6

Mathematical model

6.1 Introduction

We recall the Navier-Stokes model (1.19)-(1.21) for two-phase incompressible flows:

$$\begin{cases} \rho_i \Big(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \Big) = -\nabla p + \rho_i \mathbf{g} + \operatorname{div}(\mu_i \mathbf{D}(\mathbf{u})) \\ \operatorname{div} \mathbf{u} = 0 \end{cases} \quad \text{in } \Omega_i, \tag{6.1}$$

$$[\boldsymbol{\sigma}\mathbf{n}]_\Gamma = -\tau\kappa\mathbf{n}, \quad [\mathbf{u}] = 0 \quad \text{on } \Gamma, \tag{6.2}$$

$$V_\Gamma = \mathbf{u} \cdot \mathbf{n} \quad \text{on } \Gamma. \tag{6.3}$$

We recall the definition of the stress tensor $\boldsymbol{\sigma} := -p\mathbf{I} + \mu\mathbf{D}(\mathbf{u})$ and the deformation tensor $\mathbf{D}(\mathbf{u}) := \nabla\mathbf{u} + \nabla\mathbf{u}^T$. For the velocity we use Dirichlet boundary conditions $\mathbf{u} = \mathbf{u}_D$ on $\partial\Omega_D$ and natural boundary conditions on $\partial\Omega \setminus \partial\Omega_D$. The initial condition for the velocity is $\mathbf{u}(x, 0) = \mathbf{u}_0(x),\ x \in (\Omega_1 \cup \Omega_2)(0)$, with a given function $\mathbf{u}_0 : \Omega \to \mathbb{R}^3$. Furthermore, we assume that the initial interface $\Gamma(0)$ is given. Note that the model (6.1)-(6.3) is *not* in dimensionless form.

Remark 6.1.1 We address the formulation of the two-phase flow model (6.1)-(6.3) in dimensionless variables. In this model we have two Navier-Stokes equations in the two subdomains Ω_i, $i = 1, 2$. Therefore it is an option to consider a subdomain dependent scaling. For the dimensionless variables we use the same notation as in the derivation of the one-phase dimensionless Navier-Stokes equation in Sect. 2.1: $\bar{x}$, $\bar{t}$, $\bar{\mathbf{u}}$, $\bar{p}$. It does not make sense to use different spatial scales in the two subdomains. Hence we choose *one* typical length scale, denoted by L. We want to maintain the continuity property $[\mathbf{u}]_\Gamma = 0$ also in the transformed variables and thus we choose *one* typical velocity size U. In the pressure rescaling we allow a subdomain dependent rescaling with $\tilde{\rho}_i > 0$

a given constant in Ω_i (with unit kg/m^3). The corresponding piecewise constant function on Ω is denoted by $\tilde{\rho}$. Based on this, the dimensionless variables are given by

$$\bar{x} = \frac{1}{L}x, \quad \bar{t} = \frac{U}{L}t, \quad \bar{\mathbf{u}}(\bar{x},\bar{t}) = \frac{\mathbf{u}(x,t)}{U}, \quad \bar{p}_i(\bar{x},\bar{t}) = \frac{p(x,t)}{\tilde{\rho}_i U^2}, \ i = 1,2.$$

Furthermore, $\bar{\Omega} := \frac{1}{L}\Omega := \{\, \bar{x} \in \mathbb{R}^3 : L\bar{x} \in \Omega \,\}$ and $\bar{\mathbf{g}} := \frac{L}{U^2}\mathbf{g}$. The partial differential equations in (6.1) can be written in these dimensionless quantities as follows, where differential operators w.r.t. $\bar{x}_i$ and $\bar{t}$ are denoted with a $\bar{}$ (for example: $\bar{\nabla}$):

$$\begin{aligned} \frac{\rho_i}{\tilde{\rho}_i}\Big(\frac{\partial \bar{\mathbf{u}}}{\partial \bar{t}} + (\bar{\mathbf{u}}\cdot\bar{\nabla})\bar{\mathbf{u}}\Big) &= -\bar{\nabla}\bar{p} + \frac{\rho_i}{\tilde{\rho}_i}\bar{\mathbf{g}} + \overline{\mathrm{div}}\Big(\frac{1}{Re_i}\bar{\mathbf{D}}(\bar{\mathbf{u}})\Big) \\ &= \overline{\mathrm{div}}(\bar{\boldsymbol{\sigma}}) + \frac{\rho_i}{\tilde{\rho}_i}\bar{\mathbf{g}} \ \text{ in } \ \bar{\Omega}_i, \\ \overline{\mathrm{div}}\,\bar{\mathbf{u}} &= 0 \ \text{ in } \ \bar{\Omega}_i, \end{aligned} \tag{6.4}$$

with the dimensionless Reynolds numbers $Re_i = \frac{\tilde{\rho}_i L U}{\mu_i}$, $i = 1,2$, and

$$\bar{\boldsymbol{\sigma}} = -\bar{p}\mathbf{I} + \frac{1}{Re_i}\big(\bar{\nabla}\bar{\mathbf{u}} + \bar{\nabla}\bar{\mathbf{u}}^T\big).$$

Considering this rescaled problem it is tempting to choose $\tilde{\rho}_i = \rho_i$, since this leads to a simplification. In particular one then has a constant 1 in front of the material derivative. However, it is also necessary to rescale the interface conditions in (6.2)-(6.3). The conditions $[\mathbf{u}] = 0$, $V_\Gamma = \mathbf{u}\cdot\mathbf{n}$ transform to

$$[\bar{\mathbf{u}}] = 0, \quad \bar{V}_\Gamma = \bar{\mathbf{u}}\cdot\bar{\mathbf{n}}, \tag{6.5}$$

with $\bar{\mathbf{n}}(\bar{x}) = \mathbf{n}(x)$. The momentum balance condition $[\boldsymbol{\sigma}\mathbf{n}] = -\tau\kappa\mathbf{n}$ takes the form

$$[\tilde{\rho}U^2\bar{\boldsymbol{\sigma}}\bar{\mathbf{n}}] = -\frac{\tau}{L}\bar{\kappa}\bar{\mathbf{n}},$$

with $\bar{\kappa} = \overline{\mathrm{div}}_\Gamma\bar{\mathbf{n}}$, the curvature in transformed variables. To be able to write this momentum balance condition in the usual form $[\bar{\boldsymbol{\sigma}}\bar{\mathbf{n}}] = \alpha\,\bar{\kappa}\bar{\mathbf{n}}$, $\alpha \in \mathbb{R}$, the scaling function $\tilde{\rho}$ has to be taken constant across Γ, and thus $\tilde{\rho}_1 = \tilde{\rho}_2 = \tilde{\rho}$. Therefore, in the transformation to dimensionless variables one normally takes a *constant* density scaling factor (e.g., $\tilde{\rho} = \frac{1}{2}(\rho_1+\rho_2)$) and then the momentum interface condition is given by

$$[\bar{\boldsymbol{\sigma}}\bar{\mathbf{n}}] = -\frac{1}{We}\bar{\kappa}\bar{\mathbf{n}}, \quad We := \frac{\tilde{\rho}U^2 L}{\tau}. \tag{6.6}$$

The dimensionless so-called *Weber number* is a measure for the relative size of inertial and surface tension forces. The model in dimensionless variables is given by (6.4), (6.5), (6.6). Note that similar to (6.1), in (6.4) one has a piecewise constant density $\rho/\tilde{\rho}$ and a piecewise constant viscosity $1/Re_i$. This is an important difference compared to the dimensionless one-phase Navier-Stokes problem in (2.5).

We discuss a weak formulation of the Navier-Stokes equations and the interface conditions in (6.1)-(6.2). We consider the model in physical dimensions since there is no significant advantage if one instead uses the model in dimensionless variables (6.4), (6.5), (6.6).

We use the Sobolev spaces

$$\begin{aligned}
\mathbf{V} &:= H^1(\Omega)^3, \\
\mathbf{V}_0 &:= \{\, \mathbf{v} \in \mathbf{V} : \mathbf{v} = 0 \text{ on } \partial\Omega_D \,\}, \\
\mathbf{V}_D &:= \{\, \mathbf{v} \in \mathbf{V} : \mathbf{v} = \mathbf{u}_D \text{ on } \partial\Omega_D \,\}, \\
Q &:= L^2_0(\Omega) = \left\{ q \in L^2(\Omega) : \int_\Omega q\, dx = 0 \right\},
\end{aligned}$$

and define the bilinear forms

$$\begin{aligned}
m : \mathbf{V} \times \mathbf{V} \to \mathbb{R} : \qquad & m(\mathbf{u}, \mathbf{v}) := \int_\Omega \rho\, \mathbf{u}\mathbf{v}\, dx, \\
a : \mathbf{V} \times \mathbf{V} \to \mathbb{R} : \qquad & a(\mathbf{u}, \mathbf{v}) := \frac{1}{2} \int_\Omega \mu\ \mathrm{tr}\left(\mathbf{D}(\mathbf{u})\mathbf{D}(\mathbf{v})\right) dx, \\
& \qquad\qquad = \frac{1}{2} \int_\Omega \mu \sum_{i,j=1}^{3} \big(\mathbf{D}(\mathbf{u})\big)_{ij} \big(\mathbf{D}(\mathbf{v})\big)_{ij}\, dx \\
b : \mathbf{V} \times Q \to \mathbb{R} : \qquad & b(\mathbf{v}, q) := -\int_\Omega q\ \mathrm{div}\, \mathbf{v}\, dx,
\end{aligned} \tag{6.7}$$

and the trilinear form

$$c : \mathbf{V} \times \mathbf{V} \times \mathbf{V} \to \mathbb{R} : \qquad c(\mathbf{u}; \mathbf{v}, \mathbf{w}) := \int_\Omega \rho(\mathbf{u} \cdot \nabla \mathbf{v})\mathbf{w}\, dx.$$

For the weak formulation of the interface condition $[\boldsymbol{\sigma}\mathbf{n}]_\Gamma = -\tau\kappa\mathbf{n}$ in (6.2) we introduce the linear functional

$$f_\Gamma : \mathbf{V} \to \mathbb{R} : \qquad f_\Gamma(\mathbf{v}) := -\int_\Gamma \tau\kappa\mathbf{n} \cdot \mathbf{v}\, ds. \tag{6.8}$$

If the curvature κ is bounded on Γ we have

$$|f_\Gamma(\mathbf{v})| \leq c\, \|\kappa\|_{L^\infty(\Gamma)} \|\mathbf{v}\|_{L^2(\Gamma)} \leq \tilde{c} \|\mathbf{v}\|_1 \quad \text{for all} \quad \mathbf{v} \in \mathbf{V},$$

where in the last inequality we used a trace theorem on Γ. Hence we get that f_Γ is a *bounded* linear functional on $\mathbf{V}$, i.e., $f_\Gamma \in \mathbf{V}'$.

Remark 6.1.2 We restrict ourselves to the model with a constant surface tension coefficient τ. More general models with an interface momentum balance of the form $[\boldsymbol{\sigma}\mathbf{n}] = \mathrm{div}_\Gamma(\boldsymbol{\sigma}_\Gamma)$ are discussed in Sect. 7.6.1. For such an interface condition the surface tension functional generalizes to $f_\Gamma(\mathbf{v}) = \int_\Gamma \mathrm{div}_\Gamma(\boldsymbol{\sigma}_\Gamma) \cdot \mathbf{v}\, ds$.

A weak formulation of the Navier-Stokes equations and the coupling conditions in (6.2) is as follows:

Find $\mathbf{u}(t) = \mathbf{u}(\cdot,t) \in \mathbf{V}_D$, $p(t) = p(\cdot,t) \in Q$ such that for almost all $t \in [0,T]$

$$m(\frac{\partial \mathbf{u}}{\partial t}, \mathbf{v}) + c(\mathbf{u};\mathbf{u},\mathbf{v}) + a(\mathbf{u},\mathbf{v}) + b(\mathbf{v},p) = (\rho\mathbf{g},\mathbf{v})_{L^2} + f_\Gamma(\mathbf{v}) \quad \text{for all } \mathbf{v} \in \mathbf{V}_0, \tag{6.9}$$

$$b(\mathbf{u},q) = 0 \quad \text{for all } q \in Q, \tag{6.10}$$

and initial condition $\mathbf{u}(0) = \mathbf{u}_0$ in Ω.

The time derivative has to be taken in a suitable weak sense, cf. below. Note that in this model we have the weak formulation of *one* Navier-Stokes equation in *the whole domain* Ω. The *localized force term* f_Γ originates from the first interface coupling condition in (6.2). Also note that in general the bilinear forms $m(\cdot,\cdot)$, $a(\cdot,\cdot)$ and the trilinear form $c(\,\cdot\,;\cdot,\cdot)$ depend on t, due to the fact that we have $\Omega_i = \Omega_i(t)$ and thus the density and viscosity coefficients (which are piecewise constant in Ω_i) are time dependent.

The surface tension functional f_Γ will play an important role in the remainder of this monograph, both in the analysis of the models considered and in the numerical methods that will be treated. This functional has other useful representations, for example those given in Lemma 14.1.2.

Remark 6.1.3 The idea to replace the first interface coupling condition in (6.2) by a localized force term in the momentum equation was introduced in [47]. In the (engineering) literature this is known as the CSF ("Continuum Surface Force") approach. In [47] and in most other papers in which such a localized surface tension force is used, this force at the interface is *approximated* by some *volume* force (hence, *continuum* surface force). We briefly explain the main idea, for details we refer to [47, 64]. Take $x \in \Gamma$ and let $U \subset \Omega$ be a (small) neighborhood of x. Define $\gamma := \Gamma \cap U$. Let $\mathbf{g} : \gamma \to \mathbb{R}^3$ be a smooth vector function ("force at the interface"), for example $\mathbf{g}(x) = \tau\kappa(x)\mathbf{n}_\Gamma(x)$, and $\tilde{\mathbf{g}} : U \to \mathbb{R}^3$ a suitable smooth extension of $\mathbf{g}$. Furthermore, let d_Γ be the signed distance function: $d_\Gamma(x) = \operatorname{dist}(\Gamma,x)$ for $x \in U \cap \Omega_2$, $d_\Gamma(x) = -\operatorname{dist}(\Gamma,x)$ for $x \in U \cap \Omega_1$. For the "force acting on γ" we have:

$$\int_\gamma \mathbf{g}(s)\,ds = \lim_{\epsilon \downarrow 0} \int_U \delta_\epsilon(d_\Gamma(x))\tilde{\mathbf{g}}(x)\,dx,$$

with a one-dimensional smoothed Dirac delta function δ_ϵ, i.e. for $\xi > 0$ we have $\lim_{\epsilon\downarrow 0} \int_{-\xi}^{\xi} \delta_\epsilon(s)h(s)\,ds = h(0)$ for smooth functions h. Then in the spirit of the derivation of the Navier-Stokes equations in the *strong* formulation (as in (6.1)), based on conservation laws and forces on "arbitrary" neighborhoods

U, the volume force at $x \in \gamma$ is taken as $\delta_\epsilon(d_\Gamma(x))\tilde{\mathbf{g}}(x)$. In this approach one has freedom in choosing the extension $\tilde{\mathbf{g}}$ of $\mathbf{g}$ and in choosing the regularization of the Dirac delta function. It is shown in [241, 104] that the latter issue is nontrivial: seemingly natural regularizations, which work well in 1D, may lead to large errors in higher dimensions. In [64] an extension $\tilde{\mathbf{g}}$ of $\mathbf{g}$ based on the level set method is introduced, cf. Remark 6.2.4 below. All Dirac delta function regularizations lead to functions δ_ϵ with unbounded derivatives for $\epsilon \downarrow 0$, and thus such a regularization requires a high mesh resolution close to Γ.

