Diffuse Interface Models for Two-Phase Flows of Compressible and Incompressible Fluids

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February 4, 2009

Overview

1. Diffuse Interface Model for Incompressible Fluids – Matched Densities
2. Diffuse Interface Model for Compressible Fluids
3. Diffuse Interface Model for Incompressible Fluids – General Densities
4. Open Questions

Overview

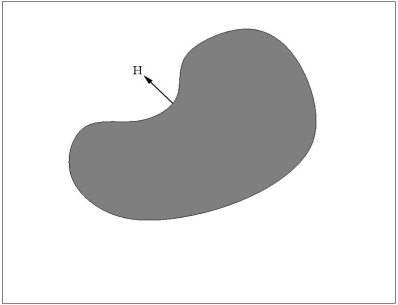
Basic Modeling Assumptions

We consider two (macroscopically) immiscible incompressible, viscous fluids like oil and water.

Classical Models: Interface is a two-dimensional surface.

Surface tension is proportional to the mean curvature.

Surface energy is proportional to the area.



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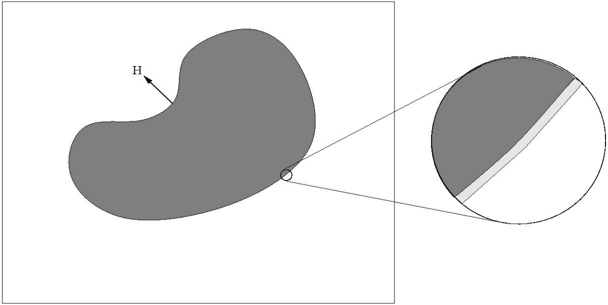


But: Sharp Interface is an idealization (van der Waals).

Fluid mix in a thin interfacial region.

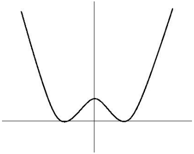
Free Energy of a Two-Component Mixture

Ansatz: We assume the fluids to be (partly) miscible.
Let $c_j \colon \Omega \to \mathbb{R}$ be the concentration of the component $j = 1, 2$, $c = c_1 - c_2$, and let

$$E_{mix}(c) = \frac{\varepsilon}{2} \int_\Omega |\nabla c(x)|^2 \, dx + \varepsilon^{-1} \int_\Omega f(c(x)) \, dx$$

be the free energy of the mixture, where $\Omega \subseteq \mathbb{R}^d$, $d = 1, 2, 3$, $\varepsilon > 0$ and

$$f \colon \mathbb{R} \to [0, \infty) \text{ with } f(c) = 0 \Leftrightarrow c = \pm 1.$$



Example:
$f(c) = \frac{1}{8}(1 - c^2)^2$

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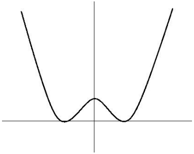
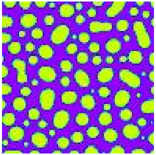


Example:
$f(c) = \frac{1}{8}(1 - c^2)^2$

Moreover, we assume

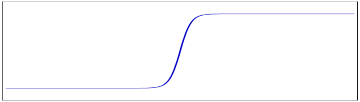
$$\frac{1}{|\Omega|} \int_\Omega c(x) \, dx = \overline{c} \in (-1, 1) \qquad \text{if } |\Omega| < \infty.$$



Remarks

- A "typical" profile of a diffuse interface is

$$c(x) = \tanh \frac{x}{2\varepsilon}, \qquad x \in \mathbb{R},$$



which minimizes E_{mix} in the case $\Omega = \mathbb{R}$ with constraint $c(x) \to_{x \to \pm\infty} \pm 1$ if $f(c) = \frac{1}{8}(1 - c^2)^2$.

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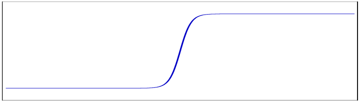

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- Modica-Mortola '77, Modica '87 proved

$$E_{mix} \equiv E_{mix,\varepsilon} \to_{\varepsilon\to 0} \sigma P$$

in the sense of Γ-convergence (w.r.t. L^1), where

$$P(v) = \begin{cases} \mathcal{H}^{d-1}(\partial^* E) & \text{if } v = 2\chi_E - 1 \\ +\infty & \text{else.} \end{cases}$$

and $\sigma = \sigma(f)$.

Modeling of a Two-Phase Flow

Ansatz: Use the free energy

$$E_{mix}(c) = \frac{\varepsilon}{2} \int_\Omega |\nabla c(x)|^2 \, dx + \varepsilon^{-1} \int_\Omega f(c(x)) \, dx$$

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Diffusion: Take diffusion of mass particles into account

$$\begin{aligned}
\partial_t c + v\cdot\nabla c &= \operatorname{div} J && \text{(continuity equation)}\\
J &= m\nabla\mu && \text{(generalized Fick's law)}\\
\mu := \frac{\delta E_{mix}}{\delta c} &:= -\varepsilon\Delta c + \varepsilon^{-1} f'(c) && \text{(chemical potential)}
\end{aligned}$$

where v is the mean velocity of the mixture and $m > 0$.

