On a thermodynamically consistent model for two-phase fluids

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Implicitly constituted materials:
Modeling, Analysis and Computing

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Highlights

- We consider a nonisothermal model for two-component fluids being thermodynamically consistent for a wide range of temperature values.
- The model describes the behavior of the variables:
  - $\boldsymbol{u}$ (macroscopic velocity),
  - φ (order parameter),
  - μ (chemical potential),
  - θ (*absolute* temperature).
- With Michela Eleuteri and Elisabetta Rocca we proved existence of "weak" solutions in 3D and existence of "strong" solutions in 2D.
- I will now describe additional results holding in the 2D case.

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The equations

$$\boldsymbol{u}_t + \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla p = \Delta \boldsymbol{u} - \operatorname{div}(\nabla\varphi \otimes \nabla\varphi) \tag{mom}$$

$$\varphi_t + \boldsymbol{u} \cdot \nabla\varphi = \Delta\mu \tag{CH1}$$

$$\mu = -\Delta\varphi + F'(\varphi) - \theta \tag{CH2}$$

$$\theta_t + \boldsymbol{u} \cdot \nabla\theta + \theta(\varphi_t + \boldsymbol{u} \cdot \nabla\varphi) - \operatorname{div}(\kappa(\theta)\nabla\theta) = |\nabla \boldsymbol{u}|^2 + |\nabla\mu|^2 \tag{heat}$$

- Heat conductivity: $\kappa(\theta) \sim 1 + \theta^q$
- Configuration potential: $F(\varphi)$ of polynomial growth

- $\Omega = [0, 1] \times [0, 1]$
- Periodic boundary conditions

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Related mathematical models

- The main feature (and also main difficulty) of the system is the non-linearized nature of the internal energy balance, given by the quadratic terms on the right hand side.
- Non-isothermal systems with these characteristics have been studied in connection with
  - phase transitions: [Luterotti, S., Stefanelli], [Miranville, S.], [Feireisl, Petzeltová, Rocca], [Benzoni-Gavage, Chupin, Jamet, Vovelle]
  - hydrogen storage: Bonetti, Colli, Laurençot, Chiodaroli
  - thermal fluids (Navier-Stokes-Fourier system): Feireisl, Novotný, Pokorný, [Bulíček, Feireisl, Málek] and many others
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The physical principles

- Starting from the system equations one can recover the energy conservation (1st law):

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathcal{E} = 0, \quad \mathcal{E} = \int_\Omega \left(\frac{1}{2}|\boldsymbol{u}|^2 + \frac{1}{2}|\nabla\varphi|^2 + F(\varphi) + \theta \right).$$

- as well as the entropy production inequality (2st law):

$$\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega -\ln\theta + \int_\Omega \frac{1}{\theta}\left(|\nabla \boldsymbol{u}|^2 + |\nabla\mu|^2\right) \leq 0.$$

- Any (reasonably defined) solution should comply with these principles (particularly from the point of view of regularity).

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  Actually, weak solutions were studied in 3D under the sole regularity assumptions on the finiteness of the initial energy and entropy.

- On the other hand, in 2D one can obtain additional regularity estimates and control the right hand side of (heat) in L^2.
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The result of ERS (Ann. Inst. Poincaré, 2016)

Theorem (Eleuteri, Rocca, S.)

Assume (all variables are Ω-periodic)

$$\boldsymbol{u}_0 \in H^1(\Omega), \quad \operatorname{div} \boldsymbol{u}_0 = 0,$$
$$\varphi_0 \in H^3(\Omega),$$
$$\theta_0 \in H^1(\Omega), \quad \theta_0 > 0 \text{ a.e.}, \quad \log\theta_0 \in L^1(\Omega).$$

Then there exists at least one "strong solution" such that

$$\boldsymbol{u} \in H^1(0,T;L^2(\Omega)) \cap L^\infty(0,T;H^1(\Omega)) \cap L^2(0,T;H^2(\Omega)),$$
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Questions left open:

1) Uniqueness of strong solutions

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Questions left open:

3) Smoothing properties and long-time behavior (attractors. . .)

Why a regularity gap?