In the *weak* formulation (6.9) this regularization (and extension) issue does not occur. The localized surface tension force is represented as a well-defined functional $f_\Gamma \in \mathbf{V}'$ (provided the curvature is bounded). In this sense the weak formulation is better suited for describing surface tension forces than the strong formulation.

The following lemma indicates that (6.9)-(6.10) is a correct weak formulation for the Navier-Stokes problems in the two subdomains with coupling conditions as in (6.2).

Lemma 6.1.4 *Assume that* (6.1)-(6.2) *has a solution* $(\mathbf{u}, p)$ *with* $\mathbf{u}_{|\partial\Omega_D} = \mathbf{u}_D$, $\int_\Omega p\,dx = 0$, $\Gamma(t)$ *is sufficiently smooth and* $\mathbf{u}$, p *are sufficiently smooth:*

$$\mathbf{u} \in C^1\big(0,T;C^2(\overline{\Omega}_i)^3\big), \quad p \in C\big(0,T;C^1(\overline{\Omega}_i)\big), \quad i = 1,2.$$

Then $(\mathbf{u}, p)$ *solves* (6.9)-(6.10).

Proof. Due to the smoothness assumption on $\mathbf{u}$ in the subdomains Ω_i and $[\mathbf{u}]_\Gamma = 0$ we have $\mathbf{u} \in \mathbf{V}_D$. Furthermore, $p(\cdot,t) \in Q$ holds. From $\operatorname{div}\mathbf{u} = 0$ it follows that (6.10) holds. We now consider the variational equation in (6.9):

$$\begin{aligned} &\int_\Omega \rho\frac{\partial \mathbf{u}}{\partial t}\mathbf{v}\,dx + \int_\Omega \rho(\mathbf{u}\cdot\nabla\mathbf{u})\mathbf{v}\,dx + \frac{1}{2}\int_\Omega \mu\,\mathrm{tr}\left(\mathbf{D}(\mathbf{u})\mathbf{D}(\mathbf{v})\right)dx \\ &-\int_\Omega p\,\operatorname{div}\mathbf{v}\,dx = \int_\Omega \rho\mathbf{g}\cdot\mathbf{v}\,dx - \int_\Gamma \tau\kappa\mathbf{n}\cdot\mathbf{v}\,ds. \end{aligned} \tag{6.11}$$

We need the following partial integration rules, which hold for functions $q : U \to \mathbb{R}$ and $\mathbf{w}, \mathbf{v} : U \to \mathbb{R}^3$ that are sufficiently smooth on $U \subset \Omega$:

$$\begin{aligned} -\int_U q\,\operatorname{div}\mathbf{w}\,dx &= \int_U \nabla q\cdot\mathbf{w}\,dx - \int_{\partial U} q\,\mathbf{w}\cdot\mathbf{n}\,ds, \\ \frac{1}{2}\int_U \mathrm{tr}\left(\mathbf{D}(\mathbf{w})\mathbf{D}(\mathbf{v})\right)dx &= -\int_U \big(\operatorname{div}\mathbf{D}(\mathbf{w})\big)\cdot\mathbf{v}\,dx + \int_{\partial U}\big(\mathbf{D}(\mathbf{w})\,\mathbf{n}\big)\cdot\mathbf{v}\,ds. \end{aligned}$$

In the equation in (6.11) we take a test function $\mathbf{v} \in C_0^\infty(\Omega)^3$, split the integrals over Ω into integrals over Ω_i, $i = 1,2$, and use the partial integration rules (with $U = \Omega_i$). Thus (6.11) can be rewritten as

$$\begin{aligned}&\sum_{i=1}^{2}\int_{\Omega_i}\Big(\rho_i\big(\frac{\partial \mathbf{u}}{\partial t}+\mathbf{u}\cdot\nabla\mathbf{u}\big)-\operatorname{div}\big(\mu_i\mathbf{D}(\mathbf{u})\big)+\nabla p\Big)\cdot\mathbf{v}\,dx\\&=\sum_{i=1}^{2}\int_{\Omega_i}\rho_i\mathbf{g}\cdot\mathbf{v}\,dx-\int_{\Gamma}[\mu\mathbf{D}(\mathbf{u})\mathbf{n}-p\mathbf{n}]_{\Gamma}\cdot\mathbf{v}\,ds-\int_{\Gamma}\tau\kappa\mathbf{n}\cdot\mathbf{v}\,ds.\end{aligned}\tag{6.12}$$

Due to the interface condition $[\boldsymbol{\sigma}\mathbf{n}]_{\Gamma}=-\tau\kappa\mathbf{n}$ the last two terms on the right-hand side cancel. From (6.1) it then follows that (6.12) and thus (6.11) holds. Since $C_0^{\infty}(\Omega)^3$ is dense in $\mathbf{V}_0$ we conclude that (6.9) is satisfied. □

Remark 6.1.5 From the proof above one can infer why we use the bilinear form $a(\cdot,\cdot)$ as in (6.7) and not the simpler one $\hat{a}(\mathbf{u},\mathbf{v})=\int_{\Omega}\mu\nabla\mathbf{u}\cdot\nabla\mathbf{v}\,dx$, which is used in the weak formulation of the one-phase Navier-Stokes equations. Partial integration on the subdomains applied to this bilinear form results in

$$\sum_{i=1}^{2}\int_{\Omega_i}\mu_i\nabla\mathbf{u}\cdot\nabla\mathbf{v}\,dx=-\sum_{i=1}^{2}\int_{\Omega_i}\mu_i\Delta\mathbf{u}\cdot\mathbf{v}\,dx+\int_{\Gamma}[\mu(\nabla\mathbf{u})^T\mathbf{n}]_{\Gamma}\cdot\mathbf{v}\,ds,$$

and thus in (6.12) instead of the term $\int_{\Gamma}[\mu\mathbf{D}(\mathbf{u})\mathbf{n}-p\mathbf{n}]_{\Gamma}\cdot\mathbf{v}\,ds=\int_{\Gamma}[\boldsymbol{\sigma}\mathbf{n}]_{\Gamma}\cdot\mathbf{v}\,ds$ one would obtain $\int_{\Gamma}[\mu(\nabla\mathbf{u})^T\mathbf{n}-p\mathbf{n}]_{\Gamma}\cdot\mathbf{v}\,ds$, which is *not* consistent with the interface condition $[\boldsymbol{\sigma}\mathbf{n}]_{\Gamma}=-\tau\kappa\mathbf{n}$ in (6.2).

For the above variational Navier-Stokes problem with the surface tension functional f_{Γ} one can derive the following energy estimate.

Lemma 6.1.6 *Consider the variational problem* (6.9)-(6.10)*, with* ρ *constant, say* $\rho=1$*, with* $\mathbf{u}_D=0$ *(homogeneous Dirichlet boundary condition) and* $\mathbf{g}=0$ *(no external forces). Assume that for* $0\leq t\leq T$ *the interface* $\Gamma(t)$ *is a sufficiently smooth compact manifold. Let* $(\mathbf{u},p)$ *be a solution of* (6.9)-(6.10) *with* $\mathbf{u}\in L^2(0,T;\mathbf{V}_0)$*. Then the following holds:*

$$\begin{aligned}&\frac{1}{2}\|\mathbf{u}(T)\|_{L^2}^2+\int_0^T a(\mathbf{u}(t),\mathbf{u}(t))\,dt+\tau\,\mathrm{meas}_2\big(\Gamma(T)\big)\\&=\frac{1}{2}\|\mathbf{u}_0\|_{L^2}^2+\tau\,\mathrm{meas}_2\big(\Gamma(0)\big).\end{aligned}\tag{6.13}$$

Proof. We take $\mathbf{v}=\mathbf{u}$ in (6.9). Using partial integration, $\rho=1$, $\mathbf{u}_{|\partial\Omega}=0$ we get $c(\mathbf{u};\mathbf{u},\mathbf{u})=0$. Furthermore, due to $\operatorname{div}\mathbf{u}=0$ we have $b(\mathbf{u},p)=0$. Thus we obtain

$$\int_{\Omega}\frac{\partial\mathbf{u}}{\partial t}\mathbf{u}\,dx+a(\mathbf{u},\mathbf{u})=-\tau\int_{\Gamma}\kappa\,\mathbf{n}\cdot\mathbf{u}\,ds.$$

Integration over $t\in[0,T]$ and applying partial integration in t results in

$$\frac{1}{2}\|\mathbf{u}(T)\|_{L^2}^2+\int_0^T a(\mathbf{u}(t),\mathbf{u}(t))\,dt=\frac{1}{2}\|\mathbf{u}_0\|_{L^2}^2-\tau\int_0^T\int_{\Gamma}\kappa\,\mathbf{n}\cdot\mathbf{u}\,ds\,dt.\tag{6.14}$$

From (14.15) and Lemma 14.2.2 we obtain

$$\int_{\Gamma(t)} \kappa\, \mathbf{n}\cdot\mathbf{u}\, ds = \int_{\Gamma(t)} \operatorname{div}_\Gamma \mathbf{u}\, ds = \frac{d}{dt}\int_{\Gamma(t)} 1\, ds.$$

Using this yields

$$-\tau \int_0^T \int_\Gamma \kappa\, \mathbf{n}\cdot\mathbf{u}\, ds dt. = -\tau\big(\operatorname{meas}_2 \Gamma(T) - \operatorname{meas}_2 \Gamma(0)\big),$$

which, combined with (6.14), completes the proof. □

Remark 6.1.7 The result in this lemma has a physical interpretation: The kinetic energy difference $\frac{1}{2}\|\mathbf{u}(T)\|^2_{L^2} - \frac{1}{2}\|\mathbf{u}(0)\|^2_{L^2}$ is balanced by the sum of kinetic energy dissipation $\int_0^T a(\mathbf{u}(t),\mathbf{u}(t))\, dt$ and the change in surface tension energy $\tau\big(\operatorname{meas}_2 \Gamma(T) - \operatorname{meas}_2 \Gamma(0)\big)$.

The question of well-posedness of the variational problem (6.9)-(6.10) combined with the immiscibility condition $V_\Gamma = \mathbf{u}\cdot\mathbf{n}$ is a very difficult one. Below we briefly address some known results.

First we consider a strongly simplified case, namely a Stokes problem with a *stationary* interface Γ. In that case the term with the trilinear form $c(\cdot;\cdot,\cdot)$ vanishes and the bilinear forms $m(\cdot,\cdot)$, $a(\cdot,\cdot)$ do *not* depend on t. We assume $\partial\Omega_D = \partial\Omega$ and $\mathbf{u}_D = 0$, i.e., a problem with homogeneous Dirichlet boundary conditions on $\partial\Omega$. We introduce the weighted L^2-scalar product $(\mathbf{v},\mathbf{w})_{L^2,\rho} := (\rho\mathbf{v},\mathbf{w})_{L^2}$. In this simplified case the variational problem (6.9)-(6.10) reduces to: determine $\mathbf{u}(t) = \mathbf{u}(\cdot,t) \in \mathbf{V}_{\mathrm{div}} = \{\, \mathbf{v}\in\mathbf{V}_0 : \operatorname{div}\mathbf{v} = 0 \,\}$ with $\mathbf{u}(0) = \mathbf{u}_0$ and

$$(\frac{\partial \mathbf{u}}{\partial t}, \mathbf{v})_{L^2,\rho} + a(\mathbf{u}(t),\mathbf{v}) = (\mathbf{g},\mathbf{v})_{L^2,\rho} + f_\Gamma(\mathbf{v}) \quad \text{for all } \mathbf{v}\in\mathbf{V}_{\mathrm{div}}, \tag{6.15}$$

for almost all $t\in[0,T]$. This variational problem is very similar to the *one-phase* Stokes problem in (2.33). Compared to (2.33), in (6.15) we have a slightly different bilinear form $a(\cdot,\cdot)$ in which a weighting with the piecewise constant viscosity μ is used, a modified L^2-scalar product (namely $(\cdot,\cdot)_{L^2,\rho}$) and an additional functional f_Γ on the right-hand side. The analysis of well-posedness of the one-phase variational Stokes problem in (2.33), cf. Theorem 2.2.10, can also be applied to the two-phase variational Stokes problem in (6.15) (notation as in Sect. 2.2.3):

Theorem 6.1.8 *Assume* $\mathbf{g}\in L^2(0,T;\mathbf{V}'_{\mathrm{div}})$, $\|\kappa\|_{L^\infty(\Gamma)} < \infty$ *and* $\mathbf{u}_0\in\mathbf{H}_{\mathrm{div}}$. *Then the variational problem* (6.15) *is well-posed.*

Proof. Use the same arguments as in the proof of Theorem 2.2.10. Note that the norms induced by the standard L^2-scalar product and by $(\cdot,\cdot)_{L^2,\rho}$ are equivalent. Furthermore, $\|\kappa\|_{L^\infty(\Gamma)} < \infty$ implies that $f_\Gamma \in \mathbf{V}' \subset \mathbf{V}'_{\mathrm{div}}$. □

For the above result to hold, the weak derivative $\mathbf{u}' = \frac{\partial \mathbf{u}}{\partial t}$ in (6.15) is defined as explained in Sect. 2.2.3. For the unique solution $\mathbf{u}$ we have

$$\mathbf{u} \in W^1(0,T;\mathbf{V}_{\mathrm{div}}) = \left\{ \mathbf{v} \in L^2(0,T;\mathbf{V}_{\mathrm{div}}) : \mathbf{v}' \in L^2(0,T;\mathbf{V}'_{\mathrm{div}}) \right\}. \quad (6.16)$$

Well-posedness results for the general Navier-Stokes case in (6.9)-(6.10) are known in the literature, however, only for special cases. In [84] well-posedness of a Navier-Stokes problem as in (6.9)-(6.10) combined with the interface condition $V_\Gamma = \mathbf{u} \cdot \mathbf{n}$ is analyzed. Instead of a bounded domain Ω, the case $\Omega = \mathbb{R}^3$ is considered (with "boundary" condition $\lim_{|x|\to\infty} \mathbf{u}(x,t) = 0$). The initial interface $\Gamma(0)$ is assumed to be a closed manifold. The main result in [84] can be summarized as follows. If the data $\Gamma(0)$, $\mathbf{u}_0$ and $\mathbf{g}$ are sufficiently smooth then for $t \in [0,T]$, *with T sufficiently small*, the two-phase Navier-Stokes problem in a weak formulation similar to (6.9)-(6.10) and with the interface condition $V_\Gamma = \mathbf{u}\cdot\mathbf{n}$ has a unique solution. The analysis is in Sobolev spaces similar to the one in (6.16). The analysis is quite technical, the main underlying idea, however, is rather easy to explain. We outline this idea. For $\xi \in \Omega$ and a given velocity field $\mathbf{u}(x,t)$ we define the characteristic $X_\xi(\tau)$:

$$\begin{cases} \frac{d}{d\tau} X_\xi(\tau) = \mathbf{u}(X_\xi(\tau),\tau), \quad \tau \geq 0, \\ X_\xi(0) = \xi. \end{cases} \quad (6.17)$$

$X_\xi(\tau)$ can be interpreted as the path of an infinitely small particle with initial position ξ. For $\mathbf{u}(x,t)$ sufficiently smooth (Lipschitz with respect to x) this system of ODEs has a unique solution. The smoothness of X_ξ depends on the smoothness of $\mathbf{u}$. To each $(x,t) \in \Omega \times [0,T]$, with T sufficiently small, there corresponds a unique $\xi \in \Omega$ such that $x = X_\xi(t)$. Physically this means that starting from (x,t) one follows the flow field backwards in time resulting in $(\xi,0)$:

$$x = \xi + \int_0^t \mathbf{u}(X_\xi(\tau),\tau)\, d\tau. \quad (6.18)$$

This defines the coordinate transformation $(x,t) = (X_\xi(t),t) \to (\xi,t)$ from *Eulerian coordinates* (x,t) to *Lagrangian coordinates* (ξ,t). The problem (6.1)-(6.3) can be transformed in Lagrangian coordinates (ξ,t) resulting in an non-stationary *Stokes* type of problem with a *stationary* interface $\Gamma(0)$. For this transformed problem well-posedness (in suitable Sobolev spaces) is shown in [85]. The length T of the time interval should be such that the coordinate transformation $(x,t) \to (\xi,t)$ is well-defined and the Jacobian of this transformation is bounded (in a suitable norm). This depends on norms of the data $\mathbf{g}$, $\mathbf{u}_0$ and the curvature of $\Gamma(0)$.

