Phase field models in fluid dynamics

Eduard Feireisl

Institute of Mathematics, Academy of Sciences of the Czech Republic, Prague

joint work with

H.Abels (Regensburg), H.Petzeltová (Praha)
E.Rocca (Milano), G.Schimperna (Pavia)

Villa Clythia, Fréjus, April 7th - 12th, 2013

Johann von Neumann [1903-1957]

In mathematics you don't understand things. You just get used to them.

Fluid equations

Mass conservation - equation of continuity

$$\partial_t \varrho + \mathrm{div}_x(\varrho \mathbf{u}) = 0$$

Momentum balance

$$\partial_t(\varrho \mathbf{u}) + \mathrm{div}_x(\varrho \mathbf{u} \otimes \mathbf{u}) = \mathrm{div}_x \mathbb{T} + \varrho \mathbf{g}$$

$\varrho = \varrho(t, x)$ .... mass density
$\mathbf{u} = \mathbf{u}(t, x)$ .... velocity field
$\mathbb{T}$ .... Cauchy stress
$\mathbf{g}$ .... external (volume) force

Phase field function - concentration difference

$$-1 \leq c(t,x) \leq 1$$

$$\partial_t(\varrho c) + \mathrm{div}_x(\varrho c \mathbf{u}) = \mathrm{div}_x \nabla_x \mu$$

$\mu = \mu(t,x)$ .... chemical potential

Cahn-Hillard type equation

$$\varrho\mu = \varrho \frac{\partial f(\varrho, c)}{\partial c} - \Delta c$$

$$\partial_t(\varrho c) + \mathrm{div}_x(\varrho c \mathbf{u}) = \Delta \left(\frac{\partial f(\varrho, c)}{\partial c} - \frac{1}{\varrho} \Delta c \right)$$

$f = f(\varrho, c)$ ....free energy

Stress relation

Young-Laplace law

$$[\mathbb{T} \cdot \mathbf{n}] = \sigma H \mathbf{n} \text{ on interface}$$

Viscous stress

$$\mathbb{S} = \nu(c) \left(\nabla_x \mathbf{u} + \nabla_x^t \mathbf{u} - \frac{2}{3} \mathrm{div}_x \mathbf{u} \mathbb{I} \right) + \eta(c) \mathrm{div}_x \mathbf{u} \mathbb{I}$$

Pressure

$$p(\varrho, c) = \varrho^2 \frac{\partial f(\varrho, c)}{\partial \varrho}$$

Extra stress

$$\mathbb{T} = \mathbb{S} - p\mathbb{I} - \boxed{\left(\nabla_x c \otimes \nabla_x c - \frac{1}{2} |\nabla_x c|^2 \mathbb{I} \right)}$$

Equation of continuity

$$\partial_t \varrho + \mathrm{div}_x(\varrho \mathbf{u}) = 0$$

Momentum balance

$$\partial_t(\varrho \mathbf{u}) + \mathrm{div}_x(\varrho \mathbf{u} \otimes \mathbf{u}) + \nabla_x p(\varrho, c)$$

$$= \mathrm{div}_x \left(\nu(c) \left(\nabla_x \mathbf{u} + \nabla_x^t \mathbf{u} - \frac{2}{3} \mathrm{div}_x \mathbf{u} \mathbb{I} \right) + \eta(c) \mathrm{div}_x \mathbf{u} \mathbb{I} \right)$$

$$- \mathrm{div}_x \left(\nabla_x c \otimes \nabla_x c - \frac{1}{2} |\nabla_x c|^2 \mathbb{I} \right) + \varrho \mathbf{g}$$

Phase field equation

$$\partial_t(\varrho c) + \mathrm{div}_x(\varrho c \mathbf{u}) = \Delta \left(\frac{\partial f(\varrho, c)}{\partial c} - \frac{1}{\varrho} \Delta c \right)$$

