NSF-CBMS Conference

The Cahn-Hilliard equation: recent advances and applications

List of lectures

The Cahn-Hilliard equation was proposed by J.W. Cahn (who died on March 14, 2016) and J.E. Hilliard in order to describe phase separation processes in binary alloys. More precisely, when an homogeneous binary alloy is cooled down sufficiently, one can observe a total phase separation (called spinodal decomposition) and one obtains a fine-grained structure. This, in turn, can have essential consequences on the mechanical properties of the system, e.g., strength or aging.

This equation is particularly popular among material scientists, engineers and physicists. Indeed, it is simple to state (it is a fourth-order in space parabolic equation), easy to implement numerically and gives very good and precise simulations (in 2 and even 3D). It reads (taking all physical contants equal to 1)

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) = 0.$$

It usually is associated with Neumann boundary conditions,

$$\frac{\partial u}{\partial \nu} = \frac{\partial \Delta u}{\partial \nu} = 0$$

on the boundary. Furthermore, one usually considers a cubic nonlinear term,

$$f(s) = s^3 - s,$$

but such a nonlinear term is an approximation of thermodynamically relevant logarithmic nonlinear terms of the form

$$f(s) = -\theta_c s + \frac{\theta}{2} \ln \frac{1+s}{1-s}, \ 0 < \theta \le \theta_c, \ s \in (-1,1).$$

From a mathematical point of view, a lot has been done (from a theoretical and also a numerical/simulation point of view); it suffices to type Cahn on mathscinet to see how popular this equation was and still is. Nevertheless, the equation still is very much studied (one can again see mathscinet) and indeed a lot has still to be done. In the lectures, we present the state of the art, but also present and discuss important open problems.

It is also interesting and important to note that the Cahn-Hilliard equation, or some of its variants, has applications in other areas/contexts, in which phase separation and/or coarsening/clustering processes can be observed or come into play. We can mention, for instance, population dynamics, bacterial films, wound healing

and tumor growth, thin films, image processing (image denoising and inpainting in particular) and even the rings of Saturn and the clustering of mussels. In particular, several interesting variants of the equation (with applications, e.g., to tumor growth and image processing) can be written in the form

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) + g(x, u) = 0.$$

Essential (mathematical) difficulties arise from the fact that, when endowing the equation with Neumann boundary conditions, one no longer has the conservation of the average of the order parameter, contrary to the original Cahn-Hilliard equation.

LECTURE 1: THE CAHN-HILLIARD EQUATION

In this lecture, we introduce the equation and its (phenomenological) derivation.

We also discuss in details the boundary conditions. In particular, we can note that the usual Neumann boundary conditions yield a contact angle (when the interface between the two components meets the boundary/walls (e.g., in a confined system)) of $\frac{\pi}{2}$. Now, in several situations (e.g., for the study of immiscible binary mixtures), it is necessary to have a contact angle which moves from its equilibrium state. Hence the necessity to introduce dynamic boundary conditions. One can consider several approaches to define such boundary conditions, based on energy principles and (different versions of) mass conservation. We present, discuss and compare the different approaches.

We finally introduce several important variants and generalizations of the Cahn-Hilliard equation.

LECTURE 2: THE CAHN-HILLIARD EQUATION WITH REGULAR NONLINEAR TERMS - PART ONE

In this lecture, we discuss the mathematical analysis of the equation. Here, we consider regular nonlinear terms (a typical choice being the usual cubic nonlinear term $f(s) = s^3 - s$) and standard (Neumann) boundary conditions.

We first present the functional framework (linear operators, linear problem, in particular).

We then discuss the well-posedness and regularity of solutions, as well as the asymptotic behavior of the system (existence of global attractors).

LECTURE 3: THE CAHN-HILLIARD EQUATION WITH REGULAR NONLINEAR TERMS - PART TWO

In this second part, we give an improved regularity result, allowing to address polynomials with arbitrary odd degree (with a strictly positive leading coefficient)

in 3D. We then discuss the finite-dimensionality of the global attractor. We finally discuss the numerical analysis of the equation.

Lecture 4: The Cahn-Hilliard equation with logarithmic nonlinear terms - Part one

In this lecture, we address the case of logarithmic nonlinear terms. Indeed, the usual cubic/regular nonlinear terms are approximations of thermodynamically relevant logarithmic nonlinear terms which follow from a mean-field model. Such nonlinear terms induce additional mathematical questions and an essential issue (not completely solved in 3D) is the separation from the pure states/singular points of the nonlinear term, namely an estimate of the form

$$||u(t)||_{L^{\infty}} \le 1 - \delta, \ \delta \in (0, 1),$$

at least after some transient time (δ possibly depending on a final time T).

