Tagungsbericht 19/1995

Mathematical models in phase transitions

14.-20.05.1995

The meeting has been organized by Hans Wilhelm Alt (Bonn) and Paul Fife (Salt Lake City). The purpose of the meeting was to bring together people from different fields so that they could exchange their knowledge and ideas on mathematical models for phase transitions. During the conference two evening discussions took place, one on "Triple junction motion" and one on "Hysteresis".
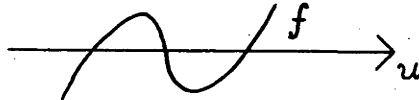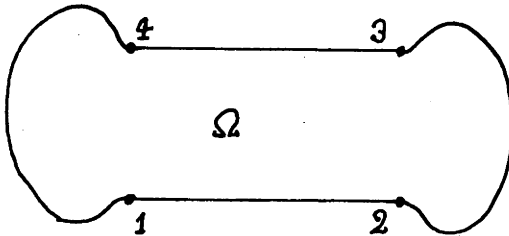
Vortragsauszüge

NICK ALIKAKOS

Finite Dimensional Dynamics and Interfaces Intersecting the Boundary — A Paradigm
(Joint work with G. Fusco and M. Kowalczyk)
We consider the Allan–Cahn (AC) equation $u_t = \varepsilon^2 \Delta u - f(u)$,

$\frac{\partial u}{\partial \eta} = 0$ on a domain with a degenerate neck, $\Omega \subset \mathbb{R}^2$ with $C^{1,\alpha}$–boundary, $\alpha > 0$,

where near corners the boundary is given by $x_2 = \phi(x_1)$ with

$$\phi^i(x_1) = \begin{cases} \kappa|x_1|^\alpha + o(|x_1|^{1+\alpha}) & , \ x_1 \le 0 \ , \\ 0 & , \ x_1 = 0 \ . \end{cases}$$

We describe the motion of single (diffused) interface solutions inside the rectangle 1234.

$$c(\xi) = \underbrace{\left[\varepsilon^{1+\alpha_3}\Gamma_3\kappa_3 + \varepsilon^{1+\alpha_4}\Gamma_4\kappa_4\right]}_{[A]} e^{-2\beta\frac{\xi}{\varepsilon}} - \underbrace{\left[\varepsilon^{1+\alpha_1}\Gamma_1\kappa_1 + \varepsilon^{1+\alpha_2}\Gamma_2\kappa_2\right]}_{[B]} e^{-2\beta\frac{1-\xi}{\varepsilon}} \ , \qquad (1)$$

where κ_i = curvature of i-th corner, Γ_i = constants related to Γ-function, α_i = Hölder exponents at i-th corner.

Theorem 1 *(Equilibria)*
1. Suppose $[A][B] > 0$. Then there exists a unique equilibrium with interface at $\xi \in (l, 1-l)$ with $|\xi - \frac{1}{2}| \leq \varepsilon |\ln \varepsilon|$.
2. Suppose $[A][B] < 0$. Then there exists no equilibrium with interface in $(l, 1-l)$

Theorem 2 *(Dynamics): $c(\xi)$ in (1) is the principal term of the speed.*

ROBERT ALMGREN

Solidification Computation
We review the current state of solidification computation. First, we discuss the reasons for performing computations: to identify interesting special behavior which may then be sought in experiment, to test theories about velocity selection and the line, and to provide detailed information about microstructure for practical engineering purposes. Second, I present the physical assumptions which lead to the most commonly used mathematical models, for large, intermediate, and small undercooling, in which kinetic effects appear differently. Third and finally, I survey several currently popular methods. In the quasi-static limit at low undercooling, boundary integrals are quite effective; we present some of our own computations showing dendrites and singularity formation with dumbbell initial data. Among methods which do not track the interface explicitly, the current favorite is phase field: we present efforts in process to implement adaptive mesh techniques. Other promising methods are level set, a variational algorithm based on the Ising model, and artificial dynamics.

PETER BATES

Traveling Waves for Higher Order and Nonlocal Models
(joint with Paul Fife, Bob Gardner, Chris Jones, Xiaofeng Pien, Xenfeng Wang)
Starting with a Helmholtz free energy for an order parameter distributed on a lattice, we derive a nonlocal evolution equation as the gradient flow of the continuized energy:

$$u_t = J * u - u + f(u) \tag{1}$$

were f is bistable.
We also consider "truncations" of the energy and obtain, as a gradient flow, the equation

$$u_t = A_N u + f(u) \tag{2}$$

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where A_N is a $2N$th order elliptic operator.

We establish existence, uniqueness and stability of traveling plane waves for (1) which connect the stable zeros of f. We also characterize those f's for which the wave is discontinuous and therefore stationary even when $\int_a^b f \neq 0$ (a, b are the stable zeros of f).

For (2) we establish the existence of a stationary solution when $\int_a^b f = 0$ and the existence of traveling waves when this is violated but under the assumption that all but the second order coefficient in A_N are sufficiently small.

YVES BRECHET

Plastic Instabilities and Plastic Waves

Travelling plastic waves are shown to occur both in strain rate softening (s type) and strain softening (h type) constitutive laws. Computer simulations both for propagative waves and for noise induced instabilities are presented.

