Math 277B:

Topics in Mathematics and Biochemistry-Biophysics

Spring 2011, Dept. of Math, UCSD.

Time: 3:00 – 3:50 MWF

Place: AP&M 7421

Instructor: Bo Li

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Course web:

http://www.math.ucsd.edu/~bli/teaching/math277Bs11/

Overview of the course

Topics:

1. PDE models + Dynamical Systems models and computation for molecular diffusion, continuum dielectrics, etc.

implicit solvation 2. Surface motion: cell shapes, cell dynamics, - geometry + field, phase-field models the level-set method.

3. Stochastic process, Brownian dynamics for molecular diffusion. multiscale method.

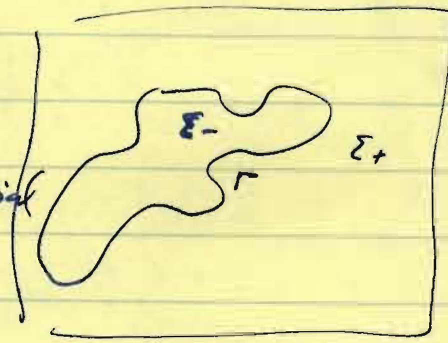
4. The Fokker-Planck equation of biomolecular ~~interfaction~~ interactions, conformational changes, protein folding, etc.

Examples. ①

$$\nabla \cdot \varepsilon \nabla \psi = -\rho$$

ρ ... charge density

ψ ... electrostatic potential



②

$$u_t = D \Delta u + f(u)$$

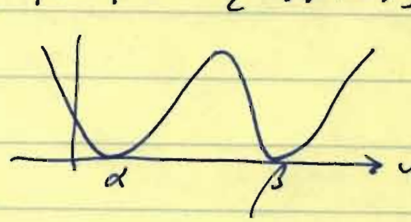
u ... concentration, order parameter

The Allen-Cahn functional.

$$\min \int_\Omega \left[\frac{\varepsilon}{2} |\nabla u|^2 + \frac{1}{\varepsilon} W(u) \right] dx.$$

Ginzburg-Landau theory for phase transitions.

$W(u) =$



$\varepsilon \to 0$?

Γ-convergence.

A model for micro RNA and messenger RNA in gene expressions.

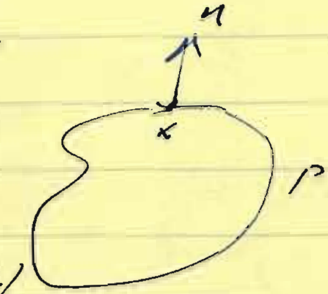
(3) $u_t = D_1 \Delta u - \beta_1 u + K_1 uv + \alpha_1$

$v_t = D_2 \Delta v - \beta_2 v + K_2 uv + \alpha_2$

$K_1 uv \longrightarrow K_1 u^{m_1} v^{n_1}$

$K_2 uv \longrightarrow K_2 u^{m_2} v^{n_2}$

(4) Surface motion.



$$v_n(x) = \frac{d\vec{x}}{dt} \cdot \vec{n}$$

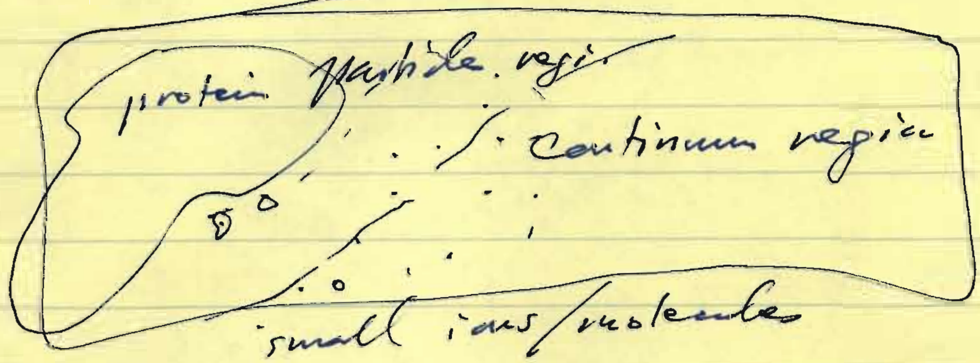
$v_n = -H$ (mean curvature)