In [232] a well-posedness result for the Navier-Stokes problem on *arbitrary* time intervals $[0,T]$ is proved, using the same Euler $\to$ Lagrange coordinate transformation. In that paper the case with a bounded domain Ω is treated. We summarize its main result. For arbitrary $T > 0$ the Navier-Stokes problem in a weak formulation similar to (6.9)-(6.10) and with the interface condition $V_\Gamma = \mathbf{u} \cdot \mathbf{n}$ has a unique solution (in suitable Sobolev spaces) if the data $\mathbf{g}$, $\mathbf{u}_0$ are sufficiently small and the initial interface $\Gamma(0)$ is sufficiently close to a sphere.

The analyses addressed above are applicable only in cases with *sufficiently smooth data* (initial and boundary data, source terms and initial interface). They do not cover situations in which the smoothness of the interface deteriorates, for example in a problem with colliding droplets. In such cases it may well happen that interface quantities like the curvature κ or the normal velocity V_Γ are not well-defined in the strong sense and suitable weak alternatives must be considered. Only few theoretical results that deal with well-posedness issues for such less regular problems are known in the literature. The analyses for less regular cases are based on *alternative characterizations of the interface*. These interface representations induce corresponding numerical techniques for the simulation of two-phase flow problems. In Sect. 6.2 we treat the most important approaches for interface representation. In the remainder of this monograph we then restrict ourselves to one of these, namely the level set representation. A suitable weak formulation of the level set interface representation combined with the weak formulation of the Navier-Stokes problem in (6.9)-(6.10) leads to the weak model that we consider for our numerical simulations. This model is presented in Sect. 6.3.

6.2 Interface representation

In this section we discuss the most important approaches for characterizing the interface. These techniques play a role both in the theoretical analysis of well-posedness and in numerical methods for simulating the two-phase flow problem.

6.2.1 Explicit interface representation: interface tracking

If the interface is sufficiently smooth then its curvature and other interface quantities like V_Γ, $\mathbf{n}_\Gamma$ are well-defined in the classical sense. For a velocity field $\mathbf{u} \in \mathbf{V}$ and a smooth interface $\Gamma(t)$ the trace $\mathbf{u}_{|\Gamma}$ and the immiscibility condition $V_\Gamma = \mathbf{u}\cdot\mathbf{n}$ in (6.3) are well-defined. The evolution of the interface can be described by using the Lagrangian coordinates. Take a (virtual) particle $\mathbf{X}$ on the interface at $t = t_0$ with Eulerian coordinates $\xi \in \Gamma(t_0)$. For $t \geq t_0$, let $X_\xi(t)$ be the Eulerian coordinates of this particle. The particles on the interface are transported by the flow field, hence for $X_\xi(t)$ we have the ODE system (6.17) and the interface $\Gamma(t)$ can be characterized as follows, cf. (6.18):

$$x \in \Gamma(t) \;\Leftrightarrow\; x = \xi + \int_{t_0}^{t} \mathbf{u}(X_\xi(\tau),\tau)\,d\tau, \quad \xi \in \Gamma(t_0), \quad t \geq t_0. \tag{6.19}$$

This Lagrangian point of view is essential for the analyses of well-posedness for two-phase flow problems with sufficient smoothness, as briefly addressed above in Sect. 6.1 (cf. [84, 232]). The interface representation in (6.19) also forms the basis for a class of numerical methods, known as *interface tracking*.

In these methods a collection of markers is put on a given interface $\Gamma(t_0)$ and then transported (numerically) by the flow field $\mathbf{u}$ to obtain the markers on the interface $\Gamma(t_0 + \Delta t)$. The collection of markers on $\Gamma(t_0)$ could be the set of vertices of a triangulation of $\Gamma(t_0)$. In such methods one usually has to redistribute the markers after a certain number of time steps. In general it is rather difficult to treat topology changes (e.g. collision of droplets) in a systematic and accurate way. Usually in interface tracking methods for two phase flows the Lagrangian approach is used only for the propagation of the interface markers. The Navier-Stokes equations are solved on a fixed grid (i.e., an Eulerian approach), cf. Fig. 6.1.

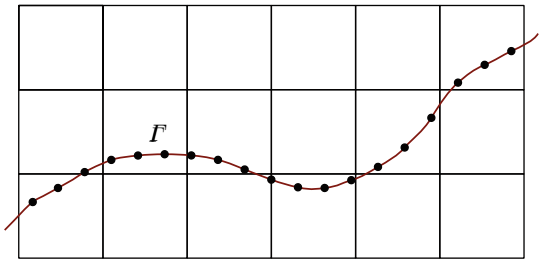


Fig. 6.1. Front tracking on an Eulerian grid for the flow problem. The interface Γ is represented by connected marker points.

Thus one needs operators for the transfer of information between the (moving) interface and the underlying fixed grid. Such front tracking methods have been successfully applied in the simulation of two-phase flows. An overview and detailed treatment of this technique can be found in [246, 243, 182]. Hybrid variants of this technique have been developed, for example so-called arbitrary Lagrangian-Eulerian (ALE) methods in which the interface (or surface) is resolved by a mesh and this mesh is moved with the flow velocity (Lagrangian interface tracking). In the interior flow domain a moving mesh is used with a mesh velocity that generally differs from the flow velocity and is taken such that strong mesh distortions are avoided. Such a mesh velocity can be obtained, for example, as the solution of a linear elasticity equation with a prescribed displacement on the boundary. Often the Navier-Stokes equations are then formulated using a *relative* velocity, which is the difference between the flow and the mesh velocity. Such ALE methods are very popular for the simulation of fluid structure interaction (FSI) problems, in which typically the movement of the boundary of the fluid domain is relatively small. ALE techniques have also been applied in the numerical simulation of one-phase flows with a free surface or of two-phase flows, e.g. [23, 28, 29, 117, 118, 185]. The Lagrangian interface tracking method can also be combined with a pure Lagrangian approach for the Navier-Stokes equations, based on an interior mesh movement that is based on the flow velocity field, cf. for example [152, 145].

6.2.2 Volume tracking based on the characteristic function

Let $\chi_1(\cdot,t) : \Omega \to \mathbb{R}$ be the characteristic function corresponding to the subdomain $\Omega_1(t)$, $t \geq 0$, i.e., $\chi_1(x,t) = 1$ for $x \in \Omega_1(t)$, $\chi_1(x,t) = 0$ otherwise. In this section we treat methods based on the simple observation $\Gamma(t) = \partial\Omega_1(t) = \partial\mathrm{supp}(\chi_1(\cdot,t))$. The function χ_1 characterizes the subdomain Ω_1 and we track this function (and thus the boundary of its support) to follow the evolution of the interface. We will derive a transport equation for χ_1 induced by the immiscibility condition $V_\Gamma = \mathbf{u}\cdot\mathbf{n}$. For this we need some additional notation. We introduce the space-time subdomain and interface:

$$\begin{aligned}
\Omega_T &:= \Omega \times [0,T] \subset \mathbb{R}^4,\\
\Omega_{i,T} &:= \left\{ (x,t) \in \mathbb{R}^4 : x \in \Omega_i(t),\ 0 \leq t \leq T \right\},\ i = 1,2,\\
\Gamma_T &:= \left\{ (x,t) \in \mathbb{R}^4 : x \in \Gamma(t),\ 0 \leq t \leq T \right\}.
\end{aligned}$$

The outward normal (not necessarily normalized) on $\partial\Omega_{1,T} \cap \Gamma_T$ is given by

$$\hat{\mathbf{n}} = \hat{\mathbf{n}}_\Gamma(x,t) = \begin{pmatrix} \mathbf{n}_\Gamma(x) \\ -V_\Gamma(x) \end{pmatrix} \in \mathbb{R}^4, \quad (x,t) \in \Gamma_T.$$

The immiscibility condition $V_\Gamma = \mathbf{u}\cdot\mathbf{n}$ on Γ can be written as:

$$\hat{\mathbf{n}} \cdot \begin{pmatrix} \mathbf{u} \\ 1 \end{pmatrix} = 0 \quad \text{on} \quad \Gamma_T. \tag{6.20}$$

Lemma 6.2.1 *Let $\chi_1(\cdot,t)$ be the characteristic function corresponding to $\Omega_1(t)$ and $\mathbf{u} \in L^2(0,T;\mathbf{V})$ with $\operatorname{div}\mathbf{u} = 0$. The condition in* (6.20) *holds iff*

$$\int_{\Omega_T} \chi_1 \big(\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla_x\phi \big)\, dx\, dt = 0 \quad \textit{for all} \quad \phi \in C_0^\infty(\Omega_T), \tag{6.21}$$

i.e., in the sense of distributional derivatives,

$$\frac{\partial\chi_1}{\partial t} + \mathbf{u}\cdot\nabla_x\chi_1 = 0 \quad \textit{in} \quad D'(\Omega_T) := C_0^\infty(\Omega_T)'. \tag{6.22}$$

Proof. Using $\operatorname{div}\mathbf{u} = 0$ and the definition of distributional derivatives we have

$$\begin{aligned}
&\int_{\Omega_T} \chi_1 \big(\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla\phi \big)\, dx\, dt = 0 \quad \text{for all} \quad \phi \in C_0^\infty(\Omega_T)\\
\text{iff} \quad &\frac{\partial\chi_1}{\partial t} + \operatorname{div}(\mathbf{u}\chi_1) = 0 \quad \text{in} \quad D'(\Omega_T),\\
\text{iff} \quad &\frac{\partial\chi_1}{\partial t} + \mathbf{u}\cdot\nabla_x\chi_1 = 0 \quad \text{in} \quad D'(\Omega_T),
\end{aligned}$$

thus the equivalence between (6.21) and (6.22) holds. For $\mathbf{u} \in L^2(0,T;\mathbf{V})$ its trace on Γ_T, denoted by $\mathbf{u}_{|\Gamma_T}$ is well-defined. The boundary of $\Omega_{1,T}$ can be partitioned as $\partial\Omega_{1,T} = (\partial\Omega_{1,T} \cap \partial\Omega_T) \cup (\partial\Omega_{1,T} \cap \Gamma_T)$. For $\phi \in C_0^\infty(\Omega_T)$ we

have $\phi = 0$ on $\partial\Omega_{1,T} \cap \partial\Omega_T$. Using partial integration and $\chi_1 = 1$ on $\Omega_{1,T}$, $\chi_1 = 0$ on $\Omega_T \setminus \Omega_{1,T}$ we obtain

$$\int_{\Omega_T} \chi_1 \big(\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla_x\phi\big)\, dx\, dt = \int_{\Omega_{1,T}} \frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla_x\phi\, dx\, dt$$
$$= \int_{\Omega_{1,T}} \begin{pmatrix}\mathbf{u}\\ 1\end{pmatrix}\cdot\nabla_{x,t}\phi\, dx\, dt = \int_{\Gamma_T} \begin{pmatrix}\mathbf{u}_{|\Gamma_T}\\ 1\end{pmatrix}\cdot\hat{\mathbf{n}}\,\phi\, dx\, dt.$$

In the last equality we used $\operatorname{div}\mathbf{u} = 0$. Since $\phi \in C_0^\infty(\Omega_T)$ is arbitrary it follows that (6.21) holds if and only if $\begin{pmatrix}\mathbf{u}_{|\Gamma_T}\\ 1\end{pmatrix}\cdot\hat{\mathbf{n}} = 0$ holds (in $L^2(\Gamma_T)$ sense). □

From this lemma it follows that the *immiscibility condition is satisfied if we solve a (weak) transport equation for the characteristic function* χ_1. The equivalence in this lemma holds in cases where the quantities that occur in the immiscibility condition (6.20) are well-defined. If this is not the case (as for example in a colliding droplet problem) then the result of this lemma offers a possibility to generalize the immiscibility condition by considering a suitable weak transport equation for the characteristic function of the subdomains. This idea is the basis of the analysis of well-posedness presented in [81] (for a two-phase Stokes problem) and [188] (for a two-phase Navier-Stokes problem).
If the velocity field $\mathbf{u}$ is *sufficiently smooth*, e.g. continuous in t and Lipschitz continuous w.r.t. x, then a strong formulation of the transport equation in the Lagrangian form

$$\dot{\chi}_1 = \frac{d}{dt}\chi_1(X_\xi(t), t) = 0,$$

with $\chi_1(X_\xi(0), 0) = 1$ if $\xi \in \Omega_1(0)$ and zero otherwise, is well-defined and has a unique solution. For general flow problems, however, one wants to relax the smoothness assumption on $\mathbf{u}$ and then for the transport equation weaker solution concepts are needed. One such a concept, namely of so-called *renormalized solutions of transport equations*, is introduced in the fundamental paper [89]. Using this, the following result can be proved (Proposition 3.3. from [188]).

Proposition 6.2.2 *Take* $\mathbf{u} \in L^2(0,\infty;\mathbf{V})$ *with* $\operatorname{div}\mathbf{u} = 0$ *and* $\mu_0 \in L^\infty(\Omega)$. *Then there is a unique weak solution* $\mu \in L^\infty(\Omega_T)$ *in the following sense:*

$$\int_0^\infty \int_\Omega \mu\big(\frac{\partial\phi}{\partial t} + \mathbf{u}\cdot\nabla_x\phi\big)\, dx\, dt = \int_\Omega \mu_0\phi(x,0)\, dx \quad \forall\ \phi \in C_0^\infty(\mathbb{R}^4). \quad (6.23)$$

Moreover, if μ_0 *is piecewise constant, i.e.,* $\mu_0 \in \{c_1, \dots c_M\}$ *a.e., with constants* c_i, *then* $\mu \in \{c_1, \dots c_M\}$ *a.e..*

Remark 6.2.3 The concept of renormalized solutions allows unique weak solutions of (6.23) even for velocity fields $\mathbf{u}$ with less regularity than $\mathbf{u} \in$

$L^2(0,\infty;\mathbf{V})$. Starting with the paper [89] there have appeared a lot of studies on well-posedness of the weak formulation (6.23). In [89] existence and uniqueness of a weak (renormalized) solution is proved for velocity fields $\mathbf{u} \in L^1(0,\infty;H^1_p(\mathbb{R}^d)^d)$. Results with even less smooth velocity fields have been derived. For example, in [12] well-posedness for velocity fields from the class of functions of bounded variation (BV) is proved. For an overview and further references we refer to [76].

