An incompressible–compressible approach for droplet impact

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Introduction

High-speed droplet impact scenarios appear in a wide range of industrial applications, for example spray coating or liquid-fuelled engines. In this context, the compressibility effects on both gaseous and liquid components cannot be neglected. As an example, Haller et al. [1] showed that the jet dynamics during high speed droplet impact are influenced by a shock wave which travels through the liquid. Since incompressible models cannot capture such features, the jetting time is not predicted correctly. Accordingly, in [1] a compressible sharp interface model has been adopted for the purpose. Unfortunately, this approach is restricted with respect to interface morphologies. For this reason, in [2] a diffuse interface approach has been developed. The authors presented a Navier–Stokes–Allen–Cahn phase field model which is capable of handling complex interface morphologies and topological changes. Both phases are compressible and allowed to mix in the interface region.

Despite the reduced prediction capabilities of incompressible models when dealing with a high-speed droplet impact, it is interesting to quantify the compressible effects on the liquid component. For this purpose, we want to develop an incompressible–compressible phase field model able to handle two components, one gaseous treated as compressible and one liquid assumed incompressible. Indeed, a direct comparison between the compressible-compressible and the incompressible-compressible models allows to get a better understanding of the effects of the liquid compressibility.

In this work we introduce an incompressible–compressible phase field model, discuss some properties, and present an approach towards a discontinuous Galerkin (dG) scheme to solve the system numerically with promising preliminary results.

Mathematical modelling

In this section we sketch the derivation of an incompressible–compressible phase field model motivated by [3]. The basic idea of phase field models is to introduce an additional variable φ named *phase field* which provides information of the phase. In the typical context of two phases, φ assumes value 0 and value 1 in the two bulk states and values in between in the interface region. Phase field models are derived based on energy principles and thus are thermodynamically consistent by construction.

We consider the balance equations in non-conservative form describing two phase flow

$$\dot{\rho} = -\rho \nabla \cdot \mathbf{u}, \tag{1}$$

$$\rho \dot{\mathbf{u}} = \nabla \cdot \mathbf{T}, \tag{2}$$

$$\rho \dot{\varphi} = \rho j, \tag{3}$$

$$\rho \dot{e} = \mathbf{T} : \mathbf{D} - \nabla \cdot \mathbf{q} + \rho r. \tag{4}$$

Here ρ denotes the density, $\mathbf{u}$ the velocity vector, $\mathbf{T} = -p\mathbf{I} + \mathbf{S} + \mathbf{C}$ the stress tensor, p the pressure, $\mathbf{S} = 2\tilde{\mu}\mathbf{D} + \tilde{\mu}_b(\nabla \cdot \mathbf{u})\mathbf{I}$ the viscous stress tensor, $\mathbf{D}$ the strain rate tensor, i.e. the symmetric part of the velocity gradient, $\mathbf{C}$ the capillarity tensor, $\mathbf{I}$ the identity matrix, $\tilde{\mu}$ the dynamic viscosity, $\tilde{\mu}_b$ the bulk viscosity, $\mathbf{q}$ the heat flux, r the energy source per unit mass and j the inter-constituent mass flow rate per unit mass. The $(\dot{\ })$ symbol specify the material derivative. In order to derive a thermodynamically consistent model, first we consider the entropy balance equation in non-conservative form

$$\rho \dot{s} = -\nabla \cdot \mathbf{\Sigma} + \frac{\rho}{T} r + s_i, \tag{5}$$

with the specific entropy s, the entropy flux $\mathbf{\Sigma}$, temperature T, and the entropy production s_i. Then we impose to verify the Clausius–Duhem inequality

$$\rho \dot{s} \geq -\nabla \cdot \left(\frac{\mathbf{q}}{T} + \mathbf{k} \right) + \frac{\rho r}{T}. \tag{6}$$

Here $\mathbf{k}$ is an entropy flux and $\mathbf{\Sigma} = -\mathbf{q}/T - \mathbf{k}$.