- The regularity framework corresponds to
  - "Strong" solutions to Navier-Stokes
  - "Second energy estimate" for Cahn-Hilliard
- But what about equation (heat)?

$$\theta_t + \boldsymbol{u} \cdot \nabla\theta + \theta(\varphi_t + \boldsymbol{u} \cdot \nabla\varphi) - \operatorname{div}(\kappa(\theta)\nabla\theta) = |\nabla \boldsymbol{u}|^2 + |\nabla\mu|^2 \qquad \text{(heat)}$$

  This is much less flexible from the point of view of regularity. We have:
  - Initial datum $\theta_0 \in H^1(\Omega)$ (not necessarily in L^∞);
  - Right hand side exactly in L^2;
  - Heat conductivity going as a power of θ.
- **Outcome:** not clear whether we can get additional "parabolic estimates" (like testing by $\kappa(\theta)\theta_t$).

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Smoother solutions

- The most critical term in (heat) is $|\nabla \boldsymbol{u}|^2$. To improve its regularity, we take the initial velocity $\boldsymbol{u}_0 \in H^{1+r}(\Omega)$ for some $r > 0$.
- Once the right hand side of (heat) is better than L^2, we can improve the regularity of the temperature. There are probably several ways to do it. We get directly a uniform in time H^1-estimate (alternative method: Moser-iterations). In any case the key point stands in the fact that the power-like growth of $\kappa(\theta)$ is no longer an obstacle.
- The uniform control of θ in $H^1(\Omega)$ is also at the basis of the uniqueness proof.

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Theorem: Well-posedness

Theorem (Eleuteri, Gatti, S., 2017)

Assume (all variables are Ω-periodic)

$$\boldsymbol{u}_0 \in H^{1+r}(\Omega), \quad r \in (0, 1/2], \quad \operatorname{div} \boldsymbol{u}_0 = 0,$$
$$\varphi_0 \in H^3(\Omega),$$
$$K(\theta_0) \in H^1(\Omega), \quad \theta_0 > 0 \text{ a.e.}, \quad 1/\theta_0 \in L^1(\Omega).$$

Then there exists one **and only one** "**stable** solution" such that

$$\boldsymbol{u} \in H^1(0, T; H^r(\Omega)) \cap L^\infty(0, T; H^{1+r}(\Omega)) \cap L^2(0, T; H^{2+r}(\Omega)),$$
$$\varphi \in H^1(0, T; H^1(\Omega)) \cap L^\infty(0, T; H^3(\Omega)),$$
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Moreover, stable solutions enjoy **parabolic smoothing** properties.

Long-time behavior

- We would like to analyze the long-time behavior of trajectories in the regularity class determined before ("stable solutions").
- In particular, we would like to characterize ω-limits of single trajectories as well as the global attractor.
- **Notice:**
  - The only source of nonconvexity is in equation (CH2) (the term $F'(\varphi)$);
  - We have conservation of mass, momentum, total energy. No external source is present;
  - In particular, in view of periodic b.c., solutions asymptotically tend to rotate around the flat torus with constant velocity $m = \int_\Omega u_0$.

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ω-limit sets

- A quadruple $(\boldsymbol{u}_\infty, \varphi_\infty, \mu_\infty, \theta_\infty)$ lies in the ω-limit set of a "stable" solution iff there exists $t_n \nearrow \infty$ such that

$$(\boldsymbol{u}(t_n), \varphi(t_n), \mu(t_n), \theta(t_n)) \to (\boldsymbol{u}_\infty, \varphi_\infty, \mu_\infty, \theta_\infty) \ \text{suitably}.$$

- By parabolic smoothing estimates, it is not difficult to prove that each trajectory has a nonempty ω-limit set all of whose elements satisfy

$$\begin{aligned}
&\operatorname{div} \boldsymbol{u}_\infty = 0, \\
&\boldsymbol{u}_\infty \cdot \nabla \boldsymbol{u}_\infty + \nabla p_\infty = \Delta \boldsymbol{u}_\infty - \operatorname{div}(\nabla\varphi_\infty \otimes \nabla\varphi_\infty), \\
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Structure of ω-limit sets, $\boldsymbol{m} = \mathbf{0}$

- In view of conservation properties and occurrence of dissipation integrals:

$$\int_0^\infty \left(\|\nabla \boldsymbol{u}\|_{L^2}^2 + \|\nabla \theta\|_{L^2}^2 + \|\nabla \mu\|_{L^2}^2 \right) < \infty,$$

the structure of reachable stationary states simplifies a lot.

