Dynamical approximation of equilibrium interfaces in contact with surfaces.

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1 Introduction. Multi-phase/multi-constituent problems. Order parameter.

- Bi-phasic. Order parameter $\phi : \Omega \subset \mathbb{R}^N \to \mathbb{R}$. Ex. $\phi = -1$ (Solid), $\phi = 1$ (Liquid).

  Effects: solidification front, dendritic formation

- Two immiscible fluids. Ex. $\phi = -1$ (oil) and $\phi = 1$ (water).

  Effects: coarsening, merging,...

- Alloys of two-materials.

  Ex. (Al-Cu). $\phi = 0$ Al, $\phi = 1$ Cu ($\phi \equiv$ volume fraction of Cu).

  If ρ_a (resp. ρ_c) is the Al mass density (resp.Cu), then the alloys mass density can be modeled by

  $$\rho = (1-\phi)\rho_a + \phi\rho_c$$

  Effects: patters formation, ...

2 Static problem. Minima of Ginzburg-Landau free-energy

- Ginzburg-Landau Free-energy:

  $$\mathcal{E}(\phi) = \frac{\varepsilon}{2}\int_\Omega |\nabla\phi|^2 + \frac{1}{\varepsilon}\int_\Omega F(\phi), \quad F(\phi) = \frac{1}{4}((1+\phi)(1-\phi))^2$$

  $F(\phi)$ double-well potential. $\varepsilon \sim$ interface width. $\Omega \subset \mathbb{R}^N$ a bounded domain.

- Static problem (non-convex minimum problem, under BCs giving contact conditions with a solid container):

  $$\min \mathcal{E}(\phi) \quad s.t. \quad \phi|_{\partial\Omega_D} = \phi_D$$

- Optimality system:

  $$\left\langle \frac{\delta\mathcal{E}}{\delta\phi}(\phi), \overline{\phi} \right\rangle = 0 \quad \forall \overline{\phi} \quad s.t. \quad \overline{\phi}|_{\partial\Omega_D} = 0.$$

- (Elliptic) boundary problem:

$$PDE \qquad -\varepsilon\Delta\phi + \frac{1}{\varepsilon}F'(\phi) = 0 \quad \Omega,$$

$$BCs \qquad \phi|_{\partial\Omega_D} = \phi_D, \quad \varepsilon\nabla\phi\cdot\boldsymbol{n}|_{\partial\Omega_N} = 0.$$

- RK: A continuum of solutions (with the same energy) could exits.

  Ex. If Ω is a disk, the problem

$$-\Delta\phi + \phi^3 = \lambda\phi \quad \Omega, \quad \phi|_{\partial\Omega} = 0,$$

  has a continuum of sols when $\lambda > 0$ is large enough [A. Haraux '91]

3 Dissipative dynamical problems, non-conserved (Allen-Cahn) o conservative (Cahn-Hilliard)

- Allen-Cahn (maximum principle):

$$\partial_t\phi + M\frac{\delta\mathcal{E}}{\delta\phi}(\phi) = 0, \quad +IC: \ \phi|_{t=0} = \phi_0, \quad +BCs$$

- Cahn-Hilliard (conservative):

$$\partial_t\phi + \nabla\cdot\left(M\nabla\frac{\delta\mathcal{E}}{\delta\phi}(\phi)\right) = 0 \quad +IC \quad +BCs+ \quad \text{Conservative BC: } M\nabla\frac{\delta\mathcal{E}}{\delta\phi}(\phi)\cdot\boldsymbol{n}\Big|_{\partial\Omega} = 0.$$

- Dissipative initial-boundary problems, based on the energy's law:

$$(EL) \qquad \frac{d}{dt}\mathcal{E}(\phi(t)) + \mathcal{D}(t) = 0$$

  where $\mathcal{D}(t)$ is the physical dissipativity:

$$\mathcal{D}(t) = \int_\Omega \left|\frac{\delta\mathcal{E}}{\delta\phi}(\phi(t))\right|^2 \quad \text{(Allen-Cahn)}, \quad \mathcal{D}(t) = \int_\Omega M\left|\nabla\frac{\delta\mathcal{E}}{\delta\phi}(\phi(t))\right|^2 \quad \text{(Cahn-Hilliard)}.$$

- **Lemma 1** *For any $\phi_0 \in X$,*

$$\mathcal{E}(\phi(t)) \le \mathcal{E}(\phi_0), \quad \int_0^{+\infty}\mathcal{D}(t)dt < +\infty$$

  In particular, since $\mathcal{E}(\phi)$ is bounded from below,

$$\mathcal{E}(\phi(t)) \downarrow \mathcal{E}_\infty \in \mathbb{R}, \quad \int_t^{t+1}\mathcal{D}(s)ds \to 0, \quad \text{as } t\uparrow +\infty$$

- Well-posedness of initial-boundary problem:

Theorem 2 *There exists a unique global in time (bounded) solution*

$$\|\phi(t)\|_X \quad \forall\, t \in (0, +\infty)$$

where $X = H^1(\Omega)$.