LIA BRONSARD

On the Multiplicity of Interfaces for the Allen–Cahn Equation

We study the radial Allen–Cahn equation

$$\varepsilon\phi_t - \varepsilon\phi_{rr} - \tfrac{1}{\varepsilon}\phi_r + \tfrac{1}{\varepsilon}\omega'(\phi) = 0 \text{ in } B(0,1) \subset \mathbb{R}^n$$
$$\text{with } u|_{\partial r} = 1 \text{ and where } \omega(\phi) = \tfrac{1}{4}(1-\phi^2)^2 \ .$$

Using the energy method of Bronsard–Kohn ([BK]), we construct solutions $\phi^\varepsilon(1,t)$ with N interfaces in $(\rho(t) - N\varepsilon^\alpha, \rho(t) + N\varepsilon^\alpha)$, $\alpha \leq \tfrac{1}{\varepsilon}$, which persist for some finite strictly positive time. Here $\rho(t)$ solves the mean curvature flow $\dot\rho = -\frac{(n-1)}{\rho}$, $\rho(0) = \rho_0 \in (\tfrac{1}{2}, 1)$. This shows that in the limit $\varepsilon \to 0$, the limiting interface $\rho(t)$ has "multiplicity" N. In particular, when N is even, this shows that there exist "phantom" interfaces separating the same phase. The assumptions are that the weighted energy functional introduced in [BK] is bounded by $NC_0 + C_1\varepsilon^{2\alpha}$, where C_0 represents the jump in energy across one interface, and that the initial data is close ($\mathcal{O}(\varepsilon^\alpha)$) in one sense to a step function with N jumps in $(\rho(t) - N\varepsilon^\alpha, \rho(t) + N\varepsilon^\alpha)$. We also construct such initial data.

This is joint work with Barbara Stoth (Bonn Univ.)

L.–Q. CHEN

A Multicomponent Order Parameter Model for Grain Growth and Ostwald Ripening in Multiphase Systems

It is proposed that an arbitrary multiphase microstructure can be described by a set of non–conserved and conserved order parameters, $\eta_1, \dots, \eta_p$, and $c_1, \dots, c_q$. The non–conserved order parameters represent the orientations of grains while the conserved order

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parameters distinguish the compositional differences among different phases. The temporal evolution of the spatially dependent order parameters is modeled by the Ginzburg–Landau (Allen–Cahn) and Cahn–Hilliard equations:

$$\frac{\partial \eta_i}{\partial t} = -L_{\eta_i} \frac{\delta F}{\delta \eta_i} \qquad 1 \le i \le p$$
$$\frac{\partial c_j}{\partial t} = \nabla \cdot \left(L_{c_j} \nabla \frac{\delta F}{\delta c_j} \right) \qquad 1 \le j \le q$$

where L_{η_i} and L_{c_j} are kinetic coefficients related to interface mobilities and diffusional coefficients, and F is totally free energy.

$$F = \int \left[(f(\eta_1, \dots, \eta_p, c_1, \dots, c_q) + \frac{\alpha_\eta}{2} \sum_i (\nabla \eta_i)^2 + \frac{\alpha_c}{2} \sum_j (\nabla c_i)^2 \right] d^3 r \ .$$

where α_η and α_c are gradient energy coefficients. Computed microstructures using this model reproduced qualitatively very similar microstructures observed experimentally and it is expected to be powerful in predicting microstructural evolution in real systems.

XINFU CHEN

Numerical Simulations for the Mullins–Sekerka Free Boundary Problem

We implemented numerical schemes to solve the following geometrical problem

$$V_{\Gamma_t} = \left[\frac{\partial}{\partial n} K_{\Gamma_t} \right]$$

where Γ_t is the position of the unknown curve at time t, V_{Γ_t} is the normal velocity of Γ_t, K_{Γ_t} is the harmonic extension of the curvature K_{Γ_t} of Γ_t, and $[\frac{\partial}{\partial n} K_{\Gamma_t}]$ represents the jump of the normal derivatives of K_{Γ_t} across Γ_t.

Our numerical scheme is implicit and is stable, allows large time steps. Various kinds of geometrical properties of the motion have been verified, several new features of the motion have also been discovered.

KLAUS DECKELNICK

Weak Solutions for the Curve Shortening Flow

We consider the curve shortening flow for curves in arbitrary codimension in the following formulation:

$$x_t = \frac{x_{uu}}{|x_u|^2} \quad \text{in } S^1 \times (0, T)$$
$$x(\cdot, 0) = x_0 \quad \text{in } S^1 \tag{1}$$

where $x_0 : S^1 \longrightarrow \mathbb{R}^n$ is a parametrization of the initial curve. (1) differs from the usual formulation $\dot{x_t} = \kappa N$ only by a motion in tangential direction. We prove that the solutions of the regularized problems

$$x_t^\varepsilon = \frac{x_{uu}^\varepsilon}{|x_u|^2 + \varepsilon^2} \quad \text{in } S^1 \times (0, \infty)$$
$$x^\varepsilon(\cdot, 0) = x_0 \quad \text{in } S^1 \tag{2}$$

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have a subsequence that converges to a function x which solves (1) in a suitable weak sense.

