45. Cahn–Hilliard equation — *phase separation and coarsening*

The Allen–Cahn equation $u_t = u - u^3 + \Delta u$ describes regions with $u \approx -1$ and $u \approx 1$ that grow and decay at the expense of one another ($\rightarrow$ *ref*). By taking minus the Laplacian of the right-hand side, we get the *Cahn–Hilliard equation*:

$$u_t = \Delta(u^3 - u) - \varepsilon \Delta^2 u. \tag{1}$$

(More generally, $u^3 - u$ may be replaced by $F'(u)$ where $F(u)$ is a double-well potential.) Again, $u \approx -1$ and $u \approx 1$ are stable steady states, but now, the total area in each state will be conserved, since integration of (1) shows that $(\mathrm{d}/\mathrm{d}t) \int u = 0$ apart from possible effects of boundary conditions.

The equation was proposed in 1958 to model certain phenomena of *phase separation* (also known as *spinodal decomposition*) in binary alloys. Cahn and Hilliard were concerned with alloys such as iron–nickel. If a blend of these metals is rapidly quenched below a critical temperature, the resulting state is unstable, and small pockets of relatively pure iron and nickel may soon appear with a characteristic length scale. As time passes, these may coarsen into larger pockets, quickly at first, then more slowly. If the two species A and B have concentrations c_A and $c_B = 1 - c_A$ at each point, then the variable u of (1) is $u(x,t) = 1 - 2c_A(x,t)$, with $u = -1$ corresponding to pure phase A and $u = 1$ to pure phase B.

One way to derive (1) is to assume that there is a free energy functional

$$E(u) = \int_\Omega \left(F(u) + \frac{1}{2}\varepsilon |\nabla u|^2 \right) \mathrm{d}x$$

in a spatial domain $\Omega \subseteq \mathbb{R}^n$, where for our special case, $F'(u) = u^3 - u$. The $|\nabla u|^2$ term reflects intermolecular interactions and can be viewed as penalising the creation of interfaces. The variation of $E(u)$ with respect to u is $\delta E/\delta u = \int_\Omega F'(u) - \varepsilon \Delta u$, again apart from any boundary effects, which can be interpreted as the integral of a kind of chemical potential $\mu(x,t)$. (The minus sign is a result of integration by parts.) Equation (1) is obtained by supposing that μ diffuses with time according to $u_t = \Delta \mu$.

The Cahn–Hilliard equation is a fourth order parabolic equation. To obtain a well-posed problem, we must complement (1) with an initial condition $u(x,0) = u_0(x)$ and boundary conditions such as the variational condition $\mathbf{n} \cdot \nabla u$ and the no-flux condition $\mathbf{n} \cdot \nabla \mu = 0$ on $\partial\Omega$, where $\mathbf{n}$ is a vector normal to $\partial\Omega$. With these boundary conditions the equation is truly mass conserving, i.e., $(\mathrm{d}/\mathrm{d}t) \int_\Omega u(x,t)\,\mathrm{d}x = 0$.

We can get an idea of how solutions of (1) may behave by considering the case of one space dimension. If the alloy is initially mixed, then $u(x) \equiv 0$. This steady state is unstable, however, and small perturbations will grow. Linearising (1) gives $u_t = -u_{xx} - \varepsilon u_{xxxx}$, the linearised Kuramoto–Sivashinsky equation ($\rightarrow$ *ref*), with negative second-order diffusion. Energy at wave numbers k with $0 < k < 1$ grows exponentially, with maximum amplification at wave number $k_{\max} = 1/\sqrt{2}$.

Figure 1 presents three snapshots of numerically computed solutions of the Cahn–Hilliard equation in 2D. The initial conditions were a small perturbation of the steady state $u(x) = 0$, and the blue and red regions represent values near -1 and $+1$, respectively. The first image shows a typical fine-grained pattern at early time. The second and third images show the solution during the middle and late stages of coarsening. In the limit $t \to \infty$ the coarsening process will leave a single region of blue and red phases separated by a semicircular boundary, with the two phases centred in opposite corners of the domain.

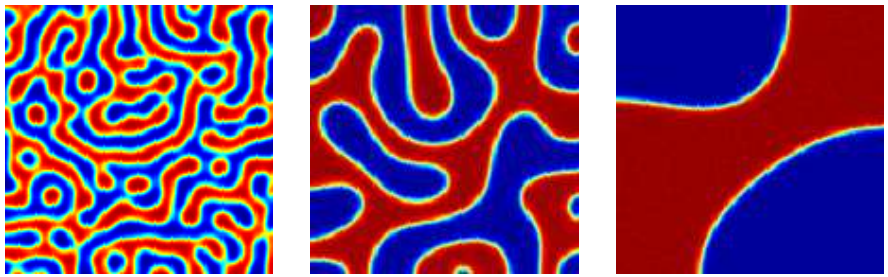

Fig. 1: Solutions in 2D for small, medium, and large t

Many aspects of the mathematics of the Cahn–Hilliard equation are well understood, including existence and uniqueness of solutions, existence of a compact attractor, the structure of equilibria (a non-local boundary value problem), the existence of inertial manifolds in one space dimension, and the moving boundary problems obtained from the equation in the limit $\varepsilon \to 0$. Many open mathematical problems remain, however, such as the characterisation of equilibria in many dimensions and the structure of heteroclinic connections on the attractor. These issues are not easy to resolve since the main analytical tool used for second order parabolic equations, the maximum principle, is not available for fourth-order problems.

Generalisations of the Cahn–Hilliard equation have been studied to model further aspects of the behaviour of alloys and related physical systems. There are systems of Cahn–Hilliard and of Cahn–Hilliard and Allen–Cahn equations, Cahn–Hilliard equations with variable mobility, Cahn–Hilliard equations coupled to equations of fluid flow or heat conduction, Cahn–Hilliard equations that are periodically perturbed (for example, by changing temperature), and more.

References

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