Boundary conditions

$$x \in \Omega \subset R^3$$

Ω .... regular (bounded) domain

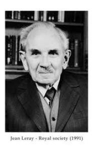
No-slip

$$\mathbf{u}|_{\partial\Omega} = 0$$

No-flux

$$\nabla_x c \cdot \mathbf{n}|_{\partial\Omega} = 0, \ \nabla_x \mu \cdot \mathbf{n}|_{\partial\Omega} = 0$$

A bit of history of global existence for large data



Jean Leray [1906-1998] Global existence of weak solutions for the incompressible Navier-Stokes system (3D)

Olga Aleksandrovna Ladyzhenskaya [1922-2004] Global existence of classical solutions for the incompressible 2D Navier-Stokes system

Pierre-Louis Lions[*1956] Global existence of weak solutions for the compressible barotropic Navier-Stokes system (2,3D)

Constitutive relations

Free energy

$$f(\varrho, c) = f_{\rm e}(\varrho) + f_{\rm mix}(\varrho, c), \ f_{\rm mix}(\varrho, c) = H(c)\log(\varrho) + G(c)$$

Pressure

$$p(\varrho, c) = \varrho^2 \frac{\partial f(\varrho, c)}{\partial \varrho} = p_{\rm e}(\varrho) + \varrho H(c), \ f_{\rm e}(\varrho) = \int_1^\varrho \frac{p_{\rm e}(z)}{z^2} \ {\rm d}z$$

$$p_{\rm e}(0) = 0, \ p_1 \varrho^{\gamma - 1} - p_2 \leq p_{\rm e}'(\varrho) \leq p_3(1 + \varrho^{\gamma - 1}), \ \gamma > \frac{3}{2}$$

Mixing

$$-H_1 \leq H'(c), H(c) \leq H_2, \ G_1 c - G_2 \leq G'(c) \leq G_3(1 + c)$$

Energy estimates

Total energy

$$E(t) = \int_\Omega \boxed{\frac{1}{2}\varrho|\mathbf{u}|^2} + \boxed{\frac{1}{2}|\nabla_x c|^2 + \varrho f(\varrho, c)} \ \mathrm{d}x$$

Total mass

$$M = \int_\Omega \varrho \ \mathrm{d}x, \ \ M(t) = \int_\Omega \varrho(t,\cdot) \ \mathrm{d}x = \int_\Omega \varrho_0 \ \mathrm{d}x, \ \ \varrho(0,\cdot) = \varrho_0$$

Energy (in)equality

$$\frac{\mathrm{d}}{\mathrm{d}t}E(t) + \int_\Omega \left(\mathbb{S} : \nabla_x \mathbf{u} + |\nabla_x \mu|^2\right) \ \mathrm{d}x \boxed{\leq} \int_\Omega \varrho \mathbf{g} \cdot \mathbf{u} \ \mathrm{d}x$$

Kinetic energy

$$\partial_t \int_\Omega \frac{1}{2}\varrho|\mathbf{u}|^2 \ \mathrm{d}x + \int_\Omega \mathbb{S} : \nabla_x \mathbf{u} \ \mathrm{d}x$$

$$= \int_\Omega p(\varrho)\mathrm{div}_x \mathbf{u} \ \mathrm{d}x + \int_\Omega \Delta c \nabla_x c \cdot \mathbf{u} \ \mathrm{d}x$$

$$\mu = \frac{\partial f(\varrho, c)}{\partial c} - \frac{1}{\varrho}\Delta c, \ \ p(\varrho, c) = \varrho^2 \frac{\partial f(\varrho, c)}{\partial \varrho}$$

"Phase field" stored energy

$$\partial_t \int_\Omega \frac{1}{2}|\nabla_x c|^2 \ \mathrm{d}x + \int_\Omega |\nabla_x \mu|^2 \ \mathrm{d}x$$

$$= - \int_\Omega \left(\varrho \frac{\partial f(\varrho, c)}{\partial c} \partial_t c + \varrho \frac{\partial f(\varrho, c)}{\partial c} \mathbf{u} \cdot \nabla_x c \right) \ \mathrm{d}x$$

$$- \int_\Omega \Delta c \nabla_x c \cdot \mathbf{u} \ \mathrm{d}x$$

Dissipative bounds and Korn's inequality

$$\int_\Omega \mathbb{S} : \nabla_x \mathbf{u} \ \mathrm{d}x \geq \int_\Omega \frac{\nu(c)}{2} \left| \nabla_x \mathbf{u} + \nabla_x^t \mathbf{u} - \frac{2}{3} \mathrm{div}_x \mathbf{u} \mathbb{I} \right|^2 \ \mathrm{d}x$$

