Weierstrass Institute for
Applied Analysis and Stochastics

On some local and nonlocal diffuse interface models

Sergio Frigeri
ERC Group “Entropy Formulation of Evolutionary Phase Transitions”

Supported by the FP7-IDEAS-ERC-StG Grant “EntroPhase”

Outline

- The motivation
- Local Cahn-Hilliard-Navier-Stokes model
- Nonlocal model for binary fluid flow and phase separation
- Analytical results
- A local diffuse interface model related to tumor growth
- Some open related problems

- An isothermal model for the flow of a **mixture of two**
  - viscous
  - incompressible
  - Newtonian fluids
  - of equal density
- Avoid problems related to interface singularities

  $\Longrightarrow$ use a **diffuse interface model**

  $\Longrightarrow$ the classical sharp interface replaced by a **thin interfacial region**
- A partial mixing of the macroscopically immiscible fluids is allowed

  $\Longrightarrow$ φ **is the order parameter**, e.g. the concentration difference

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- A partial mixing of the macroscopically immiscible fluids is allowed
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- The original idea of diffuse interface model for fluids: HOHENBERG and HALPERIN, '77
  $\Longrightarrow$ **H-model**
  Later, GURTIN ET AL., '96: continuum mechanical derivation based on microforces
- Models of two-phase or two-component fluids are receiving growing attention (e.g., ABELS, BOYER, GARCKE, GRÜN, GRASSELLI, LOWENGRUB, TRUSKINOVSKI, ...)

In $\Omega \times (0, \infty)$, $\Omega \subset \mathbb{R}^d$, $d = 2, 3$

$$\mathbf{u}_t + (\mathbf{u} \cdot \nabla)\mathbf{u} - \nu \Delta \mathbf{u} + \nabla \pi = \mu \nabla \varphi + \mathbf{h}$$

$$\mathrm{div}(\mathbf{u}) = 0$$

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- μ: **chemical potential** (Cahn-Hilliard), first variation of the (total Helmholtz) free energy

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- F double-well potential: Helmholtz free energy density
  - Singular

$$F(s) = -\frac{\theta_c}{2}s^2 + \frac{\theta}{2}\big((1+s)\log(1+s) + (1-s)\log(1-s)\big)$$

for all $s \in (-1,1)$, with $0 < \theta < \theta_c$

  - Regular

$$F(s) = (1-s^2)^2 \qquad \forall s \in \mathbb{R}$$

- **Nonlocal free energy** rigorously justified by Giacomin and Lebowitz ('97 & '98) as macroscopic limit of microscopic phase segregation models

$$E(\varphi) = \frac{1}{4}\int_\Omega\int_\Omega J(x-y)(\varphi(x)-\varphi(y))^2 dxdy + \int_\Omega F(\varphi(x))dx$$

$J : \mathbb{R}^d \to \mathbb{R}$ interaction kernel s.t. $J(x) = J(-x)$ (usually nonnegative and radial)

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- First analytical results on nonlocal CH: Giacomin & Lebowitz '97 and '98; Gajewski '02; Gajewski & Zacharias '03
- Several other contributions on nonlocal Allen-Cahn equations and phase-field systems (notably by Bates et al. and Sprekels et al.)

$$\varphi_t + \mathbf{u} \cdot \nabla\varphi = \text{div}\,(m(\varphi)\nabla\mu)$$

$$\mu = a\varphi - J * \varphi + F'(\varphi)$$

$$\mathbf{u}_t - 2\text{div}(\nu(\varphi)D\mathbf{u}) + (\mathbf{u} \cdot \nabla)\mathbf{u} + \nabla\pi = \mu\nabla\varphi + \mathbf{h}$$

$$\text{div}(\mathbf{u}) = 0$$

subject to

$$\frac{\partial\mu}{\partial n} = 0 \qquad \mathbf{u} = 0 \qquad \text{on} \quad \partial\Omega \times (0, \infty)$$

$$\mathbf{u}(0) = \mathbf{u}_0 \qquad \varphi(0) = \varphi_0 \qquad \text{in} \quad \Omega$$

- Mass is conserved

$$\overline{\varphi(t)} := |\Omega|^{-1} \int_\Omega \varphi(x,t)dx = \overline{\varphi}_0$$

