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A diffuse interface model for two-phase flow with nonlocal interactions

THE NONLOCAL CAHN-HILLIARD/NAVIER STOKES MODEL

Diffuse-interface model in which the sharp interface separating the two fluids (e.g., oil and water) is replaced by a diffuse one by introducing an order parameter φ (relative concentration of one of the fluids). The dynamics of φ is governed by a Cahn-Hilliard type equation with a transport term. φ influences the fluid velocity $\boldsymbol{u}$ through a capillarity force $\mu\nabla\varphi$. Assuming *matched densities* in $\Omega\times(0,\infty)$, $\Omega\subset\mathbb{R}^d$, $d=2,3$

(nlocCHNS)
$$\begin{aligned}&\boldsymbol{u}_t+(\boldsymbol{u}\cdot\nabla)\boldsymbol{u}-2\mathrm{div}\big(\nu(\varphi)D\boldsymbol{u}\big)+\nabla\pi=\mu\nabla\varphi+\boldsymbol{v}\\&\mathrm{div}(\boldsymbol{u})=0\\&\varphi_t+\boldsymbol{u}\cdot\nabla\varphi=\mathrm{div}\,(m(\varphi)\nabla\mu)\end{aligned}$$

μ chemical potential, first variation of the (total Helmholtz) nonlocal free energy. This system is endowed with the following boundary and initial conditions

(BIC)
$$\begin{aligned}&\partial_{\boldsymbol{n}}\mu=0\qquad \boldsymbol{u}=0\qquad \text{on}\quad \partial\Omega\\&\boldsymbol{u}(0)=\boldsymbol{u}_0\qquad \varphi(0)=\varphi_0\end{aligned}$$

- **Nonlocal free energy** (van der Waals) rigorously justified by Giacomin and Lebowitz as macroscopic limit of microscopic phase segregation models

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

  where $K:\mathbb{R}^d\to\mathbb{R}$ s.t. $K(x)=K(-x)$. Local free energy (having $\int_\Omega|\nabla\varphi|^2$ in place of the interaction integral) is an approximation of the nonlocal one

- **Nonlocal chemical potential**

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

  where

$$(K*\varphi)(x):=\int_\Omega K(x-y)\varphi(y)dy\quad a(x):=\int_\Omega K(x-y)dy$$

F double-well potential: Helmholtz free energy density of uniform mixture

- Singular

$$F(s)=-\frac{\theta_c}{2}s^2+\frac{\theta}{2}\big((1+s)\log(1+s)+(1-s)\log(1-s)\big)\quad \forall s\in(-1,1)\quad 0<\theta<\theta_c$$

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

Weak solutions (regular potential+constant or non-degenerate mobility)

Theorem 1 (Colli, F., Grasselli ’12). *Assume that $K\in W^{1,1}(\mathbb{R}^d)$, $K(z)=K(-z)$, $a(x)\geq 0$ and that $\boldsymbol{v}\in L^2_{loc}(\mathbb{R}^+;H^1_{div}(\Omega)')$. Let $\boldsymbol{u}_0\in L^2_{div}(\Omega)^d$, $\varphi_0\in L^2(\Omega)$, $F(\varphi_0)\in L^1(\Omega)$. Then, $\forall T>0$ $\exists$ a weak sol $[\boldsymbol{u},\varphi]$ to **(nloc CHNS)** s.t.*

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

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

$$\mathcal{E}(\boldsymbol{u}(t),\varphi(t))+\int_0^t(\|\sqrt{\nu(\varphi)}D\boldsymbol{u}(\tau)\|^2+\|\nabla\mu(\tau)\|^2)d\tau\leq\mathcal{E}(\boldsymbol{u}_0,\varphi_0)+\int_0^t\langle\boldsymbol{v},\boldsymbol{u}(\tau)\rangle d\tau\qquad \forall t>0$$

where we have set $\quad\mathcal{E}(\boldsymbol{u}(t),\varphi(t))=\frac{1}{2}\|\boldsymbol{u}(t)\|^2+\mathcal{E}(\varphi(t))$

Theorem 1 holds also for regular coercive potentials F of arbitrary polynomial growth. Furthermore, existence of weak sols in 2D-3D has been obtained also for: constant mobility+singular potential (F., Grasselli ’12) and degenerate mobility+singular potential (F., Grasselli, Rocca ’14).