Classical models: Pure transport of the interface (m=0).

Remark: $\mu = \frac{\delta E_{mix}}{\delta c} \equiv const. \Leftrightarrow J \equiv 0$

Diffuse Interface Model in the Case of Matched Densities

If the densities of the fluids are the same, then one can derive:

$$\partial_t v + v \cdot \nabla v - \operatorname{div}(\nu(c) Dv) + \nabla p = \underbrace{-\varepsilon \operatorname{div}(\nabla c \otimes \nabla c)}_{\text{surface tension}} \tag{1}$$

$$\operatorname{div} v = 0 \tag{2}$$

$$\partial_t c + v \cdot \nabla c = m \Delta \mu \tag{3}$$

$$\mu = -\varepsilon \Delta c + \varepsilon^{-1} f'(c) \tag{4}$$

where $Dv = \frac{1}{2}(\nabla v + \nabla v^T)$ and $\nu(c) \geq \nu_0 > 0$.
Derivation: Hohenberg & Halperin '74, Gurtin et al. '96

Moreover, let $\Omega \subset \mathbb{R}^d$ be a bounded domain with smooth boundary and

$$v|_{\partial\Omega} = 0 \tag{5}$$

$$\partial_n c|_{\partial\Omega} = \partial_n \mu|_{\partial\Omega} = 0 \tag{6}$$

$$(v, c)|_{t=0} = (v_0, c_0) \tag{7}$$

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where $Dv = \frac{1}{2}(\nabla v + \nabla v^T)$ and $\nu(c) \geq \nu_0 > 0$.
Energy dissipation: Every smooth solutions satisfies

$$\begin{aligned} \frac{d}{dt} E(c(t), v(t)) &= -\int_\Omega \nu(c) |Dv|^2 \, dx - \int_\Omega m |\nabla \mu|^2 \, dx \quad \text{with} \\ E(c(t), v(t)) &= E_{mix}(c(t)) + \int_\Omega \frac{|v(t)|^2}{2} \, dx \end{aligned}$$

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Remark: (1) can be replaced by:

$$\partial_t v + v \cdot \nabla v - \operatorname{div}(\nu(c)Dv) + \nabla g = \mu\nabla c$$

where $g = p + \varepsilon^{-1} f(c) + \frac{\varepsilon}{2}|\nabla c|^2$. – Use (4) multiplied with ∇c, which yields

$$-\varepsilon \operatorname{div}(\nabla c \otimes \nabla c) = -\varepsilon\Delta c \nabla c - \varepsilon\nabla \frac{|\nabla c|^2}{2}$$

Note: (1)-(4) is *not too strongly coupled*!

Main Results for Matched Densities

Theorem (Existence, Regularity, Uniqueness, A. (ARMA '08))

Let $d = 2, 3$. For every $v_0 \in L^2_\sigma(\Omega)$, $c_0 \in H^1(\Omega)$ with $E_{mix}(c_0) < \infty$ there is a weak solution (v, c, μ) of (1)-(4), which satisfies

$$(v, \nabla c) \in L^\infty(0,\infty; L^2(\Omega)), \quad (\nabla v, \nabla \mu) \in L^2(0,\infty; L^2(\Omega)),$$
$$\nabla^2 c, f'(c) \in L^2_{loc}([0,\infty); L^6(\Omega)).$$

For (v_0, c_0) sufficiently smooth:

1. *If $d = 2$, then the weak solution is unique and regular.*
2. *If $d = 3$, there are some $0 < T_0 < T_1 < \infty$ such that the weak solution is regular and (locally) unique on $(0, T_0)$ and $[T_1, \infty)$.*

Remark: Here $f(c)$ can be chosen as e.g.

$$f(c) = \begin{cases} \theta((1-c)\log(1-c) + (1+c)\log(1+c))c - \theta_c c^2, & \text{if } c \in [-1,1], \\ +\infty & \text{else.} \end{cases}$$

Structure of the Proof

First study the separate systems:

1. Cahn-Hilliard equation with convection and singular potential (based on $E_{mix}(c) = E_0(c) - \frac{\theta}{2}\|c\|_2^2$ with E_0 convex)
2. (Navier-)Stokes system with variable viscosity

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Existence of weak solutions:
Approximation and compactness argument

Higher Regularity: Use regularity results for separate systems

Uniqueness: Gronwall's inequality once (v, c) are sufficiently regular.