- **First mathematical results on nonlocal CHNS systems**
  - **Constant mobility+ regular potential**
    - $\exists$ **global weak sols in 2D-3D** (Colli, F. & Grasselli, J. Math. Anal. Appl. '12)
    - global attractor in 2D and trajectory attractor in 3D (F. & Grasselli, J. Dynam Differential Equations '12)
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- **More recent results**
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    - $\exists$ **global unique strong sols in 2D**, regularity of global attractor in 2D, convergence to equilibria of weak sols in 2D (F, Grasselli & Krejčí, J. Differential Equations '13)

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  - **Constant mobility+ regular or singular potential & degenerate mobility + singular potential**
    - **Uniqueness of global weak sols in 2D**
  - **Constant mobility**, **nonconstant viscosity** +regular potential
    - ∃ global unique strong sols in 2D, regularity of global attractor in 2D, convergence to equilibria of weak sols in 2D
    - weak-strong uniqueness in 2D
    - Connectedness and regularity of global attractor, ∃ exponential attractor in 2D.

Last results in: F., Gal & Grasselli, WIAS Preprint ’14

Theorem (Colli, F. & Grasselli '12)

Assume $J \in W^{1,1}(\mathbb{R}^d)$ and that $\boldsymbol{u}_0 \in L^2_{div}(\Omega)^d$, $\varphi_0 \in L^2(\Omega)$ with $F(\varphi_0) \in L^1(\Omega)$. Then, $\forall T > 0\ \exists$ a weak sol $[\boldsymbol{u}, \varphi]$ on $[0,T]$ s.t.

$$\boldsymbol{u} \in L^\infty(0,T;L^2_{div}(\Omega)^d) \cap L^2(0,T;H^1_{div}(\Omega)^d), \qquad \boldsymbol{u}_t \in L^{4/d}(0,T;H^1_{div}(\Omega)')$$

$$\varphi \in L^\infty(0,T;L^4(\Omega)) \cap L^2(0,T;H^1(\Omega)), \qquad \varphi_t \in L^2(0,T;H^1(\Omega)')$$

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which satisfies the energy inequality (identity if $d = 2$*)*

$$\mathcal{E}(\boldsymbol{u}(t),\varphi(t)) + \int_0^t (\nu\|\nabla \boldsymbol{u}(\tau)\|^2 + \|\nabla\mu(\tau)\|^2)d\tau \leq \mathcal{E}(\boldsymbol{u}_0,\varphi_0) + \int_0^t \langle \boldsymbol{h}, \boldsymbol{u}(\tau)\rangle d\tau,$$

for all $t > 0$*, where we have set*

$$\mathcal{E}(\boldsymbol{u}(t),\varphi(t)) = \frac{1}{2}\|\boldsymbol{u}(t)\|^2 + \frac{1}{4}\int_\Omega\int_\Omega J(x-y)(\varphi(x,t)-\varphi(y,t))^2 dx dy + \int_\Omega F(\varphi(t))$$

- **The nonlocal term implies that φ is not as regular as for the standard (local) CHNS system**: $\varphi \in L^2(H^1)$ (nonlocal), instead of $\varphi \in L^\infty(H^1)$ (local) $\Longrightarrow$ regularity results and uniqueness of weak sols in 2D difficult issues

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Theorem (F., Grasselli & Krejčí '13)

Assume that $J \in W^{2,1}(\mathbb{R}^2)$ *and that*

$$\boldsymbol{u}_0 \in H^1_{div}(\Omega)^2 \qquad \varphi_0 \in H^2(\Omega)$$

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Only recently we included (F., Gal & Grasselli, WIAS Preprint '14)

- **Newtonian kernels** : $J(x) = -k \log |x|$
- **Nonconstant viscosity**: $\nu = \nu(\varphi)$ with $0 < \nu_1 \leq \nu(\varphi) \leq \nu_2$

Constant mobility + regular potentials

Theorem (F., Gal & Grasselli '14)

Let $\boldsymbol{u}_0 \in L^2_{div}(\Omega)^2$, $\varphi_0 \in L^2(\Omega)$ *with* $F(\varphi_0) \in L^1(\Omega)$. *Then,* $\exists$ *a* **unique** *weak sol* $[\boldsymbol{u}, \varphi]$ *corresponding to* $[\boldsymbol{u}_0, \varphi_0]$

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Degenerate mobility + singular potential

- $\varphi-$dependent mobility in the original derivation of CH eq. (J.W. Cahn & J.E. Hilliard, 1971). Thermodynamically reasonable choice: $m(\varphi) = k(1 - \varphi^2)$
- Key assumption (cf. [Elliot & Garcke '96], [Gajewski & Zacharias '03], [Giacomin & Lebowitz '97,'98]): $mF'' \in C([-1, 1])$