GERHARD DZIUK

A Numerical Scheme for Anisotropic Curve Shortening Flow.
The gradient flow for the anisotropic length functional ($\nu =$ normal to $\Gamma(t) = x([0, 2\pi], t)$),

$$I(x) = \int_{\mathbb{R}/2\pi} g(\nu)|x_s|\, ds \ ,$$

is discretized with piecewise linear finite elements. This gives a scheme which also works for crystalline $g \in C^{0,1}$. For smooth g we prove convergence in $L^\infty((0, T), L^2(\mathbb{R}/2\pi)) \cap L^2((0, T), H^1(\mathbb{R}/2\pi))$ for the approximations of x and its time derivative x_t by the semidiscrete solution (i.e. continuous in time).

CHARLES M. ELLIOTT

Diffusion in Multicomponent Systems with Concentration Dependent Mobility Matrix
Many phenomena in the theory of phase transitions can be modelled by diffusion equations for multicomponent systems. We study evolution equations with conserved order parameters which are based on a Ginzburg–Landau free energy.
In particular we are interested in cases where the diffusion in the interfacial region is stronger than in the pure phase. This fact is reflected in a concentration dependence of the mobility matrix. Since physically reasonable mobilities degenerate in the pure component, we are let to a system of fourth order degenerate parabolic equations.
We discuss some properties of the model and give an existence proof for the degenerate parabolic system.(Joint work with C.M. Elliott (Sussex))

IRENE FONSECA

Phase Transitions, Interactions between Fracture and Damage for Solid Materials, and Related Questions
Recent progress in the understanding of material instabilities has motivated the study of nonconvex variational problems. Usually minimizing sequences develop finer and finer structure, and converge weakly to nonminimizing states which may be stable enough to be observed. The dynamical development of the microstructure and its evolution is addressed. It is well–known that interfacial energies play a pivotal role in stabilizing the microstructure; in some models, the interfacial energy is produced "naturally" by the bulk terms, while in others interfacial energy contributions are induced in the initial total energy. To illustrate the first case, the analysis of a problem of change of phase of an

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elastic material is studied; the analysis of the evolution for a continuum that undergoes both damage and fracture fits into the latter.

I.G. Götz

Kinetic Undercooling in the Stefan Problem with the Distributed Phase Function

We deal with the one–dimensional Stefan problem with distributed phase function. The phase function satisfies a Hamilton–Jacobi equation, which describes the kinetic undercooling. We prove the existence of a solution with the non–smooth initial data. For the Hamilton–Jacobi equation we find a viscosity solution, which is given as a minimum value of some functional. We study also the limit case, when a kinetic parameter tends to zero. Doing so we obtain a weak solution of the undercooled Stefan problem without the kinetic condition.(Joint work with A.M. Meirmanov (Covilha))

Gerhard Huisken

Mean Curvature Flow with Neumann Boundary Conditions

Let $\Sigma^n \subset \mathbb{R}^{n+1}$ be a smooth, fixed hypersurface. We study one–parameter families $F :$ $M^n \times [0, T) \longrightarrow \mathbb{R}^{n+1}$ of smooth immersed hypersurfaces, which move by mean curvature and meet Σ^n orthogonally at the boundary ∂M^n:

$$
\begin{cases}
\frac{d}{dt} F(p,t) & = & \vec{H}(p,t) & p \in M^n, t > 0 \\
F(p,0) & = & F_0(p) \\
\nu(p,t) & \in & T\Sigma & p \in \partial M^n, t > 0 \, ,
\end{cases}
$$

where ν is the normal of $F(M^n)$. The problem was previously studied in the case of vertical cylinders and nonparametric solutions by Huisken, Stone, Altschuler–Wu and Guan. In the talk new results in the general parametric setting due to Axel Stahl (Tübingen) were presented: Shorttime existence holds for sufficiently smooth Σ and F_0, a singularity can only occur if the curvature of M^+ becomes unbounded, a barrier principle holds if the barrier satisfies an angle condition at Σ. If $\Sigma = S^n$, any convex initial surface contracts in finite time to a point, approaching the shape of a hemisphere asymptotically.

Hans G. Kaper

Vortex Dynamics in Type–II Superconductors

In this talk, I discuss various aspects of the vortex state of type–II superconducting materials, as described by the Ginzburg–Landau equations,

$$
\begin{aligned}
&\frac{1}{\kappa^2}(\partial_t \psi + i\kappa\phi\psi) + (\frac{1}{i\kappa}\nabla - A) \cdot (\frac{1}{i\kappa}\nabla - A)\psi + (|\psi|^2 - 1)\psi = 0 && \text{in } \Omega, \\
&\sigma(\partial_t A + \nabla\phi) + \nabla \times \nabla \times A - J_s = 0 && \text{in } \Omega, \\
&J_s = \frac{1}{2i\kappa}(\psi^*\nabla\psi - \psi\nabla\psi^*) - |\psi|^2 A \, .
\end{aligned}
$$

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Here, ψ is the complex order parameter, $\psi : \Omega \to \mathbb{C}$; A is the vector potential, $A : \Omega \to \mathbb{R}^3$; and ϕ is the electric potential, $\Phi : \Omega \to \mathbb{R}$. The Ginzburg–Landau parameter κ is large ($\kappa \sim 100$ for high–temperature superconductors); σ measures the ratio of the relaxation times for the order parameter and the vector potential.