Crucial ingredient for higher regularity:
A priori estimate for $c \in BUC([0, \infty); W_q^1(\Omega))$, $q > d$!

Regularity of c

W^2_r-estimate of c: Multiplying

$$\mu(t) = -\Delta c(t) + f'(c(t))$$

with $f'(c(t))$ yields

$$\int_\Omega f'(c(t))^2\,dx \quad + \quad \int_\Omega \underbrace{f''(c(t))}_{\geq -\theta_c} |\nabla c(t)|^2\,dx \leq C\|\mu(t)\|_2^2.$$

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$$\Rightarrow \|f'(c(t))\|_2 \quad + \quad \|\nabla^2 c(t)\|_2 \leq C_r \left(\|\mu(t)\|_2 + \|\nabla c(t)\|_2\right).$$

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Similarly one derives for $2 \leq r < \infty$

$$\|f'(c(t))\|_r + \|\nabla^2 c(t)\|_r \leq C_r\left(\|\mu(t)\|_r + \|\nabla c(t)\|_2\right).$$

$$\Rightarrow c \in L^2_{loc}([0,\infty); W^2_6(\Omega)) \qquad \text{if } d = 3.$$

Modifications: Higher regularity in time in Besov spaces.

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A Compressible Model by Lowengrub and Truskinovsky '98

We consider

$$\rho\partial_t v + \rho v \cdot \nabla v - \operatorname{div} \mathbb{S} + \nabla p(\rho, c) = -\operatorname{div}\left(\nabla c \otimes \nabla c - \frac{|\nabla c|^2}{2}\mathbb{I}\right) \quad (5)$$

$$\partial_t \rho + \operatorname{div}(\rho v) = 0 \quad (6)$$

$$\rho\partial_t c + \rho v \cdot \nabla c = m\Delta\mu \quad (7)$$

$$\rho\mu = \rho\frac{\partial f}{\partial c}(\rho, c) - \Delta c \quad (8)$$

where

$$p(\rho, c) = \rho^2 \frac{\partial f}{\partial \rho}(\rho, c), \qquad \mathbb{S} = \nu(c) Dv + \eta(c) \operatorname{div} v$$

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The free energy of the system is

$$E_{free}(\rho, c) = \int_\Omega \rho f(\rho, c)\, dx + \frac{1}{2}\int_\Omega |\nabla c|^2\, dx$$

Note: There is no factor ρ in front of $|\nabla c|^2$!

Choice of the Free Energy Density

We choose

$$\begin{aligned} f(\rho, c) &= f_{\mathrm{e}}(\rho) + f_{\mathrm{mix}}(\rho, c), \\ f_{\mathrm{mix}}(\rho, c) &= H(c) \log(\rho) + G(c), \end{aligned}$$

where $H \in C_b^1(\mathbb{R})$, $|G'(c)| \leq C(1 + |c|)$ and

$$c_1 \rho^\gamma - c_1 \leq f_{\mathrm{e}}(\rho) \leq C(1 + \rho^\gamma)$$

where $\gamma > \frac{3}{2}$.

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$$p(\rho, c) = \rho^2 \frac{\partial f(\rho, c)}{\partial \rho} = p_{\mathrm{e}}(\rho) + \rho H(c),$$

Remark: The choice is motivated by

$$\begin{aligned} \rho f_{\mathrm{mix}}(\rho, c) &= \alpha_1 \rho \frac{1-c}{2} \ln\left(\rho\frac{1-c}{2}\right) + \alpha_2 \rho \frac{1+c}{2} \ln\left(\rho \frac{1+c}{2}\right) - \beta\rho c^2 \\ &= \rho \log \rho H(c) + \rho G(c) \end{aligned}$$

Main Results for Compressible Fluids

Theorem (Existence of Weak Solutions, A. & Feireisl (Indiana '08))

Let $\Omega \subset \mathbb{R}^3$ be bounded with $\partial\Omega \in C^2$, $0 < T < \infty$. For every $\rho_0 \in L^\gamma(\Omega)$, v_0 such that $\rho_0|v|^2 \in L^1(\Omega)$, $c_0 \in H^1(\Omega)$ there is a weak solution (ρ, v, c, μ) of (5)-(8), which satisfies

$$\begin{aligned} \rho &\in L^\infty(0,T;L^\gamma(\Omega)) \cap L^{\gamma+\varepsilon}(\Omega \times (0,T)), \\ \nabla c &\in L^\infty(0,T;L^2(\Omega)), \\ (\nabla v, \nabla\mu) &\in L^2(0,T;L^2(\Omega)) \end{aligned}$$

for some $\varepsilon > 0$.