We can note that such nonlinear terms force the order parameter to stay in the physically relevant interval, i.e.,

$$-1 < u < 1$$

almost everywhere; this does not hold in the case of regular nonlinear terms (we give very simple counterexamples). The separation from the pure states mentioned above, which holds in 2D, says that, actually, there is always a certain amount of the two alloys components during the phase separation.

In this first part, we discuss the well-posedness (we can mention that several approaches can be used to prove the existence of a solution) and start discussing the asymptotic behavior of the system.

Lecture 5: The Cahn-Hilliard equation with logarithmic nonlinear terms - Part two

The second part is devoted to the study of the strict separation property from the pure states and further discussions on the asymptotic behavior of the system.

LECTURE 6: THE CAHN-HILLIARD EQUATION WITH DYNAMIC BOUNDARY CONDITIONS

In this lecture, we address the Cahn-Hilliard equation with dynamic boundary conditions. As already mentioned, such boundary conditions are important to account for the interactions with the walls, in particular, as already mentioned, to account for dynamic contact angles. One possible dynamic boundary condition reads

$$\frac{\partial u}{\partial t} - \Delta_{\Gamma} u + g(u) + \frac{\partial u}{\partial \nu} = 0$$

on the boundary, where Δ_{Γ} is the Laplace-Beltrami operator and g is a surface nonlinear term, assumed regular.

We address the well-posedness, regularity and asymptotic behavior of the systems, in the case of regular nonlinear terms. In particular, we discuss different possibilities/approximation schemes for the existence of solutions. Indeed, different approaches are needed, depending on the type of dynamic boundary conditions that we consider.

We also address dynamic boundary conditions and logarithmic nonlinear terms. In that case, we can prove the nonexistence of classical solutions, i.e., of solutions in the sense of distributions, due to the fact that one of the pure states can be present in a set with non-zero measure on the walls. We thus give suitable notions of solutions to describe such solutions: these can be defined by duality techniques or by a variational inequality.

We again address the well-posedness, regularity and asymptotic behavior of the corresponding systems.

LECTURE 7: THE CAHN-HILLIARD-OONO EQUATION

The Cahn-Hilliard-Oono equation,

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) + \beta u = 0, \ \beta > 0,$$

was introduced in order to account for long-ranged (i.e., nonlocal) effects in the phase separation process.

We show in this lecture that the additional simple linear term already leads to several additional difficulties, especially when considering logarithmic nonlinear terms.

We also discuss the dynamics of the equation when β goes to 0.

LECTURE 8: THE CAHN-HILLIARD EQUATION IN IMAGE INPAINTING

In this lecture, we explain how the Cahn-Hilliard equation can be used in image processing, in particular, for image denoising and restoration. We present in particular a Cahn-Hilliard model proposed by A. Bertozzi, S. Esedoglu and A. Gillette in view of binary image inpainting which reads

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) + g(x, u) = 0,$$

where

$$g(x,s) = \lambda_0 \chi_{\Omega \setminus D}(x)(s - h(x)), \ \lambda_0 > 0, \ D \subset \Omega, \ h \in L^2(\Omega),$$

 χ denoting the indicator function. Here, h is the damaged image and D is the damaged region.

We then discuss the mathematical analysis of the models and present numerical simulations which show that such models are particularly efficient, compared to other approaches. We also address several open problems (e.g., uniqueness and regularity when considering logarithmic nonlinear terms; numerical simulations show that considering logarithmic nonlinear terms improves the efficiency of the algorithms).

We finally discuss several extensions of this model (for multicolor images and grayscale images).

LECTURE 9: THE CAHN-HILLIARD EQUATION WITH A PROLIFERATION TERM

In this lecture, we introduce variants of the Cahn-Hilliard equation in wiew of the modeling of tumor growth. More precisely, we consider the generalized equation

$$\frac{\partial u}{\partial t} + \Delta^2 u - \Delta f(u) + g(u) = 0,$$

where g is a polynomial; typically, $g(s) = s^2 - s$.

In particular, we show that the choice of the nonlinear terms is crucial, as one may have blow up in finite time if one is not careful enough; such a blow up can be avoided by considering logarithmic nonlinear terms f.

We also discuss how to account for nutrients and energitic aspects (e.g., oxygen) in tumor growth models based on the Cahn-Hilliard equation.

Lecture 10: Further generalizations of the Cahn-Hilliard equation

In this lecture, we discuss the approach due to M. Gurtin and based on a separate balance law for internal microforces. In particular, this allows to generalize the Cahn-Hilliard equation to account for important effects such as deformations and heat transfers. It is interesting to note that several such effects (e.g., heat transfers) lead to mathematically challenging (and still open) problems.