Wavenumber Selection of Turing Patterns through Boundary Conditions

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Heuristic Derivation

Let $F[u]$ be the free energy of a volume Ω defined on a non-uniform property, ϕ, of the medium.

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For an isotropic medium the free energy is invariant under the reflections $x_i \to -x_i$ and $x_i \to x_j$ so that f expands as

$$F[\phi] = \int_\Omega \left(f_0(\phi) + \kappa_1 \nabla^2\phi + \kappa_2 |\nabla\phi|^2 \right) dx$$

where $\kappa_1 = \frac{\partial f}{\partial \nabla^2 \phi}$ and $\kappa_2 = \frac{\partial f}{\partial |\nabla\phi|^2}$ are tensors given by the crystal structure of the medium.

Heuristic Derivation

Integrating by parts and dropping higher order terms we are left with an energy functional of the forming

$$F[\phi] = \int_{\Omega} \left(f_0(\phi) + \frac{c}{2} |\nabla \phi|^2 \right) dx + \int_{\partial\Omega} \kappa_1 \nabla \phi \cdot n dS$$

where $c = 2(\kappa_2 - \frac{d\kappa_1}{d\phi})$

Potentials

Assume a parameter dependent phase transition past a bifurcating value from a “random“ phase (homogeneuos ϕ) to an ”ordered“ stable phase ϕ^*. This can be modeled by a ”homogeneuos potential“ of the form

$$f_0(\phi;\lambda) = \left((a(\lambda) - (b(\lambda)\phi)^2)\right)^2$$

for stable phases given as $\phi^*(\lambda) = \frac{\sqrt{a}}{b}$.

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so that the flux of the total potential is

$$J = -D\nabla\mu$$

for a diffusion constant D.

Cahn Hilliard equation

Applying a continuity equation we have Cahn-Hilliard as a coupled second order system:

$$
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A general, phenomenalogical, 4th order, conservation law of a quantity which has a "homogeneoues" free energy and a "gradient" free energy

$$\phi_t = D\nabla^2[(1-\phi^2)^2 - \gamma\nabla^2\phi]$$

Gradient Dynamics

Under the right boundary conditions the free energy functional serves as a Lyapunov functional.

$$\frac{dF}{dt} = \int \frac{\delta F}{\delta \phi} \frac{d\phi}{dt} = \int \mu \phi_t$$

$$\frac{dF}{dt} = D \int_\Omega \mu \nabla^2 \mu = -D \int_\Omega |\nabla \mu|^2 + D \int_{\partial\Omega} \mu \frac{\partial \mu}{\partial n}$$

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For homogeneoues Neumann or homogeneoues Dirichlet boundary conditions on the potential μ, F serves as a Lyapuov functional given that the original boundary term also vanishes

$$\int_{\partial\Omega} \kappa_1 \nabla \phi \cdot n dS$$

Swift-Hohenberg

Originally developed as a model for convective instabilities in hydrodynamics, the Swift-Hohenberg equation

$$u_t = -(\nabla^2 - 1)^2 u + \mu u - u^3$$

is a well known model for pattern forming systems. The equation has equilibrium $u = 0$ which for $\mu > 0$ is linearly unstable. For particular boundary conditions, perturbations from the zero solution saturate to leading order as $u(x) = \sqrt{\frac{4\mu}{3}} \cos(kx + \varphi) + \mathcal{O}(\mu^{\frac{3}{2}})$

SH Gradient Dynamics

Similar to Cahn Hilliard the Swift Hohenberg equation has a Lyapunov functional arising from the energy fuctional

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Taking a variation we find

$$\begin{aligned}\frac{\delta F}{\delta u}v &= \int_\Omega (u_{xx}v_{xx} + u_{xx}v + uv_{xx} + uv)dx + \int_\Omega (-\mu u + u^3)vdx \\ &= \int_\Omega (u_{xxxx} + 2u_{xx} + u - \mu u + u^3)vdx + BC \\ &= \int_\Omega -u_t vdx + [(u_{xx} + u)\phi_x - (u_{xxx} + u_x)\phi]_{\partial\Omega}\end{aligned}$$

Asymptotic solutions

Perturbation Theory gives us a family of stationary solutions parameterized by wavenumber

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The only symmetry of Swift Hohenberg is translation invariance so that solutions can be paramterized by the wavenumber k and phase φ.

$$u(x;k) = \sqrt{\frac{4\mu}{3}}\cos(kx+\varphi) + \mathcal{O}(\mu^{\frac{3}{2}}).$$

But, again the boundary conditions break this symmetry (Consider Neumann.)

A Natural selection problem

We would like to understand the wavenumber and phase reationship of stationary solutions for diferent boundary conditions on the half line. And identify cases of wavenumber selection and phase selection.

$$-(\partial_x^2+1)^2 u + \mu u - u^3 = 0 \;\text{ for }\; x \in (0,\infty)$$

With the boundary conditions

$$\begin{aligned} \gamma u''(0) + (1-\gamma)u'(0) + \gamma u(0) &= 0 \\ u'''(0) + \gamma u'(0) &= 0 \end{aligned}$$

SO that $\gamma = 0$ corresponds to Neumann boundary conditions and $\gamma = 1$ corresponds to “transparent” boundary conditions.