Korn's inequality

$$\int_\Omega \frac{\nu(c)}{2} \left| \nabla_x \mathbf{u} + \nabla_x^t \mathbf{u} - \frac{2}{3} \mathrm{div}_x \mathbf{u} \mathbb{I} \right|^2 \ \mathrm{d}x \geq \underline{\nu} \| \nabla_x \mathbf{u} \|^2_{L^2(\Omega)}$$

Transport coefficients

$$\underline{\nu} \leq \nu(c) \leq \overline{\nu}$$

$$0 \leq \eta(c) \leq \overline{\eta}$$

Available a priori bounds

- $$\operatorname{ess} \sup_{t \in (0,T)} \|\varrho(t,\cdot)\|_{L^\gamma(\Omega)} \leq C(\mathrm{data})$$
- $$\operatorname{ess} \sup_{t \in (0,T)} \|\nabla_x c(t,\cdot)\|_{L^2(\Omega;R^3)} \leq C(\mathrm{data})$$
- $$\operatorname{ess} \sup_{t \in (0,T)} \|\sqrt{\varrho}\mathbf{u}(t,\cdot)\|_{L^2(\Omega;R^3)} \leq C(\mathrm{data})$$
- $$\int_0^T \left[\|\nabla_x \mathbf{u}(t,\cdot)\|^2_{L^2(\Omega;R^{3\times 3})} + \|\nabla_x \mu(t,\cdot)\|^2_{L^2(\Omega;R^3)} \right] \mathrm{d}t \leq C(\mathrm{data})$$

Div-Curl lemma

Hypotheses

$$\mathbf{U}_n \to \mathbf{U} \text{ weakly in } L^p(R^N;R^N),\ \mathbf{V}_n \to \mathbf{V} \text{ weakly in } L^q(R^N;R^N)$$

$$\frac{1}{p} + \frac{1}{q} = \frac{1}{r} < 1$$

$$\{\mathrm{DIV}[\mathbf{U}_n]\}_{n=1}^{\infty},\ \{\mathbf{CURL}[\mathbf{V}_n]\}_{n=1}^{\infty} \text{ precompact in } W^{-1,s}$$

for a certain $s \geq 1$

Conclusion

$$\mathbf{U}_n \cdot \mathbf{V}_n \to \mathbf{U} \cdot \mathbf{V} \text{ weakly in } L^r(R^N)$$

Weak compactness of the convective terms

General principle

$$\partial_t S_n + \mathrm{div}_x \mathbf{F}_n = r_n \in \text{ precompat set in } W^{-1,s}$$

$$\nabla_x H_n \in \text{ bounded in } L^p$$

Application of DIV-CURL lemma

$$\mathbf{U}_n = [S_n, \mathbf{F}_n], \ \mathbf{V}_n = [H_n, 0, 0, 0]$$

Conclusion

$$\overline{SH} = \overline{S}\ \overline{H}$$

Convective terms

Direct application of DIV-CURL lemma

$$\overline{\varrho \mathbf{u}} = \varrho \mathbf{u}, \ \overline{\varrho \mathbf{u} \otimes \mathbf{u}} = \varrho \mathbf{u} \otimes \mathbf{u}$$

$$\overline{\varrho c} = \varrho c, \ \overline{\varrho c^2} = \varrho c^2$$

Strong convergence outside vacuum

$$c_n \to c \text{ in } L^2 \text{ on the set } \{\varrho > 0\}$$

Strong convergence of $\nabla_x c$

$$-\Delta c_n = \varrho_n \frac{\partial f(\varrho_n, c_n)}{\partial c} - \varrho_n \mu_n$$

$$-\Delta c = \overline{\varrho \frac{\partial f(\varrho, c)}{\partial c}} - \overline{\varrho \mu}$$