$v_n(x) = -H(x) - F(x)$

$F(x) = \delta_\Gamma E[\Gamma]$

$$E[\Gamma] = \min_u \int \left[\frac{\varepsilon}{2} |\nabla u|^2 - fu\right] dx.$$

(5)



$$\begin{cases} dX_j = -F_j\,dt + \xi\,dW. \\ \dfrac{\partial c}{\partial t} = D \Delta c + \cdots \end{cases}$$

(6) The Fokker-Planck equation

$$\frac{\partial \rho}{\partial t} = \nabla \cdot D(\nabla \rho + \beta^{-1} \rho \nabla \phi).$$

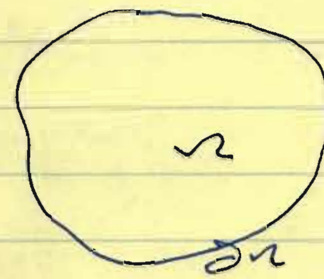
I Nonlinear Diffusion Equations

Variational approach, gradien flow.
numerical methods, etc.

1. Linear problems:

(1) $$\begin{cases} -\Delta u = f & \text{in } \Omega \\ u = u_0 & \text{on } \partial\Omega \end{cases}$$

Ω, f, u_0: known and "nice"



(2) Define $$I[u] = \int_\Omega \left(\frac{1}{2}|\nabla u|^2 - f u\right) dV$$

(3) $$K = \Big\{ u : \underbrace{\int_\Omega \left(u^2 + \int |\nabla u|^2\right) dV}_{\|u\|^2_{H^1(\Omega)} =} < \infty, \ u = u_0 \text{ on } \partial\Omega \Big\}.$$

Thm. ① There exists a unique $u \in K$ such that
$$I[u] = \min_{v \in K} I[v].$$
Call u the minimizer of I over K.

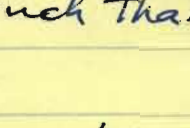
② The minimizer u is the unique solution to the BVP (1).

"Proof" ① Step 2: Let $\alpha = \inf_{v \in K} I[v]$. α is finite.
Let $u_j \in K$: $I[u_j] \to \alpha$.

Step 1: Important bound (growth condition).
$$I[v] \ge C_1 \|v\|^2_{H^1} - C_2. \quad \forall v \in K.$$
$$\|v\|_{H^1} = \sqrt{\int\int (v^2 + |\nabla v|^2) dV}.$$

Then, $u_{j_k} \longrightarrow u$. as $k \to \infty$.

Step 3 $\alpha = \liminf_{k \to \infty} I[u_{j_k}] \ge I[u] \ge \alpha$.



Step 4 convexity $\Rightarrow$ uniqueness.

② Since $u \in K$ is ~~the~~ min. (local min. — enough).

Fix $v \in K_0$ $\frac{I[u+tv] - I[u]}{t}$ ~~≥ 0 $|t|>0$ small. $\forall v$.~~

$g(t) = I[u+tv]$ is min. at $t = 0$.

$g'(0)=0.$

$$g'(0) = \frac{d}{dt}\Big|_{t=0} I[u+tv] =: \delta I[u][v].$$

$$= \frac{d}{dt}\Big|_{t=0} \int_\Omega \left[\frac{1}{2}|\nabla u + t\nabla v|^2 - f(u+tv)\right]dV$$

$$= \int_\Omega \frac{d}{dt}\Big|_{t=0} \left\{\frac{1}{2}\left(|\nabla u|^2 + 2t\,\nabla u\cdot\nabla v + t^2|\nabla v|^2\right) - fu - tfv\right]dV$$

$$= \int_\Omega (\nabla u\cdot\nabla v - fv)\,dV = 0.$$

(4) $\displaystyle\int_\Omega (\nabla u\cdot\nabla v \,\cancel{dV} - fv)\,dV = 0 \qquad \forall v\in H_0^1(\Omega)$

i.e. $v\in H^1(\Omega)$, $v=0$ on $\partial\Omega$

starting pt. of the finite element method. Sometimes called the weak formulation.

$$\int_\Omega[\Delta u\, v - fv]\,dV - \underbrace{\int_{\partial\Omega}\frac{\partial u}{\partial n} v\,dS}_{=0} = 0.$$

since $v=0$ on $\partial\Omega$.

Lemma. If $\displaystyle\int_\Omega h\,\eta\, dV = 0$ for all η, then $h=0$.