Theorem (F., Gal & Grasselli '14)

Let $\boldsymbol{u}_0 \in L^2_{div}(\Omega)^2$, $\varphi_0 \in L^\infty(\Omega)$ *with* $F(\varphi_0) \in L^1(\Omega)$ *and* $M(\varphi_0) \in L^1(\Omega)$. *Then,* $\exists$ *a* **unique** *weak sol* $[\boldsymbol{u}, \varphi]$ *corresponding to* $[\boldsymbol{u}_0, \varphi_0]$

$M \in C^2(-1, 1)$ is s.t. $m(s)M''(s) = 1$ for all $s \in (-1, 1)$ and $M(0) = M'(0) = 0$

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- A continuous dependence estimate in $L^2_{div} \times (H^1)'$ also holds

$$\|\mathbf{u}_2(t)-\mathbf{u}_1(t)\|^2 + \|\varphi_2(t)-\varphi_1(t)\|^2_{(H^1)'}$$
$$+\int_0^t \Big(c_0\|\varphi_2(\tau)-\varphi_1(\tau)\|^2 + \frac{\nu}{2}\|\nabla(\mathbf{u}_2(\tau)-\mathbf{u}_1(\tau))\|^2\Big)d\tau$$
$$\leq \Gamma_1(t)\big(\|\mathbf{u}_{02}-\mathbf{u}_{01}\|^2 + \|\varphi_{02}-\varphi_{01}\|^2_{(H^1)'}\big) + C_\eta\Gamma_2(t)|\overline{\varphi}_{02}-\overline{\varphi}_{01}|$$

$|\overline{\varphi}_{01}|, |\overline{\varphi}_{02}| \leq \eta$, with $\Gamma_i \in C(\mathbb{R}^+)$ depending on weak sols norms

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$|\overline{\varphi}_{01}|, |\overline{\varphi}_{02}| \leq \eta$, with $\Gamma_i \in C(\mathbb{R}^+)$ depending on weak sols norms

- **Uniqueness of sol and $\exists$ of the global attractor for the local CH with degenerate mobility are open issues**

Consequences

- the nonlocal CHNS system generates a **semigroup** $S(t)$ of *closed* operators: $[\mathbf{u}(t), \varphi(t)] = S(t)[\mathbf{u}_0, \varphi_0]$ on the (metric) phase-space

$$\mathcal{X}_\eta = L^2_{div}(\Omega)^2 \times \mathcal{Y}_\eta \quad \mathcal{Y}_\eta = \{\varphi \in L^2(\Omega) : F(\varphi) \in L^1(\Omega), |\bar{\varphi}| \leq \eta\}$$

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- The global attractor in $\mathcal{X}_\eta$ for $S_\eta(t)$ is **connected**
- By establishing a **smoothing property** for the difference of two sols in $L^2_{div} \times L^2$

Theorem (F., Gal & Grasselli '14)

For every $\eta \geq 0$ the dynamical system $\big(\mathcal{X}_\eta, S(t)\big)$ possesses an **exponential attractor** $\mathcal{M}_\eta$*, i.e., a compact set in $\mathcal{X}_\eta$ s.t.*

(i) *Positively invariance: $S(t)\mathcal{M} \subset \mathcal{M}\ \forall t \geq 0$*

(ii) *Finite dimensionality: $\dim_F \mathcal{M} < \infty$*

(iii) *Exponential attraction: $\exists J : \mathbb{R}^+ \to \mathbb{R}^+$ increasing and $\kappa > 0$ s.t., $\forall R > 0$ and $\forall \mathcal{B} \subset \mathcal{X}_\eta$ with $\sup_{z\in\mathcal{B}} \mathbf{d}_{\mathcal{X}_\eta}(z,0) \leq R$ there holds*

$$\mathit{dist}(S(t)\mathcal{B}, \mathcal{M}) \leq J(R)e^{-\kappa t}$$

Optimal control for nonlocal CHNS

$$\varphi_t + \mathbf{u}\cdot\nabla\varphi = \text{div}\,(m(\varphi)\nabla\mu)$$
$$\mu = a\varphi - J*\varphi + F'(\varphi)$$
$$\mathbf{u}_t - \nu\Delta\mathbf{u} + (\mathbf{u}\cdot\nabla)\mathbf{u} + \nabla\pi = \mu\nabla\varphi + \mathbf{v}$$
$$\text{div}(\mathbf{u}) = 0$$

The external force **v** is the control function.