Application of previous observations

$$\boxed{\overline{\varrho \frac{\partial f(\varrho, c)}{\partial c} c}} = \boxed{\overline{\varrho \frac{\partial f(\varrho, c)}{\partial c}}} c$$

$$\overline{\varrho \mu c} = \overline{\varrho \mu} c$$

Conclusion

$$\nabla_x c_n \to \nabla_x c \text{ (strongly) in } L^2((0, T) \times \Omega; R^3)$$

$$b \in C^1[0,\infty),\ \ b'(z) = 0 \text{ for all } z \geq z_0$$

Renormalized equation

$$\partial_t b(\varrho) + \mathrm{div}_x (b(\varrho)\mathbf{u}) + \Big(b'(\varrho)\varrho - b(\varrho) \Big) \mathrm{div}_x \mathbf{u} = 0$$

$$\partial_t (\varrho \log(\varrho)) + \mathrm{div}_x \Big(\varrho \log(\varrho) \mathbf{u} \Big) + \boxed{\varrho \mathrm{div}_x \mathbf{u}} = 0$$

Density oscillations - first approximation

Limit of renormalized equations

$$\partial_t \overline{\varrho \log(\varrho)} + \mathrm{div}_x \left(\overline{\varrho \log(\varrho)} \mathbf{u} \right) + \overline{\varrho \mathrm{div}_x \mathbf{u}} = 0$$

Renormalized limit equation

$$\partial_t \left(\varrho \log(\varrho) \right) + \mathrm{div}_x \left(\varrho \log(\varrho) \mathbf{u} \right) + \varrho \mathrm{div}_x \mathbf{u} = 0$$

Density oscillations

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \left(\overline{\varrho \log(\varrho)} - \varrho \log(\varrho) \right) \, \mathrm{d}x$$

$$+ \int_\Omega \left(\overline{\varrho \mathrm{div}_x \mathbf{u}} - \varrho \mathrm{div}_x \mathbf{u} \right) \, \mathrm{d}x = 0$$

DiPerna-Lions' regularization method

$$v_\delta = \kappa_\delta * v$$

Regularized equation

$$\partial_t \varrho_\delta + \mathrm{div}_x(\varrho_\delta \mathbf{u}) = \boxed{\mathrm{div}_x\Big(\varrho_\delta \mathbf{u}\Big) - [\mathrm{div}_x(\varrho \mathbf{u})]_\delta} \equiv r_\delta$$

$$\nabla_x \mathbf{u} \in L^p,\ \ \varrho \in L^{p'}\ \ \frac{1}{p} + \frac{1}{p'} = 1$$

$$\Rightarrow$$

$$r_\delta \to 0 \text{ as } \delta \to 0$$

Effective viscous flux identity

"Weak continuity" of the effective viscous flux

$$\overline{p(\varrho)\varrho} - \left(\frac{4}{3}\nu(c) + \eta(c) \right) \overline{\varrho \mathrm{div}_x \mathbf{u}}$$

$$= \overline{p(\varrho)}\varrho - \left(\frac{4}{3}\nu(c) + \eta(c) \right) \varrho \mathrm{div}_x \mathbf{u}$$

$$\overline{\varrho \mathrm{div}_x \mathbf{u}} - \varrho \mathrm{div}_x \mathbf{u} \geq 0$$

$$\Rightarrow$$

$$\overline{\varrho \log(\varrho)} = \varrho \log(\varrho)$$

$$\Rightarrow$$

$$\varrho_\varepsilon \to \varrho \text{ a.a. in } (0, T) \times \Omega$$

Effective viscous flux - Step I

"Approximate equation"

$$p(\varrho_n)$$
$$= \mathrm{div}_x \Delta^{-1} \mathrm{div}_x \mathbb{S}_n - \partial_t \Delta^{-1} \mathrm{div}_x [\varrho_n \mathbf{u}_n] - \mathrm{div}_x \Delta^{-1} \mathrm{div}_x [\varrho_n \mathbf{u}_n \otimes \mathbf{u}_n]$$
$$+ \text{"compact terms"}$$