A weak formulation of a transport equation as in Proposition 6.2.2 can be combined with a standard weak formulation of a two-phase Stokes problem as follows. We take an initial velocity field $\mathbf{u}_0 \in \mathbf{V}_0$ (i.e., homogeneous Dirichlet boundary conditions on $\partial\Omega$) with $\operatorname{div}\mathbf{u}_0 = 0$. Let $\mu_0 \in \{\mu_1,\mu_2\}$ be the piecewise constant viscosity in the two initial subdomains: $\mu_0(x) = \mu_i > 0$ for $x \in \Omega_i(0)$, $i = 1,2$. In [81] it is proved that there exists *at least one solution* $(\mathbf{u},p,\mu)$ with $\mathbf{u} \in L^\infty(0,\infty;\mathbf{V}_0)$, $\mathbf{u}(\cdot,0) = \mathbf{u}_0$, $p \in L^2(0,\infty;Q)$, $\mu \in L^\infty(Q_T)$, $\mu(\cdot,0) = \mu_0$ and $\mu \in \{\mu_1,\mu_2\}$ a.e. such that

$$\begin{aligned}
&\frac{1}{2}\int_\Omega \mu \operatorname{tr}\big(\mathbf{D}(\mathbf{u})\mathbf{D}(\mathbf{v})\big)\,dx + b(\mathbf{v},p) = 0 \quad \text{for all } \ \mathbf{v} \in \mathbf{V}_0, \quad t \geq 0,\\
&b(\mathbf{u},q) = 0 \quad \text{for all } \ q \in Q,\ t \geq 0,\\
&\frac{\partial \mu}{\partial t} + \mathbf{u}\cdot\nabla\mu = 0 \quad \text{in the weak sense as in (6.23).}
\end{aligned} \tag{6.24}$$

Thus we have *existence of a weak solution of a two-phase flow problem*. We briefly address some issues related to this result. In [188] a similar weak formulation of a Navier-Stokes two-phase problem is considered and an existence result is proved. The transport equation for the viscosity μ "replaces" the immiscibility condition, cf. Lemma 6.2.1. The analysis only yields existence of a weak solution; uniqueness is still an open problem. This concept of weak solutions allows singularities of the interface (e.g. collision of droplets) and yields existence global in time for "general" initial data. If we define the sets $\Omega_i(t) := \{\, x \in \Omega : \mu(t) = \mu_i \,\}$, $i = 1,2$, then, due to $\mu(\cdot,t) \in \{\mu_1,\mu_2\}$ a.e., we have $\overline{\Omega_1(t)} \cup \overline{\Omega_2(t)} = \overline{\Omega}$. It is, however, in general not clear what the "interface" should be. If we take $\Gamma(t) := \partial\Omega_1(t)$, then $\Gamma(t)$ can have a strictly positive Lebesgue measure. This effect is called "interface flattening" (or interface thickening). The fact that the interface can be "rough" and/or "flat" may be related to the fact that in the weak formulation above we do *not* take surface tension into account (which has a smoothing effect). It is, however, not known whether the analysis can be extended to the case with surface tension. An extensive treatment of several topics related to weak (or "generalized") solutions of two-phase flows with incompressible immiscible fluids which allow singular interfaces is given in [1, 2]. In particular it is remarked in these papers that if surface tension is taken into account, the existence of weak solutions (in the sense as explained above) is still an open problem. In [2] an even weaker concept of so-called measure-valued varifold solutions is introduced. Within that framework existence of a solution can be shown to hold for a suitable

weak formulation of a two-phase flow problem which allows for singularities of the interface and takes surface tension into account.

The analysis of well-posedness addressed above relies on a weak formulation of the transport equation for the viscosity μ, cf. (6.23). Since μ is piecewise constant one can equivalently consider a transport equation for the characteristic function χ_1 corresponding to the subdomain Ω_1. There is an important class of numerical methods in which the treatment of the interface is based on a weak formulation of the transport equation

$$\frac{\partial \chi_1}{\partial t} + \mathbf{u} \cdot \nabla \chi_1 = 0. \tag{6.25}$$

This is the class of *VOF-methods* (Volume of Fluid), which we now introduce. The original idea of this approach goes back to [187]. Note that the equation in (6.25) is not well-defined in the classical sense, since χ_1 is discontinuous across the interface Γ. Instead of using a weak formulation of (6.25) based on distributional derivatives one can also (formally) eliminate the gradient operator by integrating this transport equation. Take an arbitrary (small, connected) fluid volume $W \subset \Omega$. Integrating over W and formally applying partial integration results in

$$\frac{\partial}{\partial t} \int_W \chi_1 \, dx + \int_{\partial W} \chi_1 \mathbf{u} \cdot \mathbf{n} \, ds = 0. \tag{6.26}$$

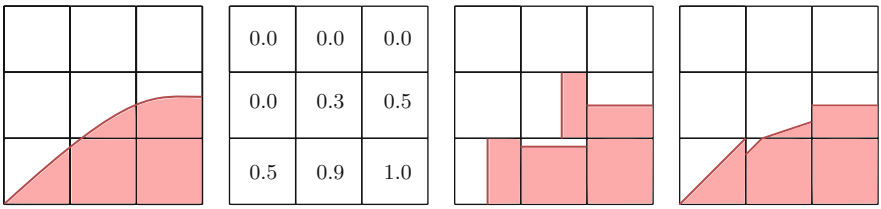
Here $\mathbf{n}$ denotes the outward unit normal on ∂W. This equation can be seen as a weak formulation of (6.25) and has a clear physical interpretation: it describes *volume conservation*. The change of volume of fluid 1 (i.e. the one in Ω_1) contained in W equals the volume flux (induced by the velocity field $\mathbf{u}$) across the boundary ∂W. Note that for an incompressible fluid conservation of volume is equivalent to mass conservation. *In VOF-methods one constructs approximations of the characteristic function χ_1 based on discretization of the conservation law* (6.26). We explain the main idea for a simple 2D case, namely with $\Omega = (0,1)^2$. Assume that Ω is partitioned in square cells $W_{ij} := [ih, (i+1)h] \times [jh, (j+1)h]$, $0 \le i, j \le m-1$ with $mh = 1$. We introduce the color function (or area fraction in 2D, volume fraction in 3D):

$$C_{ij}(t) := |W_{ij}|^{-1} \int_{W_{ij}} \chi_1(x,t) \, dx = h^{-2} \int_{W_{ij}} \chi_1(x,t) \, dx.$$

We have $0 < C_{ij} < 1$ in cells W_{ij} cut by the interface and $C_{ij} = 0$ or 1 away from it, cf. Fig. 6.2. Assume that for time $t = t_n$ (an approximation of) the color function is known in all cells, i.e., we have known values $C_{ij}^n \approx C_{ij}(t_n)$, $0 \le i, j \le m-1$. The values for the next time level $t_{n+1} = t_n + \Delta t$ are obtained by discretization of (6.26) using a standard finite volume approach:

$$C_{ij}^{n+1} = C_{ij}^n + h^{-2} \int_{t_n}^{t_{n+1}} \int_{\partial W_{ij}} \tilde{\chi}_1 \mathbf{u} \cdot \mathbf{n} \, ds \, dt, \tag{6.27}$$

where $\tilde{\chi}_1 = \tilde{\chi}_1(x, t_n)$ is a known approximation of the characteristic function χ_1, cf. below.



(a) interface (b) color function (c) SLIC (d) PLIC

Fig. 6.2. Illustration of color function C and interface reconstruction: a) interface Γ and cells W_{ij}, b) values C_{ij} of color function, c) SLIC approximation, d) PLIC approximation.

In a VOF method one distinguishes the following two steps:

1. *Reconstruction of the interface*: given the values C_{ij}^n, $0 \le i, j \le m-1$, of the color function, an approximate interface is computed. This then determines the approximate characteristic function $\tilde{\chi}_1(x, t_n)$, used in (6.27).
2. *Color function advection step*: given the function $\tilde{\chi}_1(x, t_n)$ the boundary fluxes in (6.27) are approximated, resulting in the updated values C_{ij}^{n+1}, $0 \le i, j \le m-1$.

The reconstruction is such that the consistency property

$$C_{ij}^n = h^{-2} \int_{W_{ij}} \tilde{\chi}_1(x, t_n)\, dx$$

holds (volume conservation). Since the introduction of the VOF-method there have been many papers in which interface reconstruction techniques have been treated. The earliest algorithm, denoted by SLIC ("simple line interface calculation") was introduced in the paper [187]. In this approach the reconstructed interface consists of line segments that are parallel to one of the coordinate axes, cf. Fig. 6.2. This method is only first order accurate, i.e. $\mathcal{O}(h)$, in the accuracy of the reconstruction of the interface. Modifications of this technique can be found in [144, 69, 163]. More accurate (namely second order) reconstruction methods use piecewise linear segments that are not necessarily aligned with the coordinate axes. This technique is known as PLIC ("piecewise linear interface construction). Methods of this type are studied in, for example, [204, 214, 17]. We do not treat such reconstruction methods here, but refer to the above-mentioned literature.

We briefly address the advection step. The methods known in the literature can be divided into two categories: unsplit schemes and operator split schemes.

We only discuss the latter, for the former we refer to the literature, e.g. [204]. Consider one side of the boundary of W_{ij}, say the line segment connecting (ih, jh) with $(ih, (j+1)h)$, which is denoted by ℓ. Let $\mathbf{u}^* = (u_1^*, u_2^*)$ be an approximate value of the velocity on ℓ for $t \in [t_n, t_{n+1}]$, for example the velocity value at the center of ℓ, i.e. at $(ih, (j+0.5)h)$, at time $t = t_n + 0.5\Delta t$. Assume (for ease of presentation) that $u_1^* < 0$. We consider the contribution of the segment ℓ to the boundary integral in (6.27):

$$- h^{-2} \int_{t_n}^{t_{n+1}} \int_{\ell} \tilde{\chi}_1 u_1^* \, ds \, dt \tag{6.28}$$

(we used that $\mathbf{n} = (-1, 0)$ on ℓ). After the reconstruction step we have in each cell W_{ij} an approximation $\tilde{\chi}_1(x, t_n)$ of the characteristic function $\chi_1(x, t_n)$. In (6.28) we need values for $\tilde{\chi}_1(x, t)$, $x \in \ell$, $t \in [t_n, t_{n+1}]$. For this we take the values of $\tilde{\chi}_1(\cdot, t_n)$ transported by the flow field $(u_1^*, 0)^T$ during the time $t - t_n$, i.e. we take

$$\tilde{\chi}_1(x, t) := \tilde{\chi}_1\big(x - (t - t_n) \begin{pmatrix} u_1^* \\ 0 \end{pmatrix}, t_n\big), \quad x \in \ell, \ t \in [t_n, t_{n+1}]. \tag{6.29}$$

For this to be well-defined one has to satisfy the CFL-condition

$$\Delta t \, |u_1^*| \leq h. \tag{6.30}$$

Introduce $z := -(t - t_n)u_1^*$. Using (6.29) we obtain

$$\begin{aligned} - h^{-2} \int_{t_n}^{t_{n+1}} \int_{\ell} \tilde{\chi}_1(s, t) u_1^* \, ds \, dt &= h^{-2} \int_0^{\Delta t |u_1^*|} \int_{\ell} \tilde{\chi}_1(s + \begin{pmatrix} z \\ 0 \end{pmatrix}, t_n) \, ds \, dz \\ &= h^{-2} \big| \mathrm{supp} \, \{ \, \tilde{\chi}_1(x, t_n) : \, x \in [ih, ih + \Delta t |u_1^*|] \times [jh, (j+1)h] \, \} \, \big|. \end{aligned}$$

Hence, for the area flux across the side ℓ we obtain h^{-2} times the area of the support of the reconstructed characteristic function $\tilde{\chi}_1(\cdot, t_n)$ in the cell W_{ij} between the vertical lines with x_1-coordinates ih and $ih + \Delta t |u_1^*|$. This area flux leads to new intermediate values for the color function values in the cells W_{ij} and $W_{i-1,j}$. The same is done for all other vertical cell sides in the grid. These area fluxes in the horizontal direction lead to intermediate values $C_{ij}^{n+1,*}$, $0 \leq i, j \leq m-1$. Based on these new values of the color function the reconstruction step is repeated, resulting in a new characteristic function $\tilde{\chi}_1(\cdot, t_n)$, which is then used to compute area fluxes in the vertical direction (i.e. across horizontal cell sides). Thus we obtain the final new values C_{ij}^{n+1}, $0 \leq i, j \leq m-1$. Due to this two-step procedure (three-step in 3D), first the fluxes in one direction and then those in the other direction, this approach is called an operator split scheme.

We give some comments on the VOF technique. The method is very popular for the simulation of two-phase flows, in particular in the engineering community. Most of these methods have very good mass-conservation properties. In principle topology changes (droplet collisions) can be handled easily.

Usually the method is applied on (logically) rectangular grids; it is difficult to apply an accurate VOF technique on unstructured triangular or tetrahedral grids. In the method a CFL condition as in (6.30) must be satisfied, which may lead to severe (undesirable) restrictions on the size of the time step. In general it is difficult to obtain accurate approximations of intrinsic geometric properties of the interface, such as curvature and normal direction.

6.2.3 Volume tracking based on the level set function

An important difference between the interface tracking approach in Sect. 6.2.1 and the volume tracking approach in Sect. 6.2.2 is that the former is based on a Lagrangian ODE technique, cf. (6.19), and the latter on an Eulerian PDE approach, cf. (6.25). The method presented in this section is also of Eulerian PDE type. The approach discussed in the previous section is based on (the weak formulation of) the transport equation (6.25) for the characteristic function χ_1. This function is discontinuous across the interface, which requires a special numerical treatment of the transport equation. Furthermore, the interface is *not* characterized by values of χ_1 but by the boundary of its support.

An alternative is to use instead of χ_1 another indicator function. In the level set approach a *smooth* initial function $\phi_0(x),\ x \in \Omega$ is chosen such that

$$\phi_0(x) < 0 \ \Leftrightarrow\ x \in \Omega_1(0),\ \ \phi_0(x) > 0 \ \Leftrightarrow\ x \in \Omega_2(0),\ \ \phi_0(x) = 0 \ \ \Leftrightarrow\ x \in \Gamma(0).$$

A popular choice is to take ϕ_0 (approximately) equal to a signed distance function to the initial interface, cf. Fig. 6.3.

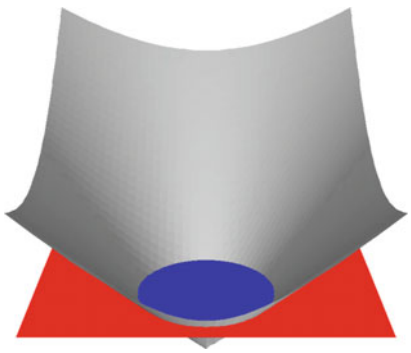


Fig. 6.3. Initial level set function ϕ_0 equals a signed distance function, 2D example.