- For $\boldsymbol{m} = \mathbf{0}$, $\boldsymbol{u}(t) \to \mathbf{0}$; moreover, μ_∞, θ_∞ are constants. The system reduces to the single equation

$$-\Delta \varphi_\infty + F'(\varphi_\infty) = \mu_\infty + \theta_\infty.$$

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The constants μ_∞, θ_∞

- Once initial data are assigned, the quantities

$$\boldsymbol{m} := \int_\Omega \boldsymbol{u} \text{ (here } \boldsymbol{m} = \boldsymbol{0}\text{)}, \qquad m := \int_\Omega \varphi, \qquad M := \mathcal{E}$$

  are conserved.

- There exists a constant $C = C(\boldsymbol{m}, m, M)$ such that

$$|\mu_\infty| + |\theta_\infty| + \|\varphi_\infty\|_{H^4(\Omega)} \leq C(\boldsymbol{m}, m, M).$$

- On the other hand, different elements of the ω-limit of a single trajectory may solve

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Structure of ω-limit sets, $\boldsymbol{m} \neq \mathbf{0}$

- If $\boldsymbol{m} \neq \mathbf{0}$, $\boldsymbol{u}(t)$ converges to $\boldsymbol{m} = \int_\Omega \boldsymbol{u}_0$: asymptotically solutions tend to "rotate" around the flat torus.
- Setting
$$\tilde{\zeta}(t,x) := \zeta(t, x + t\boldsymbol{m}), \quad \text{for } \zeta = \boldsymbol{u}, \varphi, \mu, \theta, p,$$
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The other equations are transformed analogously.
- Then, ω-limit sets exist up to controlling "rotations", namely if $t_n \nearrow \infty$, then taking a subsequence n_k such that $t_{n_k}\boldsymbol{m} \to x_0$, $\varphi(t_{n_k}) \to \varphi_\infty$ such that
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Structure of ω-limit sets, $\boldsymbol{m} \neq \mathbf{0}$

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The global attractor

- To "stable" solutions is naturally associated a solution operator (semigroup) $S(t) : z_0 \mapsto z(t)$.
- **Find** a functional space X such that $S(t) : X \to X$ has "good properties" (e.g., continuity).
- Then, the global attractor for $S(\cdot)$ is a compact and completely invariant subset $\mathcal{A} \subset X$ such that

$$\lim_{t \nearrow \infty} \mathrm{dist}_X(S(t)B, \mathcal{A}) = 0$$

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Mathematical difficulties

- **Presence of constraints:**
  - Some quantities ($\boldsymbol{m}$, m, M) do not dissipate: we have to consider this in the choice of X.
  - No way to construct a dissipative inequality directly. Absorbing sets must be constructed as neighbourhood of the set of reachable stationary solutions.
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  - just consider the case $m = 0$.
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Structure of the phase space

- The conditions on initial data for "stable solutions" are

$$\boldsymbol{u}_0 \in H^{1+r}(\Omega), \quad \varphi_0 \in H^3(\Omega), \quad K(\theta_0) \in H^1(\Omega), \quad 1/\theta_0 \in L^1(\Omega).$$

- Due to occurrence of $1/\theta$ and $K(\theta)$, this gives rise to a metric space (distance accounting, e.g., for $\|1/\theta\|_{L^1(\Omega)}$).
- Hence, we may use

$$X = X(\mathbf{0}, m, M) = \Big\{ (\boldsymbol{u}, \varphi, \theta) \in H^{1+r} \times H^3 \times H^1 : \; K(\theta) \in H^1, \\ 1/\theta \in L^1, \; \int_\Omega \boldsymbol{u} = \mathbf{0}, \; \int_\Omega \varphi = m, \; \mathcal{E} = M \Big\}.$$

- We would like to construct a compact set $\mathcal{A} = \mathcal{A}(\mathbf{0}, m, M)$ uniformly attracting any metric-bounded set $B \subset X(\mathbf{0}, m, M)$.

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- We have asymptotic compactness of trajectories, namely there exists a metric space $W \subset\subset X$ such that $S(1)B$ is bounded in W for any bounded $B \subset X$.
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- But this requires to determine $\underline{\theta} = \underline{\theta}(M, m) > 0$ such that $\theta_\infty \geq \underline{\theta}$ for any "reachable" θ_∞.
- We need to impose a (further) constraint on the initial entropy:

$$X^R := \left\{ (\boldsymbol{u}, \varphi, \theta) \in X(\boldsymbol{0}, m, M) : -\int_\Omega \theta \leq R \right\}.$$

Under this condition, we can actually prove that $\theta_\infty \geq \underline{\theta}(M, m, R)$.