Limit equation

$$\overline{p(\varrho)} = \mathrm{div}_x \Delta^{-1} \mathrm{div}_x \mathbb{S} - \partial_t \Delta^{-1} \mathrm{div}_x [\varrho \mathbf{u}] - \mathrm{div}_x \Delta^{-1} \mathrm{div}_x [\varrho \mathbf{u} \otimes \mathbf{u}]$$
$$+ \text{"compact terms"}$$

Effective viscous flux - Step II

$$\nu > 0,\ \eta = 0 \text{ constant}$$

"Approximate equation"

$$p(\varrho_n)\varrho_n - \frac{4\nu}{3}\varrho_n \mathrm{div}_x \mathbf{u}_n$$

$$= -\Delta^{-1}\mathrm{div}_x[\varrho_n \mathbf{u}_n]\mathrm{div}_x(\varrho_n \mathbf{u}_n) - \mathrm{div}_x \Delta^{-1}\mathrm{div}_x[\varrho_n \mathbf{u}_n \otimes \mathbf{u}_n]\varrho_n$$

$$+ \text{"compact terms"}$$

Limit equation

$$\overline{p(\varrho)\varrho} - \frac{4\nu}{3}\varrho \mathrm{div}_x \mathbf{u}$$

$$= -\Delta^{-1}\mathrm{div}_x[\varrho \mathbf{u}]\mathrm{div}_x(\varrho \mathbf{u}) - \mathrm{div}_x \Delta^{-1}\mathrm{div}_x[\varrho \mathbf{u} \otimes \mathbf{u}]\varrho$$

$$+ \text{"compact terms"}$$

Effective viscous flux - Step III

Effective viscous flux identity revisited

$$\overline{p(\varrho)\varrho} - \frac{4\nu}{3}\overline{\varrho \mathrm{div}_x \mathbf{u}} \approx \overline{p(\varrho)}\varrho - \frac{4\nu}{3}\varrho \mathrm{div}_x \mathbf{u}$$

$$+\mathrm{weak} - \lim_{n\to\infty} \mathbf{u}_n \cdot \boxed{\Big[\varrho_n \mathrm{div}_x \Delta^{-1} \mathrm{div}_x [\varrho_n \mathbf{u}_n] - \varrho_n \mathbf{u}_n \mathrm{div}_x \Delta^{-1} \mathrm{div}_x [\varrho_n] \Big]}$$

$$-\mathbf{u} \cdot \boxed{\Big[\varrho \mathrm{div}_x \Delta^{-1} \mathrm{div}_x [\varrho \mathbf{u}] - \varrho \mathbf{u} \mathrm{div}_x \Delta^{-1} \mathrm{div}_x [\varrho] \Big]}$$

Div-Curl lemma revisited

Hypotheses

$$\mathbf{U}_n \to \mathbf{U} \text{ weakly in } L^p(R^N; R^N), \ \mathbf{V}_n \to \mathbf{V} \text{ weakly in } L^q(R^N; R^N)$$

$$\frac{1}{p} + \frac{1}{q} = \frac{1}{r} < 1$$

$$\mathcal{R}_{i,j} = \partial_{x_i} \Delta^{-1} \partial_{x_j}$$

Conclusion

$$\sum_{i,j} \left(U^i_n \mathcal{R}_{i,j}[V^j_n] - V^i_n \mathcal{R}_{i,j}[U^j_n] \right) \to \sum_{i,j} \left(U^i \mathcal{R}_{i,j}[V^j] - V^i \mathcal{R}_{i,j}[U^j] \right)$$

weakly in $L^r(R^N)$

$$\mathbf{u}_n \to \mathbf{u} \text{ weakly in } L^2(0,T;W_0^{1,2}(\Omega;R^3))$$

$$\varrho_n \to \varrho \text{ in } C_{\rm weak}([0,T];L^\gamma(\Omega))$$

$$\varrho_n\mathbf{u}_n \to \varrho\mathbf{u} \text{ in} C_{\rm weak}([0,T];L^{2\gamma/\gamma+1}(\Omega;R^3))$$