The GL equations, supplemented by the "natural" boundary conditions, are gauge invariant under the transformation $(\psi, A\phi) \mapsto (\psi e^{i\kappa\chi}, A + \nabla\chi, \phi - \partial_t\chi)$. Possible gauges are the zero–electric potential gauge ($\phi = 0$) or the Landau gauge ($\nabla \cdot A = 0$ in Ω, $A \cdot n = 0$ on $\partial\Omega$).

Existence of global weak solutions ($\Omega \subset \mathbb{R}^2$) and existence and uniqueness of global strong solutions ($\Omega \subset \mathbb{R}^2$ or $\mathbb{R}^3$) have been established by Tang and Wang (preprint).

With proper scaling, we show that the GL equations describe the dynamics of a system of "vortices" in the limit as $\kappa \longrightarrow \infty$ ($\Omega \subset \mathbb{R}^2$).

We show the results of numerical simulations in 2 and 3 dimensions. In two dimensions, we focus on the evolution of a superstructure in the vortex lattice (point–defects, grain boundaries); in three dimensions, on the formation of vortices and the influence of thermal fluctuations.

This work was done jointly with several colleagues at Argonne. The computations were done on the IBM–SPI (128 processors, 128 Mbytes per processor).

INGO MÜLLER

The Effect of Coherency on Phase Diagrams

Usually in a binary mixture in two phases the free enthalpy of an mixture is assumed to be equal to the sum of the free enthalpies of the phases. If coherency at the phase boundaries is taken into account, a penalty term for the formation of such interfaces must be added. In the present work that penalty term is assumed to be proportional to the product of the fractions of the two phases – with a coherency coefficient as factor of proportionality. In order to investigate the consequences of such an Ansatz we consider the simplest possible phase mixture, viz. an ideal solution of incompressible liquids in equilibrium with a mixture of ideal gases consisting of the vapours of the liquid.

It turns out that – compared to the usual non–coherent case – the boiling line is lowered and the condensation line is lifted. Both lines intersect such that the pure constituents and, in fact, dilute solutions, suffer the effect of supersaturation. The mixture does not, at least not for moderate values of the coherency coefficient. The most prominent prediction of this theory is that the single boiling and condensation points – which normally characterize the pure constituents – occur at concentrations of the mixture that are unequal to 0 or 1.

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STEFAN MÜLLER

Microstructures with Multiple Scales

Many systems develop a fine scale structure that involves several small scales. Typical examples are magnetic materials where magnetic domains, Bloch walls and point or line singularities occur on separate scales or solid–solid phase transformation that often lead to a microstructure that involves a hierarchy of laminates. While there are powerful methods to deal with problems involving one small scale (singular perturbations, Γ– convergence,...) much less is known about multiple scales.

A simple mathematical model is given by the problem

$$I_\varepsilon(u) = \int_0^1 \varepsilon^2 u_{xx}^2 + (u_x^2 - 1)^2 + u^2 \, dx \xrightarrow{!} \min,$$

$$u : [0,1] \longrightarrow \mathbb{R}, \text{periodic}.$$

By rather ad-hoc methods one can show the following

Theorem 1 *Suppose that ε is small enough and u_ε is a minimizer of I_ε. Then u_ε is periodic with period $P_\varepsilon = L_0 \varepsilon^{1/3} + O(\varepsilon^{2/3})$.*

The talk discusses the development of a general approach to analyze such problems that is based on studying the Young measure related to a rescaled map

$$\hat{v}_\varepsilon : (0,1) \to L^2(-L,L)$$

where

$$(\hat{v}_\varepsilon(x))(y) = \varepsilon^{-1/3} u_\varepsilon(x + \varepsilon^{1/3} y)0, \quad x \in (0,1), \ y \in (-L,L)$$

(Joint work with G. Alberti, Pisa)

AMY NOVICK–COHEN

Cahn–Hilliard/Allen–Cahn Equations and Trijunctions

For a system of Cahn–Hilliard/Allen–Cahn equations derived in the context of simultaneous ordering and phase separation in binary alloys on a BCC lattice, formal asymptotic equations are developed in the low temperature limit and under the assumption the mobility is dependent on the concentration and on the non–conserved order parameter. This motion yields two interphase boundaries which move by motion by minus the surface Laplacian of mean curvature coupled to an antiphase boundary which moves by motion by mean curvature.

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Euza Orlandi

Ising Spin Systems with Kac Potentials Modelling Phase Separation

(Joint work with A. De Masi, E. Presutti, L. Triolo)

We consider an Ising spin system in $\mathbb{Z}^d$ with Hamiltonian

$$H_\gamma(\sigma) = -\frac{1}{2} \sum_{x \neq y} J_\gamma(x,y)\, \sigma(x)\, \sigma(y) \tag{1}$$

where $\sigma(x) = \pm 1$ for $x \in \mathbb{Z}^d$, and $\gamma > 0$ is a scaling parameter,

$$J_\gamma(x,y) = \gamma^d J(\gamma|x-y|), \quad J(|r|) \geq 0, \quad \int J(|r|)\, dr = 1.$$

We are interested in the limit $\gamma \downarrow 0$.