For weak sols in 2D with constant viscosity we have also

Theorem 2 (F., Gal, Grasselli ’14). *The weak sol $[\boldsymbol{u},\varphi]$ corresponding to $[\boldsymbol{u}_0,\varphi_0]$ is unique .*

Strong solutions in 2D (regular potential+constant mobility)

Theorem 3 (F., Grasselli, Krejčí ’13). *Let $\boldsymbol{v}\in L^2_{loc}(\mathbb{R}^+;L^2_{div}(\Omega)^2)$ and in addition $K\in W^{2,1}(\mathbb{R}^2)$ or K newtonian. If $\boldsymbol{u}_0\in H^1_{div}(\Omega)^2$, $\varphi_0\in H^2(\Omega)$ then, $\forall T>0$ $\exists$ unique strong sol $[\boldsymbol{u},\varphi]$ s.t.*

$$\begin{aligned}&\boldsymbol{u}\in L^\infty(0,T;H^1_{div}(\Omega)^2)\cap L^2(0,T;H^2(\Omega)^2)\qquad \boldsymbol{u}_t\in L^2(0,T;L^2_{div}(\Omega)^2)\\&\varphi\in L^\infty(0,T;H^2(\Omega))\qquad \varphi_t\in L^\infty(0,T;L^2(\Omega))\cap L^2(0,T;H^1(\Omega))\end{aligned}$$

Theorem 3 has been extended also for the case of nonconstant viscosity (F., Gal, Grasselli ’14)

References

–P. Colli, S. Frigeri, M. Grasselli, *Global existence of weak solutions to a nonlocal Cahn–Hilliard–Navier–Stokes system*, J. Math. Anal. Appl. **386** (2012), 428-444.
–S. Frigeri, M. Grasselli, *Nonlocal Cahn–Hilliard–Navier–Stokes systems with singular potentials*, Dyn. Partial Differ. Equ. **9** (2012), 273-304.
–S. Frigeri, M. Grasselli, P. Krejčí, *Strong solutions for two-dimensional nonlocal Cahn–Hilliard–Navier–Stokes systems*, J. Differential Equations **255** (2013), 2597-2614.
–S. Frigeri, M. Grasselli, E. Rocca, *A diffuse interface model for two-phase incompressible flows with nonlocal interactions and nonconstant mobility*, WIAS Preprint No. 1941 (2014).
–S. Frigeri, C. Gal, M. Grasselli, *On nonlocal Cahn–Hilliard–Navier–Stokes systems in two dimensions*, WIAS Preprint No. 1923 (2014).

Optimal control for nloc CHNS in 2D (regular potential+constant mobility)

Problem **(CP)**: minimize the **cost functional**

$$J(y,\boldsymbol{v}):=\frac{\beta_1}{2}\|\boldsymbol{u}-\boldsymbol{u}_Q\|^2_{L^2(Q)^2}+\frac{\beta_2}{2}\|\varphi-\varphi_Q\|^2_{L^2(Q)}+\frac{\beta_3}{2}\|\boldsymbol{u}(T)-\boldsymbol{u}_\Omega\|^2+\frac{\beta_4}{2}\|\varphi(T)-\varphi_\Omega\|^2+\frac{\gamma}{2}\|\boldsymbol{v}\|^2_{L^2(Q)^2}$$

where $y:=[\boldsymbol{u},\varphi]$ solves **(nlocCHNS)** (with $m=1$) and **BIC** and the external body force density $\boldsymbol{v}$, which plays the role of the **control**, belongs to a suitable closed, bounded and convex subset of the **space of controls** $\mathcal{V}:=L^2\big(0,T;L^2_{div}(\Omega)^2\big)$