Conclusion

$$\mathbf{u}_n \cdot \Big[\varrho_n {\rm div}_x \Delta^{-1} {\rm div}_x[\varrho_n\mathbf{u}_n] - \varrho_n\mathbf{u}_n {\rm div}_x \Delta^{-1} {\rm div}_x[\varrho_n] \Big]$$

$$\to$$

$$\mathbf{u} \cdot \Big[\varrho {\rm div}_x \Delta^{-1} {\rm div}_x[\varrho\mathbf{u}] - \varrho\mathbf{u} {\rm div}_x \Delta^{-1} {\rm div}_x[\varrho] \Big]$$

Commutator

$$\mathcal{R}_{i,j}\left[\nu(c_n)\left(\nabla_x\mathbf{u}_n+\nabla_x\mathbf{u}_n^t-\frac{2}{3}\mathrm{div}_x\mathbf{u}_n\in I\right)\right]$$

$$=\mathcal{R}_{i,j}\left[\nu(c_n)\left(\nabla_x\mathbf{u}_n+\nabla_x\mathbf{u}_n^t-\frac{2}{3}\mathrm{div}_x\mathbf{u}_n\in I\right)\right]-\frac{4}{3}\nu(c_n)\mathrm{div}_x\mathbf{u}_n$$

$$+\frac{4}{3}\nu(c_n)\mathrm{div}_x\mathbf{u}_n$$

Commutator lemma [Coifman and Meyer]

Lemma

Let $w \in W^{1,r}(R^N)$, $\mathbf{V} \in L^p(R^N; R^N)$ be given, where

$$1 < r < N, \ 1 < p < \infty, \ \frac{1}{r} + \frac{1}{p} - \frac{1}{N} < 1.$$

The for any s satisfying

$$\frac{1}{r} + \frac{1}{p} - \frac{1}{N} < \frac{1}{s} < 1$$

there exists $\beta > 0$ such that

$$\left\| \sum_{j=1}^{N} \mathcal{R}_{i,j}[wV_j] - \sum_{j=1}^{N} w\mathcal{R}_{i,j}[V_j] \right\|_{W^{\beta,s}(R^N,R^N)} \leq c \|w\|_{W^{1,r}} \|\mathbf{V}\|_{L^p},$$

$$i = 1, \dots, n$$

General constitutive relations

Oscillations defect measure

$$\omega_q[\varrho_n \to \varrho](Q) = \sup_{k>0} \left[\limsup_{n\to\infty} \int_Q |T_k(\varrho_n) - T_k(\varrho)|^q \ \mathrm{d}x \ \mathrm{d}t \right]$$

$$T_k(r) = \min\{r, k\}$$

Claim

$$\omega_q[\varrho_n \to \varrho]((0,T)\times\Omega) < \infty, \ \ q = \gamma + 1 > 2$$

Renormalized equation revisited

Lemma

$$\omega_q[\varrho_n \to \varrho]((0,T) \times \Omega) < \infty, \ \ q > 2$$

$$\Rightarrow$$

ϱ, $\mathbf{u}$ satisfy the renormalized equation

Sir Winston Churchill, [1874–1965]

However beautiful the strategy, you should occasionally look at the results

Allen-Cahn model

Allen-Cahn equation

$$\partial_t(\varrho c) + \mathrm{div}_x(\varrho c \mathbf{u}) = -\mu$$

$\mu = \mu(t,x)$ .... chemical potential

$$\varrho\mu = \varrho \frac{\partial f(\varrho, c)}{\partial c} - \Delta c$$

Singular elastic pressure

$$p_e(\varrho) \approx (\varrho - \overline{\varrho})^{-3} \text{ as } \varrho \to \overline{\varrho}-$$