4 Convergence towards an equilibrium. Stability of local minima.

- Task: Large time behavior.
- Dynamical system: $\phi_0 \in X \to \phi(t) \in X$ $(X = H^1(\Omega))$
- ω-limit set (or equilibrium):

$$\omega(\phi_0) = \{\phi_\infty \in X \ : \ \exists\, (t_n) \uparrow +\infty \ s.t.\ \phi(t_n) \to \phi_\infty \text{ in } X\}$$

- Critical points of the free-energy:

$$\mathcal{C} = \left\{ \overline{\phi} \in X \ : \ \frac{\delta \mathcal{E}}{\delta \phi}(\overline{\phi}) = 0 \right\}$$

- Stationary solutions:

$$\mathcal{S}_{AC} = \mathcal{C}, \quad \mathcal{S}_{CH} = \left\{ \overline{\phi} \in X \ : \ \nabla \cdot \left(M \nabla \frac{\delta \mathcal{E}}{\delta \phi}(\overline{\phi}) \right) = 0 \right\}$$

- Remark: $\mathcal{S}_{AC} \subset \mathcal{S}_{CH}$. In fact, we will see that $\mathcal{S}_{CH} \subset \mathcal{S}_{AC}$
- $(X, \phi(t))$ is a gradient system, because $\mathcal{E}(\phi(t))$ is a Lyapunov function, i.e.:
  - $\mathcal{E}(\phi(t))$ decreases (along trajectories $\phi(t)$)
  - If $\mathcal{E}(\phi(t)) = \mathcal{E}(\phi(t'))$ for some $t < t'$, then $\phi(t)$ is a stationary solut.
- Remark: A gradient system cannot have (nonconstant) periodic trajectories nor can have (noncostant) homoclinic trajectories. A gradient system can have heteroclinic trajectories.
- **Lemma 3** $\omega(\phi_0)$ *is nonempty, and* $\omega(\phi_0) \subset \mathcal{C}$ *(with the same energy* $\mathcal{E}_\infty$*).*

  Comments:

1. This Lemma admits a specific proof based only in the energy law, without proving that the dynamical system has relatively compact orbits in X [Petzeltova-Rocca-Schimperna '13].
2. If the set of equilibria $\omega(\phi_0)$ be discrete, then any trajectory converges to an equilibrium.
3. If this is not the case, then there are PDE with $F(\phi) \in C^\infty$ but not analytic, with sols. whose ω-limit set $\omega(\phi_0)$ is a continuum of equilibria [P. Polacik & F. Simondon'02].
4. It cannot happen for $1D$ domains [H. Matano '78]

- **Theorem 4 (Convergence towards an equilibrium)** *For any ϕ_0, there exists a unique $\phi_\infty \in \mathcal{C}$ s.t. $\phi(t) \to \phi_\infty$ (ϕ_∞ depends on ϕ_0). Moreover, the following convergence rate holds*

$$\|\phi(t) - \phi_\infty\| \le C \frac{1}{(1+t)^{\theta/(1-2\theta)}}, \quad \theta \in (0, 1/2].$$

If $\theta = 1/2$ then the convergence rate is exponential. This happens, for instance, if ϕ_∞ is isolated.

- The proof is based on:

Lemma 5 (Lojasiewicz-Simon inequality) *Let $\overline{\phi} \in \mathcal{C}$. There exist constants $C, \delta > 0$ and $\theta \in (0, 1/2]$ s.t., for any $\phi \in X$ with $\|\phi - \overline{\phi}\| \le \delta$, it holds*

$$|\mathcal{E}(\phi) - \mathcal{E}(\overline{\phi})|^{1-\theta} \le C \left\| \frac{\delta \mathcal{E}}{\delta \phi}(\phi) \right\|$$

- **Theorem 6 (Stability of local minima)** *If $\overline{\phi}$ is a (local) minimum of $\mathcal{E}(\phi)$, then $\overline{\phi}$ is (locally) stable, but not asymptotically stable in general (i.e., $\|\phi(t) - \overline{\phi}\| <<$ for all $t \ge 0$ and $\phi(t) \to \phi_\infty$, but $\phi_\infty \ne \overline{\phi}$ in general).*

In particular, if $\overline{\phi}$ is isolated then $\overline{\phi}$ is asymptotically stable ($\phi(t) \to \overline{\phi}$).