This class of models has been introduced by Kac–Uhlenbeck, Hemmer [63] to prove the validity of the Van der Waals Theory of phase transition. The equilibrium statistical properties have been studied by Lebowitz and O. Penrose [66]. We consider the Glauber (non conservative) spin–flip dynamic for the spin model with hamiltonian (1) and rescaling suitably time and space we derive the continuum equation for the order parameter of the system: the magnetization m. We prove that at time t the evolution of the spin system is very close to the solution of the following non local equation:

$$\frac{\partial m}{\partial t} = -m + tgh\beta J * m \; ; \quad \beta = \frac{1}{|r|}, \; r = \gamma x.$$

Rescaling further space and time we prove that for $\beta > \beta_c = 1$ the clusters of the two phases forming after time $\simeq \log \frac{1}{\gamma}$ will move according to the mean curvature motion of parameter θ, before developing of singularities.

Felix Otto

Viscous Fingering

We consider the flow of two fluids of different mobility in a porous medium. If the more mobile displaces the other, the interface is virtually unstable and a specific microstructure is generated and evolves in time. Within a PDE–model we prove that the mixing zone only grows linearly in time.

Since the introduction of DLA, various stochastic algorithms simulating this phenomenon have been developed. The generated clusters are fractal in the limiting case of mobility ratio $\lambda < \infty$ and compact for $\lambda = 1$. With support of numerical experiments and renormalisation–group arguments, it had been conjectured that they eventually cross over from fractal to compact for all finite $\lambda \in (1, \infty)$. Our result above confirms this conjecture.

IRENA PAWLOW

Phase Transitions Models with Second Order Free Energy

We give a thermodynamical framework for phase transitions models governed by a second order free energy, e.g. of Ginzburg–Landau type

$$f = f_0(u) + \kappa_1(u) |\nabla u|^2 + \kappa_2(u) |\Delta u|^2 ,$$

where u is an order parameter, f_0 nonconvex, κ_1 of arbitrary sign and $\kappa_2 > 0$. Such form arises in phase transition models for oil–water–surfactant mixtures. We consider the isothermal situation and single order parameter satisfying

$$\begin{cases} \partial_t u + \nabla \cdot j = \tau \\ \text{with a constitutive equation for the mass flux} \\ j = \hat{j}(Y) , \quad Y = (u_t, Du_t, u, Du, \dots , D^{m_0}u) . \end{cases}$$

Here $D^m u = (u_{i_1 \dots i_m})_{i_1, \dots , i_m = 1, \dots N}$, τ is a source term.

The goal is to determine constitutive restrictions imposed by the entropy principle. By exploiting this principle according to I. Müller's theory with (Lagrange–Liu) multipliers we obtain the following:

1. the constitutive equation for the free energy $f = \hat{f}(u, Du, D^2u)$;

2. the constitutive structure of the free energy flux;

3. a differential equation for the chemical potential (identified with the multiplier);

4. the residual inequality.

Furthermore, we formulate a general class of models with multiplier as independent variable. Sufficient conditions for the entropy principle to be satisfied are given.

OLIVER PENROSE

A Phase–Field Model for Diffussion–Induced Grain–Boundary Motion (DIGM)

(joint work with J. W. Cahn and P. Fife)

DIGM is the motion of the boundary between two grains with differing chemical compositions in a thin film of metallic alloy, in the presence of a vapour consisting of atoms of one of the component metals. The aim of this work is to find plausible mechanism for this phenomenon.

Our model uses two fields: ϕ which takes the values $+1$ and -1 in the two crystals, and u the concentration of the "vapour" atoms in the solid metal. The free energy is

$$F = \int_\Omega A[w(\phi) + \frac{1}{2}(\nabla\phi)^2] + u \log u + (1-u)\log(1-u) + \varepsilon p(\phi, u) \, d^3x$$

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where A, ε are constants, $w(\phi) = \frac{1}{2}(1 - \phi)$ if $-1 \leq \phi \leq 1$, $+\infty$ otherwise and $p(\phi, u)$ is the coupling function. The kinematic equations are

$$\phi_t = -\delta F/\delta \phi = \phi + \nabla^2 \phi - \varepsilon \frac{\partial p}{\partial \phi}$$

$$u_t = \operatorname{div}[D(\phi, u)\operatorname{grad} \frac{\delta F}{\delta u}] = \operatorname{div}[D(0)(1 - \phi^2)\operatorname{grad} u] + \Delta(\varepsilon)$$

where $D(\phi, u) = D(0)(1 - \phi^2)\,u\,(1 - u)$ and the diffusivity $D(0)(1 - \phi^2)$ is zero in the grains but large in the boundary.

A travelling wave solution is obtained by a successive approximation method, leading to the formula

$$c = \frac{-\varepsilon \iint \frac{\partial p}{\partial \phi}(u^0, \phi^0)\,\cos x\,dx dy}{\int_{-\pi/2}^{\pi/2} \cos^2 x\,dx}$$

where $\phi^{(0)} = \sin x$ and $u^{(0)}$ are the approximate (to lowest order in ε) solutions for ϕ and u, in a coordinate system with x perpendicular to the grain boundary, y perpendicular to the film.

The physical conclusion is that $p = 0$ gives no motion, $p = u(1 - \phi^2)$, corresponding to an enhanced stability in the boundary, gives a prediction disagreeing with experiment, but that a $p(\phi, u)$ representing the effect of elastic interaction is consistent with existing experimental results.