- Introducing the space $\mathcal{H}:=\big[L^\infty(0,T;H^1_{div}(\Omega)^2)\cap L^2(0,T;H^2(\Omega)^2)\big]\times L^\infty(0,T;H^2(\Omega))$, then, the **control-to-state map** $\mathcal{S}:\mathcal{V}\to\mathcal{H}$, $\boldsymbol{v}\in\mathcal{V}\mapsto\mathcal{S}(\boldsymbol{v}):=y:=[\boldsymbol{u},\varphi]\in\mathcal{H}$, where $y:=[\boldsymbol{u},\varphi]$ is the unique strong sol to Problem **(nloc CHNS)** corresponding to $\boldsymbol{v}\in\mathcal{V}$ and to fixed initial data $\boldsymbol{u}_0\in H^1_{div}(\Omega)^2$, $\varphi_0\in H^2(\Omega)$, is well defined
- Set of **admissible controls** $\mathcal{V}_{ad}:=\big\{\boldsymbol{v}\in\mathcal{V}:\ v_{a,i}(x,t)\leq v_i(x,t)\leq v_{b,i}(x,t),$ a.e. $(x,t)\in\Omega\times(0,T)\big\}$ with $\boldsymbol{v}_a,\boldsymbol{v}_b\in\mathcal{V}\cap L^\infty(Q)^2$ prescribed

Theorem 4 (F., Rocca, Sprekels ’14). *Problem **(CP)** admits a sol $\overline{\boldsymbol{v}}\in\mathcal{V}_{ad}$*

By studying the **differentiability property** of

$$\mathcal{S}:\mathcal{V}\to\big[C([0,T];L^2_{div}(\Omega)^2)\cap L^2(0,T;H^1_{div}(\Omega)^2)\big]\times\big[C([0,T];L^2(\Omega))\cap L^2(0,T;H^1(\Omega))\big]$$

First order necessary optimality conditions. Introduce the **adjoint system**

$$\begin{aligned}\widetilde{\boldsymbol{p}}_t=&-2\mathrm{div}\big(\nu(\overline{\varphi})D\widetilde{\boldsymbol{p}}\big)-(\overline{\boldsymbol{u}}\cdot\nabla)\widetilde{\boldsymbol{p}}+(\widetilde{\boldsymbol{p}}\cdot\nabla^T)\overline{\boldsymbol{u}}+\widetilde{q}\nabla\overline{\varphi}-\beta_1(\overline{\boldsymbol{u}}-\boldsymbol{u}_Q)\\\widetilde{q}_t=&-(a\Delta\widetilde{q}+\nabla K*\nabla\widetilde{q}+F''(\overline{\varphi})\Delta\widetilde{q})-\overline{\boldsymbol{u}}\cdot\nabla\widetilde{q}+2\nu'(\overline{\varphi})D\overline{\boldsymbol{u}}:D\widetilde{\boldsymbol{p}}\\&-\big(a\widetilde{\boldsymbol{p}}\cdot\nabla\overline{\varphi}-K*(\widetilde{\boldsymbol{p}}\cdot\nabla\overline{\varphi})+F''(\overline{\varphi})\widetilde{\boldsymbol{p}}\cdot\nabla\overline{\varphi}\big)+\widetilde{\boldsymbol{p}}\cdot\nabla\overline{\mu}-\beta_2(\overline{\varphi}-\varphi_Q)\\&\mathrm{div}(\widetilde{\boldsymbol{p}})=0\\&\widetilde{\boldsymbol{p}}=0,\qquad\partial_{\boldsymbol{n}}\widetilde{q}=0\quad\text{on }\Sigma\\&\widetilde{\boldsymbol{p}}(T)=\beta_3(\overline{\boldsymbol{u}}(T)-\boldsymbol{u}_\Omega),\qquad\widetilde{q}(T)=\beta_4(\overline{\varphi}(T)-\varphi_\Omega)\end{aligned}$$

Theorem 5 (F., Rocca, Sprekels ’14). *Let $\overline{\boldsymbol{v}}\in\mathcal{V}_{ad}$ be an optimal control for Problem **(CP)** with associated state $\overline{y}=[\overline{\boldsymbol{u}},\overline{\varphi}]=S(\overline{\boldsymbol{v}})$ and adjoint state $[\widetilde{\boldsymbol{p}},\widetilde{q}]$. Then*

$$\gamma\int_0^T\int_\Omega\overline{\boldsymbol{v}}\cdot(\boldsymbol{v}-\overline{\boldsymbol{v}})+\int_0^T\int_\Omega\widetilde{\boldsymbol{p}}\cdot(\boldsymbol{v}-\overline{\boldsymbol{v}})\geq 0\qquad\forall\boldsymbol{v}\in\mathcal{V}_{ad}\quad\Big(\Leftrightarrow\overline{\boldsymbol{v}}=P_{\mathcal{V}_{ad}}\big(\{-\widetilde{\boldsymbol{p}}/\gamma\}\big)\Big),$$

where $P_{\mathcal{V}_{ad}}$ is the orthogonal projector in $L^2(Q)^2$ onto $\mathcal{V}_{ad}$