- **Optimal control for nonlocal CHNS**

$$
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- Cost functional

$$
J(y,v) := \frac{\beta_1}{2}\int_0^T\int_\Omega |u-u_Q|^2 + \frac{\beta_2}{2}\int_0^T\int_\Omega |\varphi-\varphi_Q|^2
+ \frac{\beta_3}{2}\int_\Omega |u(T)-u_\Omega|^2 + \frac{\beta_4}{2}\int_0^T\int_\Omega v^2,
$$

where $y=[\mathbf{u},\varphi]$ (the state) is the weak sol to the nonlocal CHNS corresponding to the control $v\in\mathcal{U}_{ad}\subset L^\infty(Q)$ (and with smooth initial data).

- **Aim: first order necessary conditions for existence of optimal control**

(In progress with E. Rocca & J. Sprekels)

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A diffuse interface model developed by Hawkins Daarud, van der Zee and Oden.

- φ: **tumor cell concentration** ($\varphi = 1$ tumorous cell, $\varphi = -1$ healthy cell phases)
- μ: **chemical potential**
- ψ: **nutrient concentration** (density of an extra-cellular water phase)

$$\varphi_t = \Delta\mu + p(\varphi)(\psi - \mu)$$

$$\mu = -\Delta\varphi + F'(\varphi)$$

$$\psi_t = \Delta\psi - p(\varphi)(\psi - \mu)$$

$$\partial_n\varphi = \partial_n\mu = \partial_n\psi = 0 \qquad \text{on } \partial\Omega$$

$$\varphi(0) = \varphi_0, \qquad \psi(0) = \psi_0$$

- Double-well Helmholtz **free energy density** F (accounting for cell-cell adhesion)

$$F(s) = (1 - s^2)^2$$

- **Proliferation function** $p \geq 0$

$$p(s) = \begin{cases} p_0(1 - s^2) & s \in [-1, 1] \\ 0 & \text{elsewhere} \end{cases}$$

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- **Energy balance**

$$\frac{d}{dt}E(\varphi, \psi) + \|\nabla\mu\|^2 + \|\nabla\psi\|^2 + \int_\Omega p(\varphi)(\mu - \psi)^2 = 0$$

$$E(\varphi, \psi) := \frac{1}{2}\|\nabla\varphi\|^2 + \frac{1}{2}\|\psi\|^2 + \int_\Omega F(\varphi)$$

- **Total** mass conservation

$$\overline{\varphi(t)} + \overline{\psi(t)} = \overline{\varphi_0} + \overline{\psi_0}$$

- **Existence and uniqueness of weak sols**

Theorem (F., Grasselli & Rocca)

Assume that $\varphi_0 \in H^1(\Omega)$ *and* $\psi_0 \in L^2(\Omega)$. *Then,* $\forall T > 0 \; \exists$ *a* **unique** *weak solution* $[\varphi, \psi]$ *on* $[0, T]$ *s.t.*

$$\varphi \in L^\infty(0, T; H^1(\Omega)) \cap L^2(0, T; H^3(\Omega)), \qquad \varphi_t \in L^2(0, T; H^1(\Omega)')$$

$$\mu \in L^2(0, T; H^1(\Omega))$$

$$\psi \in L^\infty(0, T; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega)), \qquad \psi_t \in L^2(0, T; H^1(\Omega)')$$

satisfying the energy identity. Moreover, if $[\varphi_{0i}, \psi_{0i}] \in H^1(\Omega) \times L^2(\Omega)$, *then*

$$\|\varphi_2(t) - \varphi_1(t)\|_{(H^1)'} + \|\psi_2(t) - \psi_1(t)\|_{(H^1)'} \leq \Lambda\big(\|\varphi_{02} - \varphi_{01}\|_{(H^1)'} + \|\psi_{02} - \psi_{01}\|_{(H^1)'}\big)$$

- **Regularity result** (assuming, i.e., $\varphi_0 \in H^3(\Omega)$ and $\psi_0 \in H^1(\Omega)$)
- **Existence of the global attractor**

- **Nonlocal Cahn-Hilliard-Navier-Stokes**
  - unmatched densities (Abels, Garcke & Grün '12 for the local CHNS)
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  - **non-isothermal model(s)**
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- **Tumor dynamics**
  - coupling with Darcy laws
    (Cahn-Hilliard-Hele-Shaw **multicomponent** models, cfr. Lowengrub et al. '08 & '10)
  - singular potentials and degenerate mobilities