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Theorem: Long-time behavior

Theorem (Eleuteri, Gatti, S., 2017)

Take initial data in $X^R(\mathbf{0}, M, m)$. Then, the semiflow associated with "stable solutions" admits the global attractor $\mathcal{A}^R = \mathcal{A}^R(\mathbf{0}, M, m)$.

Moreover, there exists $C = C(M, m, R)$ such that, for any $(\boldsymbol{u}, \varphi, \theta) \in \mathcal{A}^R$,

$$\|\boldsymbol{u}\|_{H^2} + \|\varphi\|_{H^4} + \|\theta\|_{H^2} + \|1/\theta\|_{H^1} \leq C.$$

Possible extensions – singular potentials

$$\boldsymbol{u}_t + \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla p = \Delta \boldsymbol{u} - \operatorname{div}(\nabla\varphi \otimes \nabla\varphi) \tag{mom}$$

$$\varphi_t + \boldsymbol{u} \cdot \nabla\varphi = \Delta\mu \tag{CH1}$$

$$\mu = -\Delta\varphi + F'(\varphi) - \theta \tag{CH2}$$

$$\theta_t + \boldsymbol{u} \cdot \nabla\theta + \theta(\varphi_t + \boldsymbol{u} \cdot \nabla\varphi) - \operatorname{div}(\kappa(\theta)\nabla\theta) = |\nabla \boldsymbol{u}|^2 + |\nabla\mu|^2 \tag{heat}$$

- $F'(\varphi)$ derivative (subdifferential) of
- logarithmic potential: $F(\varphi) \sim (1+\varphi)\log(1+\varphi) + (1-\varphi)\log(1-\varphi) - \lambda\varphi^2$
- **Question:** can we consider strong solutions to (mom)? Note that regularity theory for (CH2) is worse.

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- (AC1) and (AC2) combine as

$$\varphi_t + \boldsymbol{u} \cdot \nabla\varphi - \Delta\varphi + F'(\varphi) = \theta \tag{AC}$$

- **Problem:** we have less regularity for φ from the energy estimate.

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Possible extensions – non-newtonian fluids

$$\boldsymbol{u}_t + \boldsymbol{u} \cdot \nabla \boldsymbol{u} + \nabla p = \operatorname{div}(|\nabla \boldsymbol{u}|^{p-2} \nabla \boldsymbol{u}) - \operatorname{div}(\nabla \varphi \otimes \nabla \varphi) \qquad \text{(mom)}$$

$$\varphi_t + \boldsymbol{u} \cdot \nabla \varphi = -\mu \ \text{ or } \Delta \mu \qquad \text{(AC1)}$$

$$\mu = -\Delta \varphi + F'(\varphi) - \theta \qquad \text{(AC2)}$$

$$\theta_t + \boldsymbol{u} \cdot \nabla \theta + \theta(\varphi_t + \boldsymbol{u} \cdot \nabla \varphi) - \operatorname{div}(\kappa(\theta) \nabla \theta) = |\nabla \boldsymbol{u}|^2 + |(\nabla)\mu|^2 \qquad \text{(heat)}$$

- The possibility to work with strong solutions of (mom) depends as usual on the value of $p \geq 2$ and on the space dimension.
- Consider, however, that the regularity analysis for $\boldsymbol{u}$ and φ may not be decoupled.

More difficult extensions

- Other types (non-periodic) boundary conditions;
- Presence of forcing terms (e.g., heat sources);
- Temperature-dependent coefficients (e.g., viscosity) or temperature-independent coefficients (choice of Fourier's law)

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References

M. Eleuteri, S. Gatti, G.S., *Regularity and long-time behavior for a thermodynamically consistent model for complex fluids in two space dimensions*, available tomorrow on **arXiv**.

See also:

M. Eleuteri, E. Rocca, G.S., *On a non-isothermal diffuse interface model for two-phase flows of incompressible fluids*, Discrete Contin. Dyn. Syst., **35** (2015), 2497–2522.

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Thanks for your attention!