A (virtual) particle $\mathbf{X}$ with Eulerian coordinates $x \in \Omega$ has a corresponding indicator value $\phi_0(x)$. Let $X_\xi(t),\ \xi \in \Omega$ be the characteristics as defined in

(6.17), assuming that the velocity field $\mathbf{u}(x,t)$ is sufficiently smooth. For $t > 0$ the level set function values $\phi(x,t)$ are defined by keeping the values constant along characteristics, i.e.,

$$\phi(X_\xi(t),t) := \phi_0(\xi), \quad \xi \in \Omega,\ t \geq 0.$$

Differentiating this with respect to t results in the transport equation

$$\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla \phi = 0 \quad \text{in} \quad \Omega, \quad t \geq 0. \tag{6.31}$$

This transport equation is of the same form as the one in (6.25). There are, however, important differences. Firstly, if the velocity field $\mathbf{u}(x,t)$ is sufficiently smooth (Lipschitz with respect to x) then the equation in (6.31) is well-defined in its *strong* formulation, due to the fact that the initial condition ϕ_0 is continuous. Due to the discontinuity in the characteristic function, the equation (6.25) is not well-defined in its strong form. Secondly, the interface $\Gamma(t)$ *can be characterized by values of the level set function* at time t:

$$\Gamma(t) = \{\, x \in \Omega :\ \phi(x,t) = 0 \,\}.$$

As already mentioned above, this is not the case for the characteristic function. For the linear hyperbolic partial differential equation in (6.31), besides the initial condition one needs suitable boundary conditions, for example, a Dirichlet boundary condition $\phi(x,t) = \phi_D(x)$ on the inflow boundary $\partial\Omega_{in} := \{\, x \in \partial\Omega :\ \mathbf{u} \cdot \mathbf{n}_\Omega < 0 \,\}$.

A suitable weak formulation of the level set equation, i.e., the transport equation (6.31) combined with continuous initial condition ϕ_0 as defined above, is used in the literature [119] for the analysis of well-posedness of a two-phase flow problem. We outline the main result from [119]. The domain Ω is taken as a d-dimensional torus (corresponding to a rectangular domain with periodic boundary conditions). For the transport of the interface the level set equation is used with a *continuous* velocity field $\mathbf{u} \in C(\overline{\Omega} \times [0,T])^d$. For general continuous $\mathbf{u}$ there is no uniqueness of a solution of the equation (6.31) in its strong formulation. However, the concept of *viscosity solutions* of transport equations with a continuous velocity field can be applied, cf. [72]. This theory yields unique so-called sub- and supersolutions of (6.31), which induce unique generalized evolutions $\Omega_1(t),\ \Omega_2(t),\ t \in [0,T]$, with $\Omega_1(0) = \{\, x \in \Omega :\ \phi_0(x) < 0 \,\}, \Omega_2(0) = \{\, x \in \Omega :\ \phi_0(x) > 0 \,\}$. One defines $\Gamma(t) := \Omega \setminus (\Omega_1(t) \cup \Omega_2(t))$. If $\mathbf{u}$ is sufficiently regular (Lipschitz with respect to x) it can be shown that $\mathrm{meas}_d(\Gamma(t)) = 0$ holds and $\Gamma(t)$ describes the interface in the usual strong sense. If, however, the velocity field $\mathbf{u}$ is (only) continuous it is not known whether $\mathrm{meas}_d(\Gamma(t)) = 0$ for $t > 0$ holds, i.e., it might be that *"interface flattening"* occurs.

For the two-phase flow problem a Stokes model of the form

$$\begin{aligned} \frac{\partial \mathbf{u}}{\partial t} - \operatorname{div}(\mu \nabla \mathbf{u}) + \nabla p &= \mathbf{g} \quad \text{in} \quad \Omega, \\ \operatorname{div} \mathbf{u} &= 0 \quad \text{in} \quad \Omega, \end{aligned}$$

is considered. A weak formulation of this problem in the Sobolev space $H_p^1(\Omega)$ with $p > 2(d+1)$ is analyzed with a piecewise constant viscosity function $\mu(x,t) = \mu_i$ for $x \in \Omega_i(t)$, $i = 1, 2$, and $\mu(x,t) = \frac{1}{2}(\mu_1 + \mu_2)$ for $x \in \Gamma(t)$. It is proved that for $|\mu_1 - \mu_2|$ sufficiently small there exists for almost all $t \in [0,T]$ a solution $\mathbf{u}$ with $\mathbf{u} \in C(\overline{\Omega} \times [0,T])^d$, $\mathbf{u}(\cdot,t) \in H_p^1(\Omega)^d$ of the Stokes problem coupled with an appropriate weak formulation of the transport problem for the evolution of the level set function ϕ. We refer to [119] for the precise results. Here we restrict ourselves to a few further comments related to this analysis. The continuity property for the velocity field $\mathbf{u}$ is needed to be able to apply the theory of viscosity solutions of transport equations as in (6.31). This theory also requires the initial condition ϕ_0 to be continuous. Note that this holds for the level set function ϕ_0 but not for the characteristic function χ_1 used in Sect. 6.2.2. For the solution $\mathbf{u}$ of the Stokes problem the regularity $\mathbf{u}(\cdot,t) \in H_p^1(\Omega)^d$ with $p > 2(d+1)$ (> 2) is proved, which due to a Sobolev embedding result implies continuity of $\mathbf{u}$. For the regularity property $\mathbf{u} \in H_p^1(\Omega)^d$ with $p > 2(d+1)$ to hold one needs that the jump in the viscosity $|\mu_1 - \mu_2|$ is sufficiently small. The analysis only applies to the case *without* surface tension and it only yields existence of a solution of the two-phase Stokes problem; uniqueness is an open problem. The existence is global in time ($t \in [0,T]$) and allows singularities of the interface (colliding droplets). However, "interface flattening" might occur, i.e., it is not clear whether the interface remains sharp.

The level set equation (6.31) is not only used in the analysis of well-posedness of a two-phase flow problem but also forms the basis of an important class of *numerical techniques* for representing the interface. These *level set methods* are used not only in two-phase flow simulations but also in many other applications with interfaces or free boundaries, cf. the overview paper [221] and the monographs [222, 198]. We outline the main ideas. The linear hyperbolic transport equation (6.31), or a weak variant of it, is considered with an initialization $\phi_0(x)$ that is continuous, close to a signed distance function and such that $\Gamma(0) = \{\, x \in \Omega : \phi_0(x) = 0 \,\}$ holds. The velocity $\mathbf{u}$ results from the Navier-Stokes flow problem. The transport equation is discretized in space and time using appropriate numerical methods. We will treat this issue in more detail in Sect. 7.2. The accurate discretization of the level set equation is (much) easier than that of the transport equation considered in the VOF method in Sect. 6.2.2 because in the latter one has to approximate the discontinuous characteristic function χ_1 whereas in the level set method the solution ϕ is smooth (close to the interface, for a sufficiently short time interval). During time evolution, in a neighborhood of the zero level it is monitored how much the discrete

solution $\phi_h(x,t)$ deteriorates from a signed distance function. For this one can use, for example, the quantity $\|\nabla\phi_h(x,t)\|_2$ as an indicator. If the deterioration exceeds a given tolerance a *re-initialization* of the given level set function, say $\phi_h(x,t_n)$, is performed. In this re-initialization one determines a new level set function $\phi_h^{\text{new}}(x,t_n)$ such that $\|\nabla\phi_h^{\text{new}}(x,t_n)\|_2 \approx 1$ (in a neighborhood of the zero level) and $\{\, x\in\Omega:\ \phi_h(x,t_n)=0\,\} \approx \{\, x\in\Omega:\ \phi_h^{\text{new}}(x,t_n)=0\,\}$ holds, i.e. one determines a re-initialization ϕ_h^{new} with (approximately) the same zero level as the current level set function but which is much closer to a signed distance function. This topic of re-initialization is addressed in more detail in Sect. 7.4.1.

Remark 6.2.4 The level set method is often combined with the CSF approach explained in Remark 6.1.3. This idea was introduced in [64]. There it is shown that (under certain smoothness assumptions) the following holds, with notation as in Remark 6.1.3:

$$\int_\gamma \kappa \mathbf{n}_\Gamma \, ds = \lim_{\epsilon\downarrow 0} \int_U \kappa(\phi)\delta_\epsilon(\phi(x))\nabla\phi \, dx, \tag{6.32}$$

with the level set function ϕ and δ_ϵ a one-dimensional smoothed Dirac delta function. For the approximation of the curvature term $\kappa(\phi)$ one can use, cf. (14.7),

$$\kappa(x) = \operatorname{div} \mathbf{n}_\Gamma(x) = \operatorname{div}\big(\frac{\nabla\phi}{|\nabla\phi|}\big), \quad x\in\Gamma,$$

and extend this relation to $x\in U$ ($|\nabla\phi|^2 := \nabla\phi\cdot\nabla\phi$). This leads to a *volume* surface tension force term of the form

$$-\tau \operatorname{div}\big(\frac{\nabla\phi}{|\nabla\phi|}\big)\delta_\epsilon(\phi(x))\nabla\phi \tag{6.33}$$

in the *strong* formulation of the momentum equation, which acts in an ϵ-neighborhood of the interface Γ. Clearly this approach induces an error due to numerical regularization with the smoothed Dirac delta function.

6.2.4 Phase field representation

In the interface representations treated above the interface is either tracked explicitly or "captured" implicitly as the discontinuity of a characteristic function or the zero level of an approximate signed distance function. In all three cases one typically has a *sharp interface*. This sharp interface property may be lost due to numerical effects, for example if one combines the level set method with the CSF technique as described in Remark 6.2.4, in which the surface tension force is approximated by a volume force using a smoothed Dirac delta function. In that approach, although the interface is represented sharply as the zero level of the level set function there is an interface smearing effect due to the smoothing of the surface tension force. In the continuous model the

sharp interface property may be lost if in cases with interface singularities an interface flattening effect occurs. In the approach discussed in this section the model is such that one *always has a non sharp or diffusive interface*. These so-called phase field models are based on the observation that even for two (macroscopically) immiscible fluids there is a very thin interfacial region in which partial mixing of the two fluids occurs, cf. Sect. 1.1.5. In this sense, the physical interface is not sharp but diffusive. The interfacial mixing region has nonzero thickness but is extremely thin (about $100\,nm$). Hence modeling it as a sharp interface (as is done in the methods discussed above) seems reasonable. There are, however, mechanisms, for example in droplet collision, that are relevant and act on length scales comparable to that of interface thickness. For an accurate modeling of these mechanisms a diffusive interface representation may be more appropriate. Quantities that in the sharp interface formulation are localized at the interface, such as surface tension or surfactant transport, are distributed in a narrow interfacial region in a phase field model. The idea of diffusive interface modeling is an old one and was already used in [208, 247]. An overview on diffusive interface methods is given in [13]. Below we describe one popular phase field model for two-phase incompressible flows, namely the Navier-Stokes equations combined with the *Cahn-Hilliard* equation for the representation of the interface.

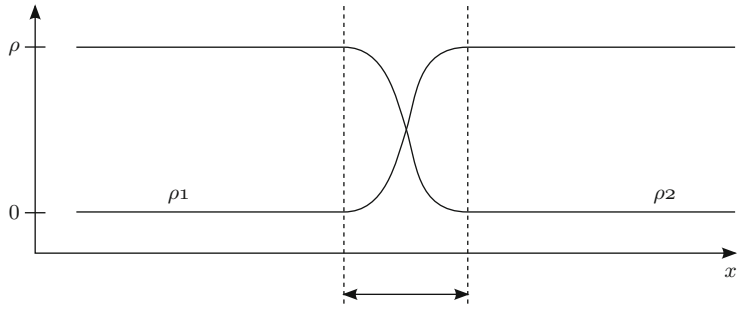


Fig. 6.4. Partial densities ρ_j, $j = 1, 2$, and diffusive interface (region between dashed lines) in the phase field representation.

Throughout this section, let $\rho_j = \rho_j(x)$, $x \in \Omega$, $j = 1, 2$, denote the *partial density* (or mass concentration) of the fluid j, i.e., for $W \subset \Omega$ the quantity $\int_W \rho_j(x)\,dx$ is the mass of the fluid j contained in W. Note that this notation differs from the one previously used, where ρ_j denoted the (constant) density of fluid j as a pure substance. The partial densities $\rho_1(x)$ and $\rho_2(x)$ are in general not constant, i. e., there is a mixing region representing the diffusive interface, cf. Fig. 6.4. The density of the *mixture* is denoted by $\rho(x)$, $x \in \Omega$, i.e., $\int_W \rho(x)\,dx$ is the total mass of the fluid contained in W. Clearly $\rho = \rho_1 + \rho_2$ holds. We restrict ourselves to the case of *matched densities*, i.e. we assume

$$\rho \text{ is constant in } \Omega. \tag{6.34}$$

It is no restriction to take $\rho = 1$. We introduce a so-called order parameter

$$c := \rho_1 - \rho_2 = 2\rho_1 - 1 \in [-1, 1].$$

This concentration (or density) difference has value -1 in regions filled by fluid 2, value 1 in regions filled by fluid 1 and values in between in the mixing region. It is assumed to be a smooth function of (x, t). Note that opposite to the characteristic function χ_1 and the level set function ϕ, which are used as indicator functions in the approaches treated above, *the order parameter c has a physical meaning*. A main issue is to derive an appropriate model for the evolution of c. We outline the derivation of the Navier-Stokes/Cahn-Hilliard model as given in [131]. It is based on a local dissipation inequality (corresponding to the second law of thermodynamics) and basic concepts from continuum mechanics, such as mass and momentum conservation, cf. Sect. 1.1.1. The mixture is considered as *one* incompressible Newtonian fluid. Its velocity field is denoted by $\mathbf{u}(x, t)$. Due to the incompressibility assumption we have $\operatorname{div} \mathbf{u} = 0$. Let $W(t)$ a material volume that is advected by the velocity field $\mathbf{u}$ and $\mathbf{h}_j$ the mass flux of fluid j, measured *relative* to the gross motion of the fluid. Due to incompressibility ($\rho = 1$) the relation $\mathbf{h}_1 = -\mathbf{h}_2$ holds. We define the (relative) mass flux quantity $\mathbf{h} := \mathbf{h}_1 - \mathbf{h}_2 = 2\mathbf{h}_1$. From mass conservation it follows that

$$\frac{d}{dt} \int_{W(t)} \rho_j \, dx + \int_{\partial W(t)} \mathbf{h}_j \cdot \mathbf{n} \, ds = 0,$$

where $\mathbf{n}$ is the outward unit normal on $W(t)$. Using Reynolds' transport theorem and $c = 2\rho_1 - 1$ this yields the mass conservation equation

$$\dot{c} = \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c = -\operatorname{div} \mathbf{h}. \tag{6.35}$$