G. PURDY

Phase Equilibria and Diffusion in Multicomponent Systems

Two examples are considered of the application of thermodynamics to multicomponent diffusion–transformation systems.

1. Ostwald Ripening (with I. Manal): Classical mean–field theory is reviewed; it is shown that the thermodynamic properties of the parent solution enter both the diffusion coefficients and the Gibbs–Thomson relationships through the same factor, (the Hessian of the free energy). These thermodynamic terms cancel, leaving only mobilities in the final kinetic expression.

2. Coherent Equilibrium and Diffusion in Multilayers (with Yves Brechet): Multi-component equilibrium and diffusion equations can be extended to include biaxial coherency strains. Ternary two–phase equilibria are described by a construction in which compositions of phases in equilibrium are determined as points of contact of planes, doubly tangent to the isothermal coherent free energy surfaces. In single–phase multicomponent multilayers one can always choose sets of initial compositions to give a strain–free multilayer. In these choices, strain energy will first increase, then decrease with the course of diffusional homogenization.

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Piotr Rybka

Solid to Solid Phase Transitions in the Framework of Viscoelasticity

We study some qualitative properties of the system of viscoelasticity

$$u_{tt} = \operatorname{div}\sigma(\nabla u) + \Delta u_t , \quad u : \Omega \subset \mathbb{R}^n \to \mathbb{R}^n \tag{1}$$

in many dimensions. Here $\sigma(F) = DW(F)$. If W has several local minima the above system may be considered as a model for martensit phase transitions in solids.

We show that this equation does not permit any motion of singularities of ∇u. (Surfaces of jumps of ∇u are interpreted as interfaces). Moreover, a priori bounds for $\nabla u(t)$ in L^∞ in terms of initial data are impossible. Thus, equation (1) may not be appropriate model for phase transitions in solids.

Alfred Schmidt

An Adaptive Method for the Computation of Mean Curvature Motion by the Allen–Cahn Equation

(joint work with M. Paolini, C. Verdi, Milano)

Up to now, no local a–posteriori estimate is known which gives criteria how to choose the local meshsize and order parameter ε to reach a given error bound for the moving interface.

We propose to make these values dependent on the width of the strip around the interface, where the distance function is smooth. For an implementation in 2D and 3D, the maximal principal curvature must be computed and global effects taken into account, when different parts of the interface come close together.

R.F. Sekerka

Optimum Stability Conjecture for the Role of Interface Kinetics of the Dendrite Operating State

The dendrite operating state consists of a specification of the grown speed, v, and the tip radius, ρ, of a dendrite growing from a pure supercooled melt. The supercooling is $\Delta T = T_M - T_\infty$ where T_M is the melting point and T_∞ is the far field temperature. The dimensionless supercooling is $S = \frac{\Delta T}{L_v/C_v}$ where L_v is the latent heat and C_v is the specific heat. The Pectet number is $P = \frac{v\rho}{2k}$ where k is the thermal diffusivity. Conservation of energy (Ivantsov) gives

$$S = I(P).$$

To determine v and ρ separately, one needs an additional condition: Specify

$$\sigma = \frac{2kd_0}{\rho^2 v}$$

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where d_0 is a capillary length. Current theories give $T = \text{const}$ (independent of S) which is violated experimentally by Pivalic Acid. We conjecture that ρ is given by the wavelength, λ, of morphological stability theory that is related to the fastest growing model. This gives $\frac{1}{\sigma} = A + \frac{B}{\rho}$ where A and B are constants. This fits the experimental data for Pivalic Acid. One can combine this with the energy equation $S = I(P)$ to obtain ρ and v separately. The fit is better than for constant σ but not good at low supercoolings, due to convection in the melt that is not accounted for by the theory.

R.F. SEKERKA

Stagnant Film Model of the Effect of Natural Convection on the Dendrite Operating State

HALIL METE SONER

Vector–valued Ginzburg Landau Equations

I consider the $\varepsilon \downarrow 0$ asymptotics of the reaction diffusion system

$$u_t^\varepsilon - \Delta u^\varepsilon = \frac{u^\varepsilon}{\varepsilon^2}(1 - |u^\varepsilon|^2) \,, \qquad \text{on } (0, \infty) \times \mathbb{R}^d$$

for the unknown $u^\varepsilon \in \mathbb{R}^2$. Using energy estimates, we show that, as $\varepsilon \downarrow 0$, the zero level set of $u^\varepsilon(t, \cdot)$ moves by mean curvature. This result is valid for $d > 2$ and when starting from $\Gamma_0 = \{u^\varepsilon(0, x) = 0\}$ there is a smooth mean curvature flow $\{\Gamma_t\}_{t \in [0,T]}$. The main ingredient is a parabolic type Pohozaev inequality

$$\frac{d}{dt} \int \eta(t, x) \, E^\varepsilon(t, x), dx \leq \int (\eta_t - \Delta\eta)E^2 + D^2\eta\nabla u^\varepsilon - \nabla u^\varepsilon$$

where $E^\varepsilon(t, x) = \frac{1}{2}|\nabla u^\varepsilon(t, x)|^2 + \frac{1}{\varepsilon}\omega(u^\varepsilon)$, $\omega(u) := \frac{1}{4}(1 - |u|^2)^2$ and

$$\eta(t, x) = \begin{cases} (\text{dist}\,(x, \Gamma_t))^2/2 \,, & x \text{ near } \Gamma_t \\ \text{smooth} \geq \eta_0 \,, & x \text{ away from } \Gamma_t \,. \end{cases}$$

For $d = 2$, the zero set of $u^\varepsilon(t, \cdot)$ is discrete and after rescaling of time by $1/\ln(1/\varepsilon)$, the vortices (=zeroes) move according to a simple differential equation.