Reference

–S. Frigeri, E. Rocca, J. Sprekels, *Optimal distributed control of a nonlocal Cahn–Hilliard/Navier–Stokes system in 2D*, WIAS Preprint No. 2036 (2014)

Nonlocal Cahn-Hilliard/Navier-Stokes system with unmatched densities

The following system is the nonlocal version of the model derived by Abels, Garcke and Grün describing the two-phase flow of incompressible newtonian viscous fluids with different densities

(nloc AGG)
$$\begin{aligned}&(\rho\boldsymbol{u})_t+\mathrm{div}(\rho\boldsymbol{u}\otimes\boldsymbol{u})-\nu\Delta\boldsymbol{u}+\nabla\pi+\mathrm{div}(\boldsymbol{u}\otimes\widetilde{\boldsymbol{J}})=\mu\nabla\varphi\\&\mathrm{div}(\boldsymbol{u})=0\\&\varphi_t+\boldsymbol{u}\cdot\nabla\varphi=\mathrm{div}(m(\varphi)\nabla\mu)\\&\mu=a\varphi-K*\varphi+F'(\varphi)\\&\widetilde{\boldsymbol{J}}:=-\beta m(\varphi)\nabla\mu,\qquad\beta=(\widetilde{\rho}_2-\widetilde{\rho}_1)/2\end{aligned}$$

where

$$\rho(\varphi)=(\widetilde{\rho}_2+\widetilde{\rho}_1)/2+(\widetilde{\rho}_2-\widetilde{\rho}_1)(\varphi/2)$$

and where $\widetilde{\rho}_1,\widetilde{\rho}_2>0$ are the specific constant mass densities of the unmixed fluids.

Assuming **singular potential** and nonconstant and **non-degenerate mobility**, i.e. satisfying

$$m_*\leq m(s)\leq m^*,\qquad\forall s\in\mathbb{R},$$

for some $m_*,m^*>0$, we can prove

Theorem 6. *Assume that $K\in W^{1,1}(\mathbb{R}^d)$, $K(z)=K(-z)$, $a(x)\geq 0$. Let $\boldsymbol{u}_0\in L^2_{div}(\Omega)^d$, $\varphi_0\in L^\infty(\Omega)$ such that $F(\varphi_0)\in L^1(\Omega)$ and $|\overline{\varphi}_0|<1$. Then, $\forall T>0$ and $\forall p\in[2,\infty)$ Problem **(nloc AGG)** admits a weak sol $[\boldsymbol{u},\varphi]$ such that*

$$\begin{aligned}&\boldsymbol{u}\in L^\infty(0,T;L^2_{div}(\Omega)^d)\cap L^2(0,T;H^1_{div}(\Omega)^d)\\&\varphi\in L^\infty(0,T;L^p(\Omega))\cap L^2(0,T;H^1(\Omega))\\&|\varphi(x,t)|<1,\qquad\text{a.e. }(x,t)\in\Omega\times(0,T)\\&\mu\in L^2(0,T;H^1(\Omega))\\&(\rho\boldsymbol{u})_t\in L^{4/3}(0,T;D(A)')\qquad\varphi_t\in L^2(0,T;H^1(\Omega)')\end{aligned}$$

(A is the Stokes operator with non-slip boundary condition) satisfying the following energy inequality

$$\int_\Omega\frac{1}{2}\rho\boldsymbol{u}^2+\mathcal{E}(\varphi)+\nu\int_0^t\|\nabla\boldsymbol{u}\|^2d\tau+\int_0^t\big\|\sqrt{m(\varphi)}\nabla\mu\big\|^2d\tau\leq\int_\Omega\frac{1}{2}\rho(\varphi_0)\boldsymbol{u}_0^2+\mathcal{E}(\varphi_0)\qquad\forall t\in[0,T]$$

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