5 Energy-stable time-schemes. Time adaptivity.

- For simplicity, we reduce to the Allen-Cahn problem.
- Ex. Unconditional solvable and energy-stable Implicit-Explicit first-order time-scheme [Eyre'99]:

- Convex-concave decomposition: $F(\phi) = F_c(\phi) + F_e(\phi)$, s.t. $F_c'' \geq 0$ (convex) and $F_e'' \leq 0$ (concave)

- Given $\phi^n \sim \phi(t^n)$, compute ϕ^{n+1} as:

$$\frac{1}{M}\frac{\phi^{n+1}-\phi^n}{dt^n} - \Delta\phi^{n+1} + F_c'(\phi^{n+1}) + F_e'(\phi^n) = 0, \quad +\text{BCs on } \phi^{n+1}$$

- **Lemma 7 (Local discrete energy law)** *It holds*

$$EL^n := \frac{\mathcal{E}(\phi^{n+1}) - \mathcal{E}(\phi^n)}{dt^n} + \int_\Omega \frac{1}{M}\left|\frac{\phi^{n+1}-\phi^n}{dt^n}\right|^2 \leq 0.$$

  In particular, $\mathcal{E}(\phi^{n+1})$ is a discrete Lyapunov functional, because

  - *the discrete energy decreases: $\mathcal{E}(\phi^{n+1}) \leq \mathcal{E}(\phi^n)$.*
  - *If $\mathcal{E}(\phi^{n+1}) = \mathcal{E}(\phi^n)$ then $\phi^{n+1} \equiv \phi^n$ in Ω.*

- Remark: This scheme can be seen as an implicit-explicit descent method, based on the time dynamic.

- **Theorem 8 (Long-time convergence)** *There exits $\phi^\infty \in \mathcal{C}$ s.t. $\phi^n \to \phi^\infty$ as $n \uparrow +\infty$.*

- Open question: Do the limits of continuum and discrete problems coincide as $dt^n \to 0$?

- Some extensions:

  - energy stable linear time-scheme
  - second-order time-schemes

- Time adaptivity: Given dt^n, to compute ϕ^{n+1} and EL^n (energy law approximation criterium).

  - If $|EL^n| << $ then ϕ^{n+1} is valid and dt^n can increase.
  - If $|EL^n| >> $ then ϕ^{n+1} is not valid and dt^n must decrease.

6 Space Finite-Element (FE) approximation. Mesh adaptation

- Discrete approximation of the variational formulation of time-discrete problem.
- Mesh adaptation criterium, refining where local spatial variation of ϕ^n be large.

7 Bi-parametric test problem in a wedge geometry; angle and contact parameter.

- Physical problem: liquid-gas phase-transitions in contact with a surface Γ (with a coin).
- Order parameter: $\phi = -1$ (gas), $\phi = 1$ (liquid)
- $2D$ domain, surface with acute angle $\alpha \in (0, \pi/2)$.
- Contact parameter $\phi_s \in (0, 1)$ s.t. $\phi|_{surface} = \phi_s$ (enforcing that some liquid remains near of the surface).

  PICTURES (domain and BCs)
- Task: To detect numerically locally stable interfaces in the liquid-gas phase-transitions wrt. α and ϕ_s.
- Physical arguments for an (infinite) surface say that:
  - If $\alpha <<$ then there exists only one stable interface in contact with the surface.
  - If $\alpha >>$ then there exists two stable interfaces in contact with the surface for a determined range of ϕ_s
- Question:

  How is the transition between these two possibilities ? (Physics)

  Is there bifurcation ? (Mathematics)

8 Numerical simulations of liquid-vapor phase-transitions in a wedge geometry. Bifurcations ?

- PICTURES: equilibrium interfaces,
- GRAPHICS: energy vs. ϕ_s
- Conclusion: There is bifurcation starting from $\alpha = 15^{o}$ approx. and ϕ_s near of a critical value $\phi_s^\star$