Sketch of the Proof (I)

1.) First one solves a system with artificial pressure:

$$\rho\partial_t v + \rho v \cdot \nabla v - \operatorname{div} \mathbb{S} + \nabla(p(\rho, c) + \delta\rho^\Gamma) = -\operatorname{div}\left(\nabla c \otimes \nabla c - \frac{|\nabla c|^2}{2}\mathbb{I}\right)$$

$$\partial_t \rho + \operatorname{div}(\rho v) = 0$$

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where $\delta > 0$ and $\Gamma > 3$ (e.g. by an implicit time discretization).

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where $\delta > 0$ and $\Gamma > 3$ (e.g. by an implicit time discretization).
2.) Next one shows an improved integrability of ρ, i.e,

$$\|\rho\|_{L^\infty(0,T;L^{\gamma+\varepsilon})} \leq C \qquad \text{uniformly in } \delta > 0.$$

by testing with $B[\rho^\varepsilon - \frac{1}{|\Omega|}\rho^\varepsilon]$ and using

$$-\operatorname{div}\left(\nabla c \otimes \nabla c - \frac{|\nabla c|^2}{2}\right) = -\Delta c \nabla c = \rho\mu\nabla c - \frac{\partial f}{\partial c}(\rho, c)\nabla c$$

Sketch of the Proof (II)

3.) Compactness of $\nabla c \equiv \nabla c_\delta$: Using

$$\rho_\delta \mu_\delta = \rho_\delta \frac{\partial f}{\partial c}(\rho_\delta, c_\delta) - \Delta c_\delta$$

and $c_\delta \to_{\delta \to 0} c$ on $\{\rho > 0\}$ a.e., one shows

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4.) Convergence of ρ_δ a.e.:
Based on weak continuity of the effective viscous flux:

$$\overline{b(\rho) p} - (\frac{4}{3}\nu(c) + \eta(c))\overline{b(\rho) \operatorname{div} u} = \overline{b(\rho)} \cdot \overline{p} - (\frac{4}{3}\nu(c) + \eta(c))\overline{b(\rho)} \cdot \overline{\operatorname{div} u},$$

where $\overline{f} = w - \lim_{\delta \to 0} f_\delta$ and renormalized solutions for the transport equation, cf. Feireisl '03.

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Quasi-Incompressible Model (Lowengrub & Truskinovsky)

Generalization for $\rho = \rho(c) \not\equiv const.$:

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Difficulties:

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- g possesses low regularity.
- Singular free energies cannot be used.
- How to define $\rho(c)$ for $c \notin [-1, 1]$? (E.g. $\frac{1}{\rho(c)} = \frac{1-c}{\rho_1} + \frac{c}{\rho_2}$)

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A. '07/'08: Existence of weak solutions for modified free energy/system

$$E_{mix}(c) = \frac{1}{q}\int_\Omega |\nabla c|^q \, dx + \int_\Omega \rho f(c(x))\, dx \qquad \text{with } q > d!$$

Decomposition of the Pressure and Velocity

Reformulation: (9),(12) are equivalent to

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Key point: Use that

$$g_0 = g_1 - \partial_t G(v),$$

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$$\Delta G(v(t)) = \operatorname{div} v(t), \qquad \partial_n G(v(t))|_{\partial\Omega} = n \cdot v(t)|_{\partial\Omega}.$$

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Then $v(t) = P_\sigma v(t) + \nabla G(v(t))$ and

$$\partial_t P_\sigma v + v \cdot \nabla v - \rho^{-1} \operatorname{div}(\nu(c) Dv) + \nabla g_1 = \mu_0 \nabla c.$$

$$\Rightarrow \Delta g_1 = -\operatorname{div}\operatorname{div} \underbrace{\left(v \otimes v - \frac{|v|^2}{2} I \right)}_{\in L^2(0,\infty;L^r)} + \ldots$$

and therefore $g_1 \in L^2(0,\infty; L^r(\Omega))$, $r \in (1, \frac{d}{d-1})$, due to Navier-BCs.

Overview

Open Questions

- More detailed analysis of the asymptotics as $t \to \infty$.
  What are the stable stationary solutions?
  Do similar effects occur as for the Cahn-Hilliard system?
- Incompressible fluids with different densities:
  Short-time existence of strong solutions. – Numerical properties?
  Alternative models? – Low Mach-number limit of the compressible model?
- Sharp Interface Limes Question: What is the limit system as $\varepsilon \to 0$?
  If $m = m(\varepsilon) \to_{\varepsilon\to 0} 0$: Do solution converge to the classical model for a two-phase flow?
  Problem: Existence of weak solution for the limit system is open.
  If $m = m(\varepsilon) \to_{\varepsilon\to 0} m_0 > 0$: Do solutions converge to a Navier-Stokes/Mullins-Sekerka-System?
  So far: Convergence as $\varepsilon \to 0$ to varifold solutions similarly to X. Chen'95.
  Existence of weak solution is known in this case, cf. A. & Röger '08.