To obtain similar results for $u^\varepsilon \in \mathbb{R}^k$, I consider a slightly different equation:

$$(E^\varepsilon(t, x))^{\frac{k}{2}-1}u_t^\varepsilon = -\delta I^\varepsilon = \text{div}((E^\varepsilon)^{\frac{k}{2}-1}\nabla u^\varepsilon) + (E^\varepsilon)^{\frac{k}{2}-1}\frac{u^\varepsilon}{\varepsilon^2}(1 - |u^\varepsilon|^2)$$

where

$$I^\varepsilon(\phi) := \int_{\mathbb{R}^d} \frac{2}{k}(E^\varepsilon)^{\frac{k}{2}} \,, \quad E^2 = \frac{1}{2}|\nabla\phi|^2 + \frac{1}{\varepsilon^2}\omega(\phi) \,.$$

Above equation becomes:

$$u_t^\varepsilon - \Delta u^\varepsilon - (\tfrac{k}{2} - 1)\frac{\nabla E^\varepsilon - \nabla u^\varepsilon}{E^\varepsilon} = \frac{u^\varepsilon}{\varepsilon^2}(1 - |u^\varepsilon|^2) \,, \quad \text{on } (0, \infty) \times \mathbb{R}^d$$

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for the unknown $u^\epsilon \in \mathbb{R}^k$. Results analogous to the $k = 2$ case hold. These are joint results with R. Jerrard (Carnegie Mellon and University of Illinois)

BARBARA STOTH

The Ginzburg–Landau Equations for Type–I Superconductors and Sharp Interface Limit

In this talk I present rigorous asymptotics of the Ginzburg–Landau equations for type–I superconductors. These equations model the penetration of a normal region into an initially superconducting wire, when a sufficiently strong external field is applied. The Ginzburg–Landau equations for the magnetic field $H = \text{curl } Q$ and the scalar order parameter f take the form (cf. Chapman–Harrison–Ochendon / SIAM Rev. 1992)

$$\begin{cases} \frac{\lambda^2}{\kappa^2}(\alpha\partial_t f - \frac{1}{r}(rf')') + \omega'(f) + \frac{1}{\lambda^2}fQ^2 = 0 \\ \partial_t Q - (\frac{1}{r}(rQ)')' + \frac{1}{\lambda^2}f^2Q = 0 \end{cases}$$

where λ is a material constant measuring the penetration depth of H, $W(f) = \frac{1}{4}(1-f^2)^2$ the potential and κ the Ginzburg–Landau parameter. We impose Neumann conditions for f and Dirichlet conditions for $H = \text{curl } Q$ on the surface of the wire.

We prove rigorously that, as $\lambda \longrightarrow 0$, the magnetic field converges to a solution of the classical, one–phase, well–posed Stefan problem: $H = 0$ in the superconducting region, $\partial_t rH - \Delta H = 0$ in the normal region, and $H = \frac{1}{\sqrt{2}}$ and $\nabla H \cdot \nu = \frac{-1}{\sqrt{2}}V$ on the interface separating normal– and superconducting regions.

We assume an initially stable situation.

The analysis holds true for any value of κ, but the radial model seems only appropriate for $\kappa \leq \frac{1}{\sqrt{2}}$, which corresponds to type–I superconductors.

These results are joint work with Lia Bronsard (McMaster).

JEAN E. TAYLOR

Crystalline Surface Diffusion

We consider the motion of polyhedral curves bounding regions in $\mathbb{R}^2$ by the law $v = -\Delta_S K_\Phi$ for a crystalline "surface" energy Φ, where v is the normal velocity, κ_Φ is the weighted mean curvature κ and Δ_S is the surface Laplacian. (Terms are defined below). For such motion, we establish the right formulation, develop the bases of the theory, and implement it computationally.

Given a function $\Phi : S^{n-1} \longrightarrow \mathbb{R}^+$ which is the surface free energy per unit area, the Wulff shape $W = \{x \in \mathbb{R}^n : x \cdot n \leq \gamma(n)\}$ is the (unique to translations) solution to the isoperimetric problem of enclosing a region of volume equal to that of W by a surface of minimum surface free energy (as measure by $\int_S \Phi(\hat{n}_S(x))d\mathcal{H}^{n-1}$). The crystalline case is where W is a polyhedron (in $\mathbb{R}^2$, a polygon). We fix W in $\mathbb{R}^2$, and require the initial

polyhedral curves to have their normals by normals of W. The crystalline (weighted mean) curvature of a line segment s_i in a polyhedral curve is $-\frac{\sigma_i \Lambda(n_i)}{l_i}$, when l_i is the length of s_i, $\Lambda(n_i)$ is the length of the line segment of ∂W with normal $n_i =$ normal of s_i, and $\sigma_i = 1,\ 0$ or -1, depending on the geometry around s_i. A major technical difficulty is deciding where and when to stop edges.