We now turn to the conservation of momentum $\int_{W(t)} \rho \mathbf{u} \, dx$, cf. Sect. 1.1.1. For simplicity we assume that there are no external forces like gravity. Based on fundamental principles from continuum mechanics (Cauchy's theorem) one obtains from momentum conservation and using $\rho = 1$ the equation

$$\rho \dot{\mathbf{u}} = \frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} = \operatorname{div} \boldsymbol{\sigma}, \tag{6.36}$$

with a symmetric stress tensor $\boldsymbol{\sigma}$ that is associated with the macroscopic motion of the fluid. For a one-phase incompressible Newtonian fluid one has $\boldsymbol{\sigma} = -p\mathbf{I} + \mu \mathbf{D}(\mathbf{u})$, cf. (1.11). In [131] a stress tensor for the case of a fluid mixture is derived using local energy inequalities that are based on the second law of thermodynamics. The resulting stress tensor is given in (6.42) below. We sketch the main idea, for more details we refer to [131, 3]. We consider a

total energy $e_W(\mathbf{u}, c)$ in a volume W which is the sum of a kinetic energy and a *free energy*:

$$e_W(\mathbf{u}, c) = \int_W \rho \frac{1}{2}\mathbf{u} \cdot \mathbf{u} + \psi(c, \nabla c)\, dx.$$

The free energy $\int_W \psi(c, \nabla c)\, dx$ is used to describe energy changes due to mixing of the fluids. Since there is significant mixing only in a very thin interfacial region, this energy is also called surface energy. Cahn and Hilliard [60] proposed the following form for the mixing energy density

$$\psi(c, \nabla c) = \varepsilon \frac{1}{2}|\nabla c|^2 + \varepsilon^{-1}\psi_0(c), \tag{6.37}$$

with $|\nabla c|^2 = \nabla c \cdot \nabla c$, $\varepsilon > 0$ a small parameter and ψ_0 a double well potential. The latter means that ψ_0 should have exactly two global minima, namely at $c = \pm 1$ in our case. For this double well potential there are several possibilities used in the literature, e.g.,

$$\psi_0(c) = (1 - c^2)^2, \quad c \in \mathbb{R},$$
$$\psi_0(c) = \frac{\theta}{2}\big((1 + c)\ln(1 + c) + (1 - c)\ln(1 - c)\big) - \frac{\theta_c}{2}c^2, \quad 0 < \theta < \theta_c, \quad |c| < 1,$$
$$\psi_0(c) = -\frac{\theta_c}{2}c^2 \quad \text{if} \quad c \in [-1, 1], \quad \infty \quad \text{otherwise},$$

cf. [3, 6] for a discussion of these and other double well potentials. Since both fluids are assumed to be present, it follows that $0 < |\Omega|^{-1} \int_\Omega \rho_1\, dx < 1$ and thus $-1 < |\Omega|^{-1} \int_\Omega c\, dx < 1$ holds. Hence, $c(x)$ can not have a constant value equal to -1 or 1, which corresponds to a minimum of ψ_0. A "diffusive interface" is represented by the region where $c(x)$ varies between $-1 + \xi$ and $1 - \xi$ (with $0 < \xi \ll 1$).

Remark 6.2.5 As an example, consider for given $a > 0$,

$$e_{\text{free}}(c) := \int_{-a}^{a} \varepsilon \frac{1}{2}c'(x)^2 + \varepsilon^{-1}(1 - c(x)^2)^2\, dx,$$

and minimization of this functional over the set V consisting of all piecewise linear $c = c_\delta$ with $c(x) = -1$ if $x \le -\delta$, $c(x) = 1$ if $x \ge \delta$, $c(x) = \frac{x}{\delta}$ if $-\delta \le x \le \delta$, and with $\delta \in (0, a)$ arbitrary. A straightforward computation yields

$$\min_{c_\delta \in V} e_{\text{free}}(c_\delta) = e_{\text{free}}(c_{\delta^*}) = \frac{8}{\sqrt{15}}, \quad \text{for} \quad \delta^* = \frac{1}{4}\sqrt{15}\, \varepsilon.$$

Hence, in this example we have a transition region of width $2\delta^* = \frac{1}{2}\sqrt{15}\, \varepsilon$ between the extrema ± 1.

The macroscopic stresses in the mixture, modeled by contact forces $\boldsymbol{\sigma}\mathbf{n}$ that act on $\partial W(t)$, induce a corresponding energy exchange across $\partial W(t)$ (force times distance, per time unit), also called working, given by

$$\int_{\partial W(t)} \boldsymbol{\sigma}\mathbf{n}\cdot\mathbf{u}\,ds. \tag{6.38}$$

A second energy transport is due to the microscopic diffusion (i.e. diffusive effect within the mixture). This can be modeled as follows. Let μ_j^{chem} be the chemical potential of fluid j and $\mu^{\text{chem}} := \frac{1}{2}(\mu_1^{\text{chem}} - \mu_2^{\text{chem}})$. Related to the notation we remark that μ^{chem} should not be confused with $\mu = \mu(x,t)$, which we use to denote the viscosity of a fluid. Using $\mathbf{h}_1 + \mathbf{h}_2 = 0$ (as ρ is constant) and $\mathbf{h} = 2\mathbf{h}_1$ we obtain that

$$-\sum_{j=1}^{2}\int_{\partial W(t)} \mu_j^{\text{chem}}\mathbf{h}_j\cdot\mathbf{n}\,ds = -\int_{\partial W(t)} \mu^{\text{chem}}\mathbf{h}\cdot\mathbf{n}\,ds, \tag{6.39}$$

which models the energy transported into $W(t)$ due to microscopic diffusion. The third energy exchange is related to so-called microforces. In [131] these forces are introduced and it is assumed that the working of these forces accompanies changes in the concentration c. i.e., these forces cause the microscopic mixing. These forces are modeled as *contact forces* and denoted by $\boldsymbol{\xi}$. A corresponding scalar body force is given by

$$\pi := -\operatorname{div}\boldsymbol{\xi}, \tag{6.40}$$

i.e., we have a microforce balance $\int_{W(t)}\pi\,dx + \int_{\partial W(t)}\boldsymbol{\xi}\cdot\mathbf{n}\,ds = 0$. The energy exchange induced by these microforces is given by

$$\int_{\partial W(t)} \dot{c}\,\boldsymbol{\xi}\cdot\mathbf{n}\,ds. \tag{6.41}$$

The three energies in (6.38), (6.39) and (6.41) are related to the total energy $e_W(\mathbf{u},c)$ of the system, and based on the second law of thermodynamics (increase of entropy) the following *energy dissipation inequality* is assumed to hold:

$$\frac{d}{dt}e_W(\mathbf{u},c) \le \int_{\partial W(t)} \boldsymbol{\sigma}\mathbf{n}\cdot\mathbf{u}\,ds + \int_{\partial W(t)} \dot{c}\,\boldsymbol{\xi}\cdot\mathbf{n}\,ds - \int_{\partial W(t)} \mu^{\text{chem}}\mathbf{h}\cdot\mathbf{n}\,ds.$$

Based on this, in [131] the following constitutive relations are derived:

$$\begin{aligned}
\boldsymbol{\sigma} &= -p\mathbf{I} + \mu\mathbf{D}(\mathbf{u}) - \varepsilon\nabla c\nabla c^T,\\
\boldsymbol{\xi} &= \varepsilon\nabla c,\\
\mathbf{h} &= -m(c)\nabla\mu^{\text{chem}},\\
\pi &= \mu^{\text{chem}} - \varepsilon^{-1}\psi_0'(c).
\end{aligned} \tag{6.42}$$

The relations $\boldsymbol{\xi} = \varepsilon\nabla c$ and $\mathbf{h} = -m(c)\nabla\mu^{\text{chem}}$ can be seen as generalized Fick's laws. For simplicity we *assume the mobility constant $m = m(c) > 0$ to be a constant*. Using this and (6.40) we obtain

$$\mu^{\text{chem}} = \varepsilon^{-1}\psi_0'(c) - \varepsilon\Delta c.$$

Using the conservation laws (6.35), (6.36) and the generalized Fick's law for $\mathbf{h}$ in (6.42) we obtain the following *Navier-Stokes/Cahn-Hilliard phase field model*.

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \operatorname{div}\big(\mu(c)\mathbf{D}(\mathbf{u})\big) - \varepsilon \operatorname{div}(\nabla c \nabla c^T), \tag{6.43a}$$

$$\operatorname{div}\mathbf{u} = 0, \tag{6.43b}$$

$$\frac{\partial c}{\partial t} + \mathbf{u}\cdot\nabla c = m\Delta\mu^{\text{chem}}, \tag{6.43c}$$

$$\mu^{\text{chem}} = \varepsilon^{-1}\psi_0'(c) - \varepsilon\Delta c. \tag{6.43d}$$

For the general case in which $m = m(c)$ is *not* constant, the term on the right-hand side in (6.43c) has to be replaced by $\operatorname{div}(m(c)\nabla\mu^{\text{chem}})$. Suitable initial and boundary conditions for the functions c and μ^{chem} are needed, for example, homogeneous Neumann boundary conditions both for c and μ^{chem} ($\nabla c\cdot\mathbf{n} = \nabla\mu^{\text{chem}}\cdot\mathbf{n} = 0$ on $\partial\Omega$) and an initial condition $c(x,0) = c_0(x)$ for $x\in\Omega$. A simple model for $\mu(c)$ is to use a convex combination between the constant viscosities μ_1, μ_2 of the pure fluids:

$$\mu(c) = \frac{c+1}{2}\mu_1 + \frac{1-c}{2}\mu_2.$$

The model (6.43) is a fundamental phase field model that occurs at many places in the literature and forms the basis for many other phase field models. Below we briefly address the following issues: theoretical results, generalizations, numerical methods, relation to other approaches.

Theoretical results. First we consider an alternative form of (6.43a) and an energy conservation result. For general smooth scalar functions v the identity

$$\operatorname{div}(\nabla v\nabla v^T) = \frac{1}{2}\nabla|\nabla v|^2 + \Delta v\,\nabla v \tag{6.44}$$

holds. Using this (with $v = c$), the definition of the free energy density ψ in (6.37) and the expression in (6.43d) we obtain

$$\begin{aligned}\nabla\psi(c,\nabla c) &= \varepsilon\frac{1}{2}\nabla|\nabla c|^2 + \varepsilon^{-1}\psi_0'(c)\nabla c\\ &= \varepsilon\operatorname{div}(\nabla c\nabla c^T) - \varepsilon\Delta c\nabla c + \varepsilon^{-1}\psi_0'(c)\nabla c\\ &= \varepsilon\operatorname{div}(\nabla c\nabla c^T) + \mu^{\text{chem}}\nabla c.\end{aligned}$$

From this we see that the Navier-Stokes equation in (6.43a) can be replaced by

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla\tilde{p} + \operatorname{div}\big(\mu(c)\mathbf{D}(\mathbf{u})\big) + \mu^{\text{chem}}\nabla c, \tag{6.45}$$

where we introduced a new pressure variable $\tilde{p} := p + \psi(c, \nabla c)$. Using this Navier-Stokes equation we derive the following lemma.

Lemma 6.2.6 *Assume that for $t \in [0,T]$ the Navier-Stokes/Cahn-Hilliard equations (6.43a)-(6.43d) have a sufficiently smooth solution $(\mathbf{u}, c, \mu^{\text{chem}})$ with boundary conditions $\mathbf{u}_{|\partial\Omega} = 0,\ \nabla c\cdot\mathbf{n} = \nabla\mu^{\text{chem}}\cdot\mathbf{n} = 0$ on $\partial\Omega$. Then for the total energy*

$$e_\Omega(\mathbf{u}, c) = \int_\Omega \frac{1}{2}\mathbf{u}\cdot\mathbf{u} + \psi(c,\nabla c)\,dx = \frac{1}{2}\|\mathbf{u}\|_{L^2}^2 + \int_\Omega \psi(c,\nabla c)\,dx$$

the following holds:

$$\frac{d}{dt}e_\Omega\big(\mathbf{u}(t), c(t)\big) = -a\big((\mathbf{u}(t),\mathbf{u}(t)\big) - m\|\nabla\mu^{\text{chem}}(t)\|_{L^2}^2, \tag{6.46}$$

$$\begin{aligned} &e_\Omega\big(\mathbf{u}(T), c(T)\big) + \int_0^T a\big((\mathbf{u}(t),\mathbf{u}(t)\big)\,dt + m\int_0^T \|\nabla\mu^{\text{chem}}(t)\|_{L^2}^2\,dt \\ &= e_\Omega\big(\mathbf{u}(0), c(0)\big). \end{aligned} \tag{6.47}$$

Proof. First we consider the time derivative of the free energy part in the total energy:

$$\begin{aligned} \frac{d}{dt}\int_\Omega \psi(c,\nabla c)\,dx &= \int_\Omega \varepsilon\frac{d}{dt}\frac{1}{2}|\nabla c|^2 + \varepsilon^{-1}\psi_0'(c)\frac{\partial c}{\partial t}\,dx \\ &= \int_\Omega -\varepsilon\Delta c\frac{\partial c}{\partial t} + \varepsilon^{-1}\psi_0'(c)\frac{\partial c}{\partial t}\,dx = \int_\Omega \mu^{\text{chem}}\frac{\partial c}{\partial t}\,dx. \end{aligned}$$

Thus

$$\frac{d}{dt}e_\Omega\big(\mathbf{u}(t), c(t)\big) = \int_\Omega \frac{\partial \mathbf{u}}{\partial t}\cdot\mathbf{u} + \mu^{\text{chem}}\frac{\partial c}{\partial t}\,dx \tag{6.48}$$

holds. We multiply the Navier-Stokes equation (6.45) by $\mathbf{u}$, integrate over Ω, use that $c(\mathbf{u};\mathbf{u},\mathbf{u}) = b(\tilde{p},\mathbf{u}) = 0$ and obtain

$$\int_\Omega \frac{\partial \mathbf{u}}{\partial t}\cdot\mathbf{u}\,dx = -a\big((\mathbf{u}(t),\mathbf{u}(t)\big) + \int_\Omega \mu^{\text{chem}}\nabla c\cdot\mathbf{u}\,dx.$$

Using (6.43c) results in

$$\begin{aligned} \int_\Omega \frac{\partial \mathbf{u}}{\partial t}\cdot\mathbf{u}\,dx &= -a\big((\mathbf{u}(t),\mathbf{u}(t)\big) - \int_\Omega \mu^{\text{chem}}\frac{\partial c}{\partial t}\,dx + m\int_\Omega \mu^{\text{chem}}\Delta\mu^{\text{chem}}\,dx \\ &= -a\big((\mathbf{u}(t),\mathbf{u}(t)\big) - \int_\Omega \mu^{\text{chem}}\frac{\partial c}{\partial t}\,dx - m\|\nabla\mu^{\text{chem}}\|_{L^2}^2, \end{aligned}$$

and using this in (6.48) proves the result in (6.46). The result in (6.47) is a direct consequence of the one in (6.46). □

The result in this lemma can be compared with the one in Lemma 6.1.6. The result in (6.47) has a physical interpretation: the energy difference $e_\Omega\big(\mathbf{u}(T), c(T)\big) - e_\Omega\big(\mathbf{u}(0), c(0)\big)$ is balanced by the sum of the kinetic energy dissipation $\int_0^T a\big((\mathbf{u}(t), \mathbf{u}(t)\big)\, dt$ and energy dissipation $m \int_0^T \|\nabla \mu^{\mathrm{chem}}(t)\|_{L^2}^2\, dt$ that is related to the microscopic diffusion of the two phases close to the interface.
In the phase field model that we consider the free energy $\int_\Omega \psi(c, \nabla c)\, dx$ replaces the interfacial energy $\tau \int_\Gamma 1\, ds$ that occurs in a sharp interface model. For $\varepsilon \to 0$ this free energy tends to $\tau \int_\Gamma 1\, ds$, in some suitable weak sense, cf. the following remark.

