplet between two walls sliding in the opposite directions with speed \( U \). Under the shear flow the droplet deforms (towards an ellipsoid) and a steady state is achieved if the surface tension is high enough to balance the viscous forces. The deformation of the droplet depends on the capillary number defined now as \( Ca = We/Re \). The domain size is set to \( 4 \times 2 \times 2 \) and the droplet diameter is \( D = 0.5 \). The spatial resolution is \( 256 \times 128 \times 128 \). The Reynolds number is \( Re = 1 \). Thus, the capillary number value is changed by modifying the Weber number only. In Fig. 2 the final droplet shape is shown for \( Ca=0.1 \). Let \( l \) and \( s \) denote the large and small axes of the ellipsoid. Assuming creeping flow, Taylor [11] has shown that:

\[
E = \frac{l - s}{l + s} = \frac{35}{32} Ca. \tag{19}
\]

Table 1. Left: steady droplet, spurious currents. Right: droplet deformation in Couette flow.

| La    | Ca     | \( Ca \) | \( E_{\text{comp}} \) | \( E \) |
|-------|--------|----------|------------------------|--------|
| \( 10^2 \) | \( 1.2 \times 10^{-2} \) | 0.1      | 0.1072                 | 0.1094 |
| \( 10^4 \) | \( 5.6 \times 10^{-4} \) | 0.2      | 0.2228                 | 0.2188 |
Figure 2. The deformation of a droplet in the Couette flow at Ca=0.1. The line marks the interface; the velocity field in the $x - y$ plane passing through the droplet centre is also shown.

In Table 1 (right panel) the results of our computations are gathered. A good agreement with the theoretical correlation, Eq. (19), is visible and the errors are $\sim 2\%$ which is as accurate as the phase field model based on the Cahn-Hilliard equation [5]. In the above simulations we set $Ma=0.1$ and therefore the time step is restricted by the viscous effects, resulting in the Courant number $\sim 0.2$ so the explicit discretisation is far from optimal choice in this case.

5. Conclusions and additional remarks
The proposed complete approach for the simulation of two-phase flows with interfaces gives good results for standard benchmark tests. In our opinion, the important advantages are the simplicity of the method and very high efficiency that can be obtained on the desktop computers.

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