Jean E. Taylor

The Variational Approach to Motion by Weighted Mean Curvature and Other Motions

A variational approach is given for the motion of boundaries of regions in $\mathbb{R}^n$ by weighted mean curvature for any given surface free energy function (per unit area) $\Phi : S^{n-1} \to \mathbb{R}^t$ and for *all* time $t \geq 0$. Existence is proved for all time of flow $\kappa(t)$ of surfaces, given a initial region κ_0 of finite perimeter, this flow agrees with any classical motion by weighted mean curvature of any viscosity solution wherever such solutions are defined. This motion, however, applies to any Φ and passes through all singularities.

One thereby obtains a piecewise constant flow $K_j(t)$ for each $j = 1, 2, \ldots$, and Cantor diagonalization produces a limit flow $K(t)$ defined for a chosen set of time t. The crucial step is the proof of a Hölder bound on the $K_j(k\Delta t)$ which enables $K(t)$ to be extended continuously to *all* time t.

More recent work extends this to cover grain growth (including multijunctions) with different Φ_{ij} and mobility M_{ij} for each pair of adjacent regions (Carabello – there are certain conditions the Φ_{ij} and M_{ij} must satisfy) and motion by surface diffusion (Chung)

Augusto Visitin

Models of Phase Nucleation

Extending the classical Stefan model, we represent surface tension by the *Gibbs–Thomson law*, and account for solid *nucleation* in an undercooled liquid.

This phenomenon includes *bistability* (e.g., temperature does not necessarily determine the phase), and *symmetry breaking*.

We distinguish two modes of phase evolution: front motion and discontinuous phase transition (like nucleation).

On account of the smallness of the capillarity scale, we propose a model involving both a *macroscopic* and a *mesoscopic* space–scale. Transition from the finer to the coarser scale is provided by an average procedure, which we represent by convolution with a Gaussian kernel. This accounts for fast diffusion of latent heat of fusion, and allows us to represent solid nucleation at low undercooling.

This also provides an interpretation of *mushy regions.*

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ADAM WHEELER

Anisotropic Phase Field Models

A natural way to incorporate an anisotropic surface energy into a phase field model is based on a free–energy functional of the form

$$\phi = \int_\Omega \frac{\varepsilon^2}{2}[\Gamma(\nabla\phi)]^2 + f(\phi, T)\, dV$$

where $\Gamma(\nabla\phi)$ is a homogeneous function of degree one. We show that the corresponding Euler–Lagrange equation for ϕ may be expressed as

$$\varepsilon^2 \nabla \cdot [\Gamma(\nabla\phi)\vec{\xi}(\nabla\phi)] - f\phi = 0$$

where $\vec{\xi}(\nabla\phi)$ provides a natural generalisation of the Cahn–Hoffman xi–vector previously employed for sharp interfaces.

We go onto report an asymptotic analysis in the sharp interface limit $\varepsilon \to 0$, and show that we obtain the appropriate form of the Gibbs–Thomson equation, expressed in terms of the xi–vector:

$$u = -\nabla_S \cdot \vec{\xi}$$

where $\nabla_S\cdot$ is the surface divergence on the interface S. (Joint work with G.B. McFadden, NIST, USA)

DARIUSZ WROZEK

Infinite System of Reaction–Diffusion Equations in the Theory of Sol–Gel Transition

The following system of reaction–diffusion equations is studied:

$$\frac{\partial u_1}{\partial t} = d_1 \Delta u_1 = a_1 u_1 \sum_{j=1}^{\infty} a_j u_j \ ,$$

$$\vdots$$

$$\frac{\partial u_k}{\partial t} = d_k \Delta u_k + \frac{1}{2} \sum_{i=1}^{k-1} a_i a_{k-i} u_i u_{k-i} - a_k u_k \sum_{j=1}^{\infty} a_j u_j \quad k = 2, 3, \ldots$$

on $\Omega \times (0, T)$, where Ω is a bounded open set in $\mathbb{R}^n$, $n \geq 1$, with smooth boundary $\partial\Omega$, d_k, a_k are positive constants. We impose homogeneous Neumann boundary conditions

$$\frac{\partial u}{\partial \nu} = 0 \quad \text{on } \partial\Omega \times (0, T) \ k = 1, 2, \ldots$$

and initial data

$$u_1(x, 0) = U_0(x) \ , \ u_k(x, 0) = 0 \text{ for } k \geq 2 \ , \ x \in \Omega$$

where U_0 is a given function, such that $U_0 \in L^\infty(\Omega)$, $U_0 \geq 0$. The variables u_k represent concentrations of k–mers (polymers). The relevant o.d.e. system was derived by Smoluchoski in 1917. We study the problem under two different hypotheses

(H1) $\lim\limits_{k \to \infty} \frac{a_k}{k} = 0$, $d_k > 0$ $k = 1, 2, \ldots$

(H2)   1. there exists $M \geq 1$ such that $d_k = d = \text{const}$, for $k \geq M$

       2. $\limsup\limits_{k \to \infty} \frac{a_k}{k} < \infty$.

Existence, uniqueness and asymptotic behaviour of solutions are investigated. In some cases, the mass $M = \int_\Omega^\infty k u_k(x, t) \, dx$ is violated in a finite time. This phenomenon is related to a sol–gel transition. (Joint work with Ph. Bènilan)

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