Compressible phase field models like [2,4,5] are based on the Helmholtz free energy F and the pressure is obtained from the specific Helmholtz free energy f as $p = \rho^2\, \partial f / \partial \rho$. However, in incompressible phase field models such a derivation is not possible due to the constant density assumption and, therefore, the Gibbs free energy G is needed which allows to define the density ρ as

$$\frac{1}{\rho} = \frac{\partial g}{\partial p}. \tag{7}$$

Considering the specific Gibbs free energy in the form $g = g(T, p, \varphi, \nabla\varphi)$ and exploiting thermodynamic relations, one can derive conditions for permissible constitutive relations to achieve a thermodynamic consistent model. Among different constitutive relations [6] one possible choice leads to the set of *Navier–Stokes–Cahn–Hilliard* (NSCH) equations which comprises (1)-(4) with the capillarity parameter $\gamma > 0$ and

$$\frac{1}{\rho} = \frac{\varphi}{\rho_\alpha(T,p)} + \frac{1-\varphi}{\rho_\beta(T,p)}, \tag{8}$$

$$g = g_0(T,\varphi,p) + \frac{\gamma}{2}|\nabla\varphi|^2, \tag{9}$$

$$\mathbf{C} = -\rho\gamma\nabla\varphi \otimes \nabla\varphi, \tag{10}$$

$$\overline{\mu} = \frac{\partial g_0}{\partial\varphi}(T,p) - \frac{T}{\rho}\nabla\cdot\left(\gamma\frac{\rho}{T}\nabla\varphi\right), \tag{11}$$

$$j = \nabla\cdot\left(\zeta\nabla\frac{\overline{\mu}}{T}\right). \tag{12}$$

g_0 is a suitable function that define the specific Gibbs free energy as function of temperature, pressure and phase field variable. For (8)-(12) the entropy flux and entropy production read as

$$\mathbf{\Sigma} = -\frac{\mathbf{q}}{T} - \nabla\cdot\left(\zeta\nabla\frac{\overline{\mu}}{T}\right)\frac{\partial g}{\partial\nabla\varphi} - \zeta\frac{\overline{\mu}}{T}\nabla\frac{\overline{\mu}}{T}, \tag{13}$$

$$s_i = 2\frac{\tilde{\mu}}{T}|\mathbf{D}|^2 + \tilde{\mu}_b(\nabla\cdot\mathbf{u})^2 + \frac{\beta}{T^2}|\nabla T|^2 + \zeta\left|\nabla\frac{\overline{\mu}}{T}\right|^2 \geq 0. \tag{14}$$

Notice that the entropy production s_i is nonnegative and therefore the model thermodynamically consistent.
Up to now no assumptions have been made on the densities ρ_α and ρ_β of the two phases and thus the derived NSCH system is valid either for compressible or incompressible phases. In the following we restrict ourselves to the isothermal case, i.e. $T = const.$, and consider a compressible gaseous phase which obeys the perfect-gas equation of state, $\rho_g = p/\alpha$, and an incompressible liquid phase with constant liquid density, $\rho_L > 0$

$$\frac{1}{\rho} = \frac{\varphi}{\rho_L} + \alpha\frac{1-\varphi}{p}. \tag{15}$$

Combining with the Cahn–Hillard relation [7] and equation (7), the specific Gibbs free energy writes

$$g = \varphi\frac{p-p_0}{\rho_L} + (1-\varphi)\alpha\ln\frac{p}{p_0} + \frac{\gamma}{2}|\nabla\varphi|^2 + W(\varphi), \tag{16}$$

using the double well potential $W(\varphi) = b\,\varphi(1-\varphi)^2, b > 0$, and the reference pressure $p_0 > 0$.

Introducing the pseudo-Mach number M, the Reynolds number Re, the Cahn number C, and the Peclet number Pe, see [4], the incompressible–compressible Navier–Stokes–Cahn–Hilliard (ICNSCH) model in nondimensional form reads as

$$\partial_t\rho + \mathbf{u}\cdot\nabla\rho + \rho\nabla\cdot\mathbf{u} = 0, \tag{17}$$

$$\rho\partial_t\mathbf{u} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \frac{1}{\mathrm{M}^2}\nabla p = \frac{1}{\mathrm{Re}}\nabla\cdot\mathbf{S} - \frac{\mathrm{C}}{\mathrm{M}^2}\nabla\cdot(\rho\nabla\varphi\otimes\nabla\varphi), \tag{18}$$

$$\rho\partial_t\varphi + \rho\mathbf{u}\cdot\nabla\varphi = \frac{1}{\mathrm{Pe}}\Delta\mu, \tag{19}$$

where,

$$\mu = W'(\varphi) + \frac{p}{\rho_L} - \alpha\ln(p) - \frac{\mathrm{C}}{\rho}\nabla\cdot(\rho\nabla\varphi) \tag{20}$$

$$\rho^{-1} = \frac{\varphi}{\rho_L} + (1-\varphi)\frac{\alpha}{p}. \tag{21}$$

Properties

In this section we state some properties of the ICNSCH system.