Remark 6.2.7 We discuss a result from [179] on properties of the Cahn-Hilliard free energy functional. We introduce a scaled version of this functional and for simplicity we choose a specific form of ψ_0, namely $\psi_0(c) = (1 - c^2)^2$. The corresponding *scaled* (by ε) free energy is given by

$$\tilde{e}_{\mathrm{free}}(c) = \varepsilon e_{\mathrm{free}}(c) := \int_\Omega \varepsilon^2 |\nabla c|^2 + (1 - c^2)^2\, dx.$$

We consider minimization of this functional over the set

$$V_\alpha := \left\{ c \in L^1(\Omega) :\ -1 \le c(x) \le 1 \ \text{ a.e. },\ \ |\Omega|^{-1} \int_\Omega c\, dx = \alpha \right\},$$

with $-1 < \alpha < 1$. For $\varepsilon = 0$ the problem $\min\{\, \tilde{e}_{\mathrm{free}}(c) :\ c \in V_\alpha \,\}$ has infinitely many solutions, namely all "piecewise constant" functions c, with $c(x) = 1$ for $x \in \Omega_1$, and $\Omega_1 \subset \Omega$ an arbitrary measurable set with $|\Omega|^{-1}|\Omega_1| = \frac{1}{2}(\alpha + 1)$, $c(x) = -1$ for $x \in \Omega_2 := \Omega \setminus \Omega_1$. For such a function c we have $|\Omega|^{-1} \int_\Omega c\, dx = |\Omega|^{-1}(|\Omega_1| - |\Omega_2|) = 2|\Omega|^{-1}|\Omega_1| - 1 = \alpha$, i.e., $c \in V_\alpha$ and $\tilde{e}_{\mathrm{free}}(c) = 0$ (if $\varepsilon = 0$). We define $\Gamma := \partial\Omega_1 \cap \Omega$. Even if we restrict to cases in which this boundary Γ is assumed to be sufficiently smooth it can have *arbitrary area*. We now treat $\varepsilon > 0$ with $\varepsilon \downarrow 0$ and show that then the situation is quite different. We outline a main result from [179]. Consider the minimization problem

$$\min\{\, \tilde{e}_{\mathrm{free}}(c) :\ c \in V_\alpha \,\}. \tag{6.49}$$

Let $(\varepsilon_n)_{n \ge 0}$ be a sequence of strictly positive numbers with $\lim_{n\to\infty} \varepsilon_n = 0$ and (u_{ε_n}) a sequence of solutions of (6.49) with $\varepsilon = \varepsilon_n$. Then there exists a subsequence, which we also denote by (u_{ε_n}), which tends to a limit u_0 in $L^1(\Omega)$, i.e. $\lim_{n\to\infty} \int_\Omega (u_{\varepsilon_n} - u_0)\, dx = 0$. The limit function takes only the extremum values 1 or -1 on Ω: $u_0 = \pm 1$ a.e. on Ω. Define $\Omega_1 := \{\, x \in \Omega :\ u_0(x) = 1 \,\}$, and Γ, Ω_2 as above. Thus $\frac{1}{2}(u_{\varepsilon_n} + 1)$ tends to the characteristic function corresponding to Ω_1. To simplify the presentation we assume that Γ is smooth, say Lipschitz continuous (cf. [179] for the general case). Note that $u_0 \in V_\alpha$ and from $|\Omega|^{-1} \int_\Omega u_0\, dx = \alpha$ it follows that $|\Omega|^{-1}\big(|\Omega_1| - (|\Omega| - |\Omega_1|)\big) = \alpha$, and thus $|\Omega|^{-1}|\Omega_1| = \frac{1}{2}(\alpha + 1)$.

The following holds:

$$\lim_{n\to\infty} \varepsilon_n^{-1} \tilde{e}_{\text{free}}(u_{\varepsilon_n}) = 2c_0 \int_\Gamma 1\, ds, \quad c_0 := \int_{-1}^{1} \psi_0(c)^{\frac{1}{2}}\, dc = \frac{4}{3}, \tag{6.50}$$

$$\int_\Gamma 1\, ds = \min \left\{ \int_{F\cap\Omega} 1\, ds : \ F = \partial W, \ \ W \subset \Omega, \ \frac{|W|}{|\Omega|} = \frac{1}{2}(\alpha+1) \right\}. \tag{6.51}$$

We refer to [179] for more details. This means that the free energy $e_{\text{free}}(u_{\varepsilon_n}) = \int_\Omega \psi(u_{\varepsilon_n})\, dx$ converges to $2c_0 \int_\Gamma 1\, ds$ and that the interface Γ *has minimal area*, in the sense as in (6.51). For these results to hold, *it is essential that in the free energy functional* e_{free} *the "regularization term" with* ∇c *is included.*

In the Navier-Stokes/Cahn-Hilliard model the chemical potential μ^{chem} can be eliminated by substitution of (6.43d) into (6.43c). Furthermore, in the Navier-Stokes problem the pressure can be eliminated by restricting to the subspace of divergence-free velocity fields. This results in a strongly coupled highly nonlinear system of PDEs for the unknowns $\mathbf{u}$ and c. For the analysis it may be convenient not to eliminate μ^{chem}. For the Navier-Stokes/Cahn-Hilliard model (6.43a)-(6.43d), with suitable initial and boundary conditions, the state of the art concerning existence and uniqueness of solutions is much better than for the models considered in Sects. 6.2.2 and 6.2.3. To a large extent this is due to the following two (related) facts. Firstly, if we substitute (6.43d) into (6.43c) this results in a time-dependent *convection-diffusion* problem for the concentration c. The diffusion term $-\varepsilon m \Delta^2 c$ that occurs in this equation is not present in the pure convection equations (6.25) and (6.31) and has a regularizing effect. Secondly, in this diffusive interface model we have an energy estimate such that $\|\nabla \mu^{\text{chem}}\|_{L^2}$ can be controlled, cf. Lemma 6.2.6. Such a term is not present in the energy estimate for a sharp interface model as in Lemma 6.1.6. Recently, an extensive analysis of the model (6.43a)-(6.43d) has been given in [3]. Results on existence and uniqueness of weak solutions of this model are presented which are comparable to the results for the *one*-phase Navier-Stokes model for an incompressible Newtonian fluid. For $d = 2$ existence and uniqueness of a weak solution $(\mathbf{u}, c, \mu^{\text{chem}})$ has been proved, provided the initial data for $\mathbf{u}$ and c are sufficiently regular. For $d = 3$ existence is shown to hold, but (as for the one-phase Navier-Stokes equations) uniqueness only in special cases, for example for $t \in [0, T]$ with T sufficiently small. We refer to [3, 5] for precise statements and a discussion of further results.

Generalizations. Above we considered the case of *matched densities*, cf. (6.34). In many two-phase systems the assumption $\rho =$ constant is not reasonable, since it implies that both pure fluids must have (approximately) the same density. There are generalizations of the Navier-Stokes/Cahn-Hilliard model (6.43a)-(6.43d) for the case that the two fluids have different (or "non-matched") densities, cf. e.g. [171, 3]. These models are much more complicated as in the case of matched densities.

One important difference is that instead of the equation $\operatorname{div} \mathbf{u} = 0$ one obtains $\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{u}) = 0$, which implies that in general $\operatorname{div} \mathbf{u} = 0$ does not hold. Hence, although the two pure fluids are incompressible, the mixture does not have this property; it is called quasi-incompressible. This complicates the analysis because one can not eliminate the pressure unknown by restricting to the space of divergence free velocity fields. Another difference is that the pressure p enters the partial differential equation for c, which makes the coupling between the Navier-Stokes and the Cahn-Hilliard equations even less transparent. There are existence results for weak solutions of the diffuse interface model for the case with non-matched densities only for some special cases, cf. [4] for a discussion. A phase field model based on the Cahn-Hilliard free energy functional for a three-(or more) phase flow problem, in which the three fluids can have different densities, is derived in [156].

In the literature there are studies on phase field models with free energies that differ from the Cahn-Hilliard form.

Numerical methods. In order to have a proper modeling of relevant physical phenomena, the parameter ε in the Navier-Stokes/Cahn-Hilliard model (6.43a)-(6.43d) has to be taken extremely small. As a consequence the order parameter c has very large gradients that must be resolved numerically. The equation for c (after elimination of μ^{chem}) is of convection-diffusion type with a *fourth* order diffusion term $-\varepsilon m \Delta^2$. The numerical treatment of such biharmonic type of equations is known to be difficult. Furthermore there is a strong nonlinear coupling between the Navier-Stokes (for $(\mathbf{u}, p)$) and Cahn-Hilliard (for (c, μ^{chem})) equations. Hence, even for the case of matched densities the Navier-Stokes/Cahn-Hilliard model has a very high numerical complexity. For non-matched densities (which are physically much more relevant) there is a further significant increase in the numerical complexity. Some early numerical results for a Navier-Stokes/Cahn-Hilliard model (6.43a)-(6.43d) of a two-dimensional two-phase flow problem are presented in [149]. This model is also simulated, again for a two-dimensional problem, in [155]. In both cases uniform grids and finite difference or finite volume discretization methods are used. Numerical simulations of a spatially three-dimensional Navier-Stokes/Cahn-Hilliard model with matched densities are given in [20]. Recent work on numerical simulations of two-phase flows based on phase field models is found in [233, 234]. The numerical simulation of a spatially two-dimensional *three*-phase system with matched densities is treated in [156].

It appears that up to now numerical simulations of two-phase flows based on phase field interface representations are used and studied much less than those based on interface tracking or interface capturing (with VOF or level set) techniques.

Comparison to other approaches. One important difference between the diffusive and the sharp interface approach was already mentioned above: the energy estimates are different, cf. Lemma 6.1.6 and Lemma 6.2.6. This has strong implications for the theoretical analysis. Furthermore, in the volume tracking techniques (VOF or level set) discussed above we have a pure transport

equation for an indicator function (characteristic function or level set function), whereas as in the phase field method we have a convection-diffusion type of equation for the concentration c. In the Navier-Stokes equation (6.43a) of the phase field model a "localized force" term

$$-\varepsilon \operatorname{div}(\nabla c \nabla c^T) \tag{6.52}$$

occurs. We comment on this term and its relation to the surface tension forces used in other approaches. First we consider the force term that occurs in the *strong* formulation if one uses a level set CSF approach, as explained in Remark 6.2.4. We assume a (highly) idealized situation in which the zero level of c describes the interface Γ and the scaled order function $\tilde{c} := \varepsilon c$ is a signed distance function to Γ in a neighborhood U_ε of Γ. Hence, $\varepsilon|\nabla c| = |\nabla \tilde{c}| = 1$ holds in U_ε. Using $\phi = \tilde{c}$ in (6.33) and $\delta_\epsilon(\phi(z)) \approx \epsilon^{-1}$ for z sufficiently close to Γ, we obtain

$$\begin{aligned} -\tau \operatorname{div}\big(\frac{\nabla\phi}{|\nabla\phi|}\big)\delta_\epsilon(\phi(z))\nabla\phi &\approx -\tau\epsilon^{-1}\operatorname{div}(\nabla\tilde{c})\nabla\tilde{c} \\ &= -\tau\epsilon^{-1}\varepsilon^2\Delta c\nabla c = -\tau\epsilon^{-1}\varepsilon^2\operatorname{div}(\nabla c\nabla c^T), \end{aligned}$$

in a sufficiently small neighborhood of Γ. In the last equality we used the relation (6.44) and $\nabla|\nabla c|^2 = 0$. This agrees with the localized force as in (6.52) if we take ϵ (in Dirac delta function) and ε (in Cahn-Hilliard) such that $\epsilon \sim \tau\varepsilon$.

In the *weak* formulation the force term in the Cahn-Hilliard model (6.43a) takes the form

$$\tilde{f}_\Omega(\mathbf{v}) := -\varepsilon \int_\Omega \operatorname{div}(\nabla c \nabla c^T)\mathbf{v}\, dx, \tag{6.53}$$

which we now compare with the functional $f_\Gamma(\mathbf{v}) = -\tau \int_\Gamma \kappa\, \mathbf{n}\cdot\mathbf{v}\, ds$ in (6.8) that is used for surface tension representation in the weak formulation of a sharp interface representation. For this we use another formula, cf. Lemma 14.1.2:

$$f_\Gamma(\mathbf{v}) = -\tau \int_\Gamma \operatorname{tr}(\mathbf{P}\nabla\mathbf{v})\, ds, \quad \mathbf{P} = \mathbf{I} - \mathbf{n}\mathbf{n}^T.$$

We consider only test functions with $\operatorname{div}\mathbf{v} = 0$ (which is reasonable, since by elimination of the pressure one can restrict to the subspace of divergence free velocities). Then we have $\operatorname{tr}\nabla\mathbf{v} = \operatorname{div}\mathbf{v} = 0$ and thus we get

$$f_\Gamma(\mathbf{v}) = \tau \int_\Gamma \operatorname{tr}(\mathbf{n}\mathbf{n}^T\nabla\mathbf{v})\, ds = \tau \int_\Gamma \mathbf{n}^T\nabla\mathbf{v}\,\mathbf{n}\, ds, \tag{6.54}$$

with $\mathbf{n} = \mathbf{n}_\Gamma$. Using partial integration the volume force in (6.53) can be reformulated as

$$\tilde{f}_\Omega(\mathbf{v}) = \varepsilon \int_\Omega \operatorname{tr}(\nabla c\nabla c^T\nabla\mathbf{v})\, dx = \varepsilon \int_\Omega \nabla c^T\nabla\mathbf{v}\nabla c\, dx.$$

As above we assume that $\tilde{c} = \varepsilon c$ is a signed distance function to Γ in U_ε. Note that then $\nabla\tilde{c}(x) = \mathbf{n}(x)$ for $x \in \Gamma$ and $\nabla\tilde{c}(y) = \mathbf{n}(x)$ for $y \in U_\varepsilon$, $x \in \Gamma$ and $y - x = \alpha\mathbf{n}(x)$ with $\alpha \in \mathbb{R}$. Assume that $\mathbf{v}$ is sufficiently smooth and that $|\nabla\tilde{c}(y)| \ll 1$ for $y \notin U_\varepsilon$, cf. Fig. 6.4. Using a suitable coordinate transformation one obtains

$$\begin{aligned}\tilde{f}_\Omega(\mathbf{v}) &= \varepsilon^{-1}\int_\Omega \nabla\tilde{c}^T\nabla\mathbf{v}\nabla\tilde{c}\,dx \approx \varepsilon^{-1}\int_{-\varepsilon}^{\varepsilon}\int_\Gamma \nabla\tilde{c}(s,0)^T\nabla\mathbf{v}(s,r)\nabla\tilde{c}(s,0)\,ds\,dr \\ &\approx \varepsilon^{-1}\int_{-\varepsilon}^{\varepsilon}\int_\Gamma \mathbf{n}(s,0)^T\nabla\mathbf{v}(s,0)\mathbf{n}(s,0)\,ds\,dr \approx 2\int_\Gamma \mathbf{n}^T\nabla\mathbf{v}\mathbf{n}\,ds,\end{aligned}$$

which is of the same form as the functional in (6.54).

6.3 Weak formulation

In the remainder of this monograph we restrict to the level set method for interface representation. Our choice is motivated by the following requirements. We want to develop a solver that can handle interface singularities (droplet collision), too. Therefore an interface tracking approach based on the interface condition $V_\Gamma = \mathbf{u}\cdot\mathbf{n}$ in (6.3) is less suitable. A representation of the interface as a surface in $\mathbb{R}^3$, which corresponds to a sharp interface model, is desirable since we want to use a model for mass transport between the phases, in which a Henry condition *at* the interface occurs, and a model for surfactant transport *on* the interface. It is not clear how (variants of) these models can be combined with a phase field approach. Therefore, we decided not to use a phase field method for interface representation. Comparing the VOF and level set interface capturing methods we decided to use the latter, since the numerical treatment of the transport equation for the level set function (which is smooth) is easier than for the characteristic function (which is discontinuous) and because the level set approach fits better in a finite element discretization framework than the VOF approach. The latter is more natural in a finite volume discretization context. Furthermore, the task of interface reconstruction is much easier using the discrete level set function instead of the discrete VOF color function. A disadvantage of the level set method compared to VOF is that it has a worse mass conservation property.

In this section we present a two-phase Navier-Stokes/level set model. We start with the strong formulation. Then a weaker variational model is formulated, which forms the basis of the finite element discretization method treated in the next chapter.

The jumps in the coefficients ρ and μ can be described using the level set function ϕ in combination with the Heaviside function $H : \mathbb{R} \to \mathbb{R}$:

$$H(\zeta) = 0 \quad \text{for} \quad \zeta < 0, \qquad H(\zeta) = 1 \quad \text{for} \quad \zeta > 0.$$

For ease one can set $H(0) = \frac{1}{2}$. We define

$$\begin{aligned} \rho(\phi) &:= \rho_1 + (\rho_2 - \rho_1)H(\phi), \\ \mu(\phi) &:= \mu_1 + (\mu_2 - \mu_1)H(\phi). \end{aligned} \tag{6.55}$$

We reconsider the strong formulation of the two-phase flow problem in (6.1)-(6.2). Instead of the Lagrangian interface propagation condition $V_\Gamma = \mathbf{u} \cdot \mathbf{n}$ in (6.3) we use the level set function for the representation of the interface and therefore add the level set equation (6.31) to the model. This results in the following model for the two-phase problem in $\Omega \times [0, T]$:

$$\begin{aligned} &\begin{cases} \rho(\phi)\Big(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u}\Big) = -\nabla p + \operatorname{div}(\mu(\phi)\mathbf{D}(\mathbf{u})) + \rho(\phi)\mathbf{g} \\ \operatorname{div} \mathbf{u} = 0 \end{cases} \quad \text{in } \Omega_i,\ i = 1, 2, \\ &[\boldsymbol{\sigma}\mathbf{n}]_\Gamma = -\tau\kappa\mathbf{n}, \quad [\mathbf{u}]_\Gamma = 0 \quad \text{on } \Gamma, \\ &\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla\phi = 0 \quad \text{in } \Omega, \end{aligned} \tag{6.56}$$

together with suitable initial and boundary conditions for $\mathbf{u}$ and ϕ, cf. Sect. 1.2. For the level set function ϕ, the initial condition is $\phi(x, 0) = \phi_0(x)$, in which ϕ_0 is given and should be such that $\{\, x \in \mathbb{R}^3 : \phi_0(x) = 0 \,\} = \Gamma(0)$. Moreover, ϕ_0 should be an (approximate) signed distance function to $\Gamma(0)$. To make the problem with the linear hyperbolic level set equation well-posed one needs boundary conditions on the inflow boundary $\partial\Omega_{in} := \{\, x \in \partial\Omega : \mathbf{u} \cdot \mathbf{n}_\Omega < 0 \,\}$. There are no natural (e.g., physics based) boundary conditions for ϕ at the inflow boundary. We are only interested in values of ϕ close to the interface (= zero level on ϕ) and ϕ is evolved according to $\frac{\partial \phi}{\partial t} + \mathbf{u} \cdot \nabla\phi = 0$ only for a short time interval. After this short time a re-initialization of ϕ is applied, cf. Sect. 7.4.1. Due to this the issue of the choice of the boundary condition for the level set function on $\partial\Omega_{in}$ is of minor importance.

Note that the model (6.56) is *not* in dimensionless form. A dimensionless formulation can be derived in a similar way as in Remark 6.1.1.

As discussed in Sect. 6.2.3 a general weak formulation of the model (6.56) for which well-posedness has been proved, is not known in the literature. As basis for the finite element discretization we will use the weak formulation of the Navier-Stokes problem given in (6.9)-(6.10) and combine it with a weak formulation of the level set equation.

We address this weak formulation of the level set equation. We do not apply the approach based on viscosity solutions of transport equations, briefly discussed in Sect. 6.2.3, since this requires the velocity field to be continuous: $\mathbf{u} \in C(\overline{\Omega} \times [0, T])^3$, which is not compatible with the usual weak formulations of the Navier-Stokes equation.

We also do not use a weak formulation as in Proposition 6.2.2 which is based on the concept of renormalized solutions of transport equations. A disadvantage of this formulation is that it leads to a space-time variational problem. In our setting we want to have a variational formulation only in space, cf. (6.9)-(6.10). We introduce a "space-only" variational formulation of the level set equation as in [106], Sect. 6.3. We consider a transport equation of the form

$$\frac{\partial \phi}{\partial t} + \mathbf{w} \cdot \nabla \phi = 0, \tag{6.57}$$

with $\mathbf{w} \in H^1(\Omega)^3$, $\operatorname{div} \mathbf{w} = 0$ and (for simplicity) $\mathbf{w}_{|\partial\Omega} = 0$. Then $\partial\Omega_{in} = \emptyset$ and thus we do not need boundary conditions for ϕ. The initial condition is given by $\phi(x,0) = \phi_0(x)$. Note that opposite to $\mathbf{u}$ used in the level set equation in (6.56) the velocity field $\mathbf{w}$ is *independent of* t. We introduce a so-called anisotropic Sobolev space, in which only derivatives in a particular direction, namely the flow direction $\mathbf{w}$, are considered. On $C^\infty(\Omega)$ we introduce the norm (and corresponding scalar product) $\|u\|^2_{1,\mathbf{w}} := \|u\|^2_{L^2} + \|\mathbf{w} \cdot \nabla u\|^2_{L^2}$. Let $W_\mathbf{w}$ be the completion of $C^\infty(\Omega)$ with respect to this norm. Then $W_\mathbf{w}$ is a Hilbert space and this space can also be characterized as

$$W_\mathbf{w} = \left\{ u \in L^2(\Omega) : \ \mathbf{w} \cdot \nabla u \in L^2(\Omega) \right\}$$

(where the derivative is defined in a distributional sense). This appears to be an appropriate space for a weak formulation of the transport equation (6.57):

Proposition 6.3.1 *Take $\phi_0 \in W_\mathbf{w}$. There exists a unique $\phi(t) = \phi(\cdot,t) \in C^1\big([0,T]; L^2(\Omega)\big) \cap C([0,T]; W_\mathbf{w})$ such that $\phi(0) = \phi_0$ and*

$$(\frac{d\phi}{dt}, v)_{L^2} + (\mathbf{w} \cdot \nabla \phi, v)_{L^2} = 0 \quad \textit{for all} \ \ v \in L^2(\Omega), \quad t \in [0,T].$$

Proof. This result is given in Theorem 6.52 in [106]. Its proof is based on a fundamental result known as the Hille-Yosida theorem. We only present some key ingredients which indicate that $W_\mathbf{w}$ and $L^2(\Omega)$ are the right spaces for the variational formulation. For a complete proof we refer to [106] and the references therein.

We outline the Hille-Yosida theorem. Let H be a Hilbert space and $C : D(C) \subset H \to H$ a linear operator. This operator is called monotone if $(Cv, v)_H \geq 0$ for all $v \in D(C)$ holds, and maximal if $I + C : D(C) \to H$ is bijective. The operator is maximal monotone if both properties hold. The Hille-Yosida theorem essentially states that if C is maximal monotone then an initial value problem of the form

$$\frac{du}{dt} + Cu = f, \quad t \in [0,T], \quad u(0) = u_0,$$

with $f \in H$ and $u_0 \in D(C)$, has a unique solution $u \in C^1([0,T]; H) \cap C\big([0,T]; D(C)\big)$. In our context we have $H = L^2(\Omega)$ and $C : W_\mathbf{w} = D(C) \to$

$L^2(\Omega)$ is defined by $(C\phi, v)_H = (\mathbf{w} \cdot \nabla\phi, v)_{L^2} =: c(\phi, v)$. The operator C is monotone, since:

$$(C\phi, \phi)_H = \int_\Omega \mathbf{w} \cdot \nabla\phi \, \phi \, dx = -\int_\Omega \phi\big(\phi \operatorname{div} \mathbf{w} + \mathbf{w} \cdot \nabla\phi\big) \, dx = -(C\phi, \phi)_H,$$

and thus $(C\phi, \phi)_H = 0$ for all $\phi \in W_{\mathbf{w}}$. In order to show that C is also maximal we consider the bilinear form $id + c : W_{\mathbf{w}} \times L^2(\Omega) \to \mathbb{R}$ given by $id(\phi, v) + c(\phi, v) = (\phi + \mathbf{w} \cdot \nabla\phi, v)_{L^2}$. This bilinear form is bounded on $W_{\mathbf{w}} \times L^2(\Omega)$. Now note that for $\phi \in W_{\mathbf{w}}$ we have

$$\begin{aligned}
\sup_{v \in L^2(\Omega)} \frac{id(\phi, v) + c(\phi, v)}{\|v\|_{L^2}} &= \sup_{v \in L^2(\Omega)} \frac{(\phi + \mathbf{w} \cdot \nabla\phi, v)_{L^2}}{\|v\|_{L^2}} = \|\phi + \mathbf{w} \cdot \nabla\phi\|_{L^2} \\
&= \big(\|\phi\|_{L^2}^2 + 2(\phi, \mathbf{w} \cdot \nabla\phi)_{L^2} + \|\mathbf{w} \cdot \nabla\phi\|_{L^2}^2\big)^{\frac{1}{2}} \\
&= \big(\|\phi\|_{L^2}^2 + \|\mathbf{w} \cdot \nabla\phi\|_{L^2}^2\big)^{\frac{1}{2}} = \|\phi\|_{1,\mathbf{w}},
\end{aligned}$$

and thus the inf-sup property

$$\inf_{\phi \in W_{\mathbf{w}}} \sup_{v \in L^2(\Omega)} \frac{id(\phi, v) + c(\phi, v)}{\|\phi\|_{1,\mathbf{w}} \|v\|_{L^2}} \geq 1$$

holds. Furthermore, it can be shown that $id(\phi, v) + c(\phi, v) = 0$ for all $\phi \in W_{\mathbf{w}}$ implies $v = 0$. From the boundedness of the bilinear form $id + c$, the inf-sup bound and the latter result it follows that $I + C : W_{\mathbf{w}} \to L^2(\Omega)$ is bijective, cf. Theorem 15.1.1. Hence, C is maximal monotone and the Hille-Yosida theorem yields existence and uniqueness of $\phi \in C^1\big([0, T]; L^2(\Omega)\big) \cap C([0, T]; W_{\mathbf{w}})$ such that $(\frac{d\phi}{dt}, v)_{L^2} + c(\phi, v)_{L^2} = 0$ for all $v \in L^2(\Omega)$. □

Motivated by this result we introduce a weak formulation of the level set equation in (6.56). We want to allow $\mathbf{u}_{\partial\Omega} \neq \emptyset$ and therefore use a subspace $W_{\mathbf{u},D} := \big\{ w \in W_{\mathbf{u}} : w_{|\partial\Omega_{in}} = \phi_D \big\}$ of $W_{\mathbf{u}}$. The weak formulation is as follows: find $\phi(\cdot, t) \in W_{\mathbf{u},D}$ such that $\phi(\cdot, 0) = \phi_0$ and

$$(\frac{\partial\phi}{\partial t}, v)_{L^2} + (\mathbf{u} \cdot \nabla\phi, v)_{L^2} = 0 \quad \text{for all} \quad v \in L^2(\Omega), \quad t \in [0, T]. \tag{6.58}$$

Note that in this problem the velocity $\mathbf{u}$ *depends on* t and therefore Proposition 6.3.1 can not be applied. Related to this, the space $W_{\mathbf{u},D}$ depends on $\mathbf{u}$ and thus on t.

Summarizing, we obtain the following two-phase incompressible flow model:

Find $\mathbf{u}(t) = \mathbf{u}(\cdot, t) \in \mathbf{V}_D$, $p(t) = p(\cdot, t) \in Q$, $\phi(t) = \phi(\cdot, t) \in W_{\mathbf{u},D}$ such that for almost all $t \in [0, T]$

$$m(\frac{\partial \mathbf{u}}{\partial t}, \mathbf{v}) + c(\mathbf{u}; \mathbf{u}, \mathbf{v}) + a(\mathbf{u}, \mathbf{v}) + b(\mathbf{v}, p) = (\rho \mathbf{g}, \mathbf{v})_{L^2} + f_\Gamma(\mathbf{v}) \quad \text{for all} \quad \mathbf{v} \in \mathbf{V}_0, \tag{6.59a}$$

$$b(\mathbf{u}, q) = 0 \quad \text{for all } q \in Q, \tag{6.59b}$$

$$(\frac{\partial \phi}{\partial t}, v)_{L^2} + (\mathbf{u} \cdot \nabla \phi, v)_{L^2} = 0 \quad \text{for all } v \in L^2(\Omega), \tag{6.59c}$$

initial conditions $\mathbf{u}(0) = \mathbf{u}_0, \quad \phi(0) = \phi_0 \quad \text{in } \Omega.$

Thus we have a Navier-Stokes equation (in weak form) in the *whole domain* Ω coupled with a linear hyperbolic equation (in weak form) for the level set function ϕ. The spaces used for velocity $\mathbf{u}$ and pressure p are the same as those used in the weak formulation of a one-phase flow problem. In the two-phase Navier-Stokes equation we have *discontinuous* viscosity and density coefficients. Furthermore, we have a source term f_Γ which is (only) a functional and which requires integration over the (unknown) interface Γ. This is a *sharp interface model*: there is no regularization ("numerical diffusion") caused by a smoothed Dirac delta function, cf. Remark 6.2.4.

The issue of well-posedness of this weak formulation is largely unsolved. Only under strong (unrealistic) smoothness assumptions on the data (including the initial interface) well-posedness results for (6.59a)-(6.59b) are known in the literature, cf. the discussion in Sect. 6.1. If the velocity field $\mathbf{u}(x, t)$ is sufficiently smooth (Lipschitz w.r.t. x) then the strong formulation of the level set equation is well-posed and thus also the weaker formulation in (6.59c). This weak model, however, is supposed to be suitable for less regular problems, too. Theoretical analysis that shows correctness of this claim is lacking.

In the next chapter we treat finite element methods for the discretization of this model.