By construction, the ICNSCH system fulfils an energy inequality. Let $p, \mathbf{u}$, and φ be smooth solutions of (17)-(21) with boundary conditions

$$\mathbf{u} = \mathbf{0}, \quad \nabla\varphi \cdot \mathbf{n} = \nabla\mu \cdot \mathbf{n} = 0 \quad \text{on } \partial\Omega. \tag{22}$$

Then the following energy inequality holds:

$$\frac{\mathrm{d}}{\mathrm{d}t}E = \frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \frac{1}{2}\rho|\mathbf{u}|^2 + \frac{1}{\mathrm{M}^2}\rho g(p,\varphi,\nabla\varphi) - \frac{1}{\mathrm{M}^2}p\,\mathrm{d}\mathbf{x} = -\int_\Omega \frac{1}{\mathrm{Re}}\mathbf{S}:\nabla\mathbf{u}\,\mathrm{d}\mathbf{x} - \int_\Omega \frac{1}{\mathrm{M}^2\mathrm{Pe}}|\nabla\mu|^2\,\mathrm{d}\mathbf{x} \le 0. \tag{23}$$

It is interesting to note that for a pseudo-Mach number M that tends to zero, i.e., the so called low-Mach limit, the ICNSCH converge to the quasi-incompressible model of Lowengrub and Truskinovsky [8].

More in particular for $\varepsilon > 0$, let us consider the following regime

$$\mathrm{M} = \varepsilon, \quad \mathrm{C} = \varepsilon^2, \quad \mathrm{Re} = 1, \quad \mathrm{Pe} = \varepsilon^2, \quad b = \varepsilon^2, \quad \alpha = 1. \tag{24}$$

In the limit $\varepsilon \to 0$, the solution of the system (17)-(21) are expected to converge to solutions of the quasi-incompressible system [8]

$$\nabla\cdot\mathbf{u} = -\frac{1}{\rho}\frac{\partial\rho}{\partial\varphi}(\partial_t\varphi + \mathbf{u}\cdot\nabla\varphi), \tag{25}$$

$$\rho\partial_t\mathbf{u} + \rho(\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla p = \nabla\cdot\mathbf{S} - \nabla\cdot(\rho\nabla\varphi\otimes\nabla\varphi), \tag{26}$$

$$\rho\partial_t\varphi + \rho\mathbf{u}\cdot\nabla\varphi = \Delta\mu. \tag{27}$$

Here

$$\mu \quad = W'(\varphi) - \frac{p}{\rho^2}\frac{\partial\rho}{\partial\varphi} - \frac{1}{\rho}\cdot\nabla(\rho\nabla\varphi) \tag{28}$$

$$\rho^{-1} = \frac{\varphi}{\rho_L} + \frac{(1-\varphi)}{\rho_V}. \tag{29}$$

Idea of proof: Formally by assuming an asymptotic expansion, $u = u^{(0)} + \varepsilon u^{(1)} + \varepsilon^2 u^{(2)} + \cdots, u = \rho, \varphi, \mathbf{u}$, and comparing terms with different orders of magnitude with respect to the pseudo-Mach number.

Towards a discontinuous Galerkin solver

A popular class of solvers for phase field systems are the so-called *energy consistent dG* schemes [2,3,9]. They are based on the idea that the energy inequality (23) of the phase field system should be recovered on the discrete level without introducing numerical dissipation. This prevents parasitic currents in a near equilibrium situation. In [3] such a solver was proposed for the ICNSCH system (17)-(21) but not implemented by the authors. As main drawback, these schemes show restrictions with respect to the step-size of the time integration. Indeed, at best a second order convergence in time can be achieved. Additionally, the solver is sensitive with respect to larger variations in energy. Because of the above-mentioned drawbacks and our interest in simulations away from equilibrium, where parasitic currents are negligible, we want to design a novel solver which can achieve higher order in time and circumvent the timestep restriction by means of implicit schemes.

The idea is to develop a fully implicit dG scheme based on Godunov fluxes. In order to compute the numerical fluxes, we exploit the exact solution of local Riemann problems at inter-element boundaries. However, due to the incompressible nature of the liquid phase, the time derivative of the continuity equation vanishes, thus making impossible a definition of a Riemann problem solution. In order to circumvent the issue an artificial compressibility approach is adopted. Indeed, following the work of Bassi et al. [10] an artificial compressibility is added for the liquid phase only at the inter-element level thus ensuring the hyperbolic nature of local problems. Hence, a natural approach is to add artificial compressibility with parameter $a_0 > 0$, only for the incompressible phase, i.e.

$$\frac{1}{\rho} = \frac{\varphi}{\rho_L} + (1-\varphi)\frac{\hat{a}}{p}, \tag{30}$$

with $\hat{a} := \varphi a_0 + (1-\varphi)$. This leads to the speed of sound $c^2 = u^2 + \hat{a}^2\left(1 - \frac{1-\varphi}{p^2}\alpha(\rho u)^2\right)$.

However, this approach cannot be applied since hyperbolicity cannot be guaranteed and the sound speed depends both on the velocity and pressure, which results in the fact that a Riemann solution cannot be explicitly computed. Therefore, we introduce an artificial equation of state, namely

$$\rho = \varphi\left(\frac{p - p_0}{a_0^2} + \rho_L\right) + (1 - \varphi)\frac{p}{\alpha}. \tag{31}$$

With (31) the square of the speed of sound is $c^2 = \frac{a_0^2 \alpha}{\varphi\alpha + (1-\varphi)a_0^2} > 0$ and the corresponding system hyperbolic. Note that for $\varphi = 0$ we obtain $c^2 = \alpha$ and for $\varphi = 1$ we obtain $c^2 = a_0^2$.

To test the applicability of this novel approach we implemented it for the simpler case of a single-phase incompressible Navier–Stokes system with the artificial equation of state

$$\rho = \frac{p - p_0}{a_0^2} + \rho_L. \tag{32}$$

First results are promising, see Figure 1, where the following test case T1 was considered:

$$p = \begin{cases} p_l, & x < 0.5 \\ p_r, & x \geq 0.5' \end{cases} \quad u = \begin{cases} u_l, & x < 0.5 \\ u_r, & x \geq 0.5' \end{cases} \quad \text{with } p_l = 1, u_l = 0, p_r = 0.1, u_r = 0 \tag{33}$$

For finer grids the solution converges nicely to the exact solution. In a forthcoming publication we will extend this approach to the ICNSCH system.

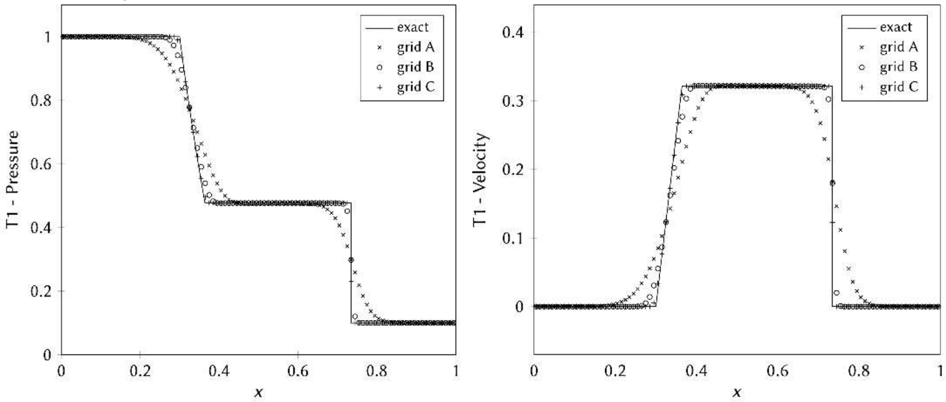

Figure 1. DG $\mathbb{P}^0$ method applied to test T1. Comparison between numerical and exact solutions on three grids of 100 (grid A), 1000 (grid B) and 10000 (grid C) elements. For the grid B and grid C only the solution of 1/10 and 1/100 of the elements is shown, respectively.

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