Hence $-\Delta u = f$ in Ω.

pf of Lemma in 1d.

step 1. assume h is continuous.

Let η be positive in $(x_0-\delta, x_0+\delta)$ and 0 elsewhere.

step 2. assume h is integrable.

~~Appr. h by cont. function~~:

Use mollifiers. or use measure-theoretical method. Good exercise for math students!

2. Nonlinear problems (steady state)

(5) $$\begin{cases} -\nabla\cdot\varepsilon(x)\nabla u + B'(u) = f & \text{in } \Omega. \\ u = u_0 & \text{on } \partial\Omega \end{cases} \qquad f:\Omega\to\mathbb{R}$$

Ω, $\varepsilon:\Omega\to\mathbb{R}$, $B:\mathbb{R}\to\mathbb{R}$, $u_0:\partial\Omega\to\mathbb{R}$: all given, nice.

$0<\varepsilon_1\le\varepsilon(x)\le\varepsilon_2<\infty$. Assume: B satisfies some properties!

The corresponding energy functional

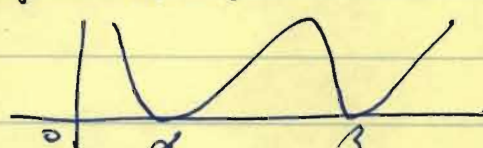
~~Example~~

(6) $$I[u] = \int_\Omega \left[\frac{\varepsilon(x)}{2}|\nabla u|^2 + B(u) - fu\right] dV$$

$u\in K$ (defined as in (3)).

Examples ① $B(u)\equiv 0$. $\varepsilon(x)=1$ $\Longrightarrow$ The previous case. linear prob.

② $I[u]=\int_\Omega\left[\frac12|\nabla u|^2+B(u)\right]dV$ — The Cahn-Hilliard.

$B(u) =$ 

a double-well potential. — nonconvex!

$B(u) = u^2(u-1)^2$, $(u^2-1)^2$.

③ $I_\varepsilon[u]=\int_\Omega\left[\frac{\varepsilon}{2}|\nabla u|^2+\frac{1}{\varepsilon}B(u)\right]dV$.

$\varepsilon>0$. $\varepsilon<<1$.

③ $I[u]=\int_\Omega\left[\frac{\varepsilon}{2}|\nabla u|^2+B(u)\right]dV$.

$B(u)=\beta^{-1}\sum_{j=1}^{m} c_j^{\infty}\left(e^{-\beta q_j u}-1\right)$.

ionic solution $c_j(x)=c_j^{\infty}e^{-\beta q_j u}$

The Poisson-Boltzmann equation.

u — electrostatic potential

c_j — ionic concentration.

$q_j = z_j e$. z_j: valence.

$\beta^{-1} = K_B T$. K_B: Boltzmann const.

T: temperature

c_j^{∞} — bulk concentration.

$B''(u) > 0$

(4). $$\begin{cases} D_1 \Delta u - \beta_1 u - k_1 u v = \alpha_1 \\ D_2 \Delta v - \beta_2 v - k_2 u v = \alpha_2 \end{cases}$$ in Ω.

$\boxed{\begin{array}{l} D_i, \beta_i, k_i > 0 \\ \text{constants,} \\ \alpha_i = \alpha_i(x) \ge 0 \end{array}}$

$D_1 = 0. \Longrightarrow \quad -\beta_1 u - k_1 u v = \alpha_1$

$$u(k_1 v + \beta_1) = -\alpha_1$$

$$u = -\frac{\alpha_1}{k_1 v + \beta_1}$$

$$D_2 \Delta v - \beta_2 v + k_2 \cdot \frac{\alpha_1}{k_1 v + \beta_1} v = \alpha_2.$$

$$D_2 \Delta v - \beta_2 v + \frac{\alpha_1 k_2 v}{k_1 v + \beta_1} = \alpha_2(x)$$

$$\frac{\alpha_1 k_2 v}{k_1 v + \beta_1} = \frac{\alpha_1 k_2}{k_1} \cdot \frac{k_1 v + \beta_1 - \beta_1}{k_1 v + \beta_1}$$

$$= \frac{\alpha_1 k_2}{k_1}\left(1 - \frac{\beta_1}{k_1 v + \beta_1}\right)$$

$$\boxed{D \Delta v - \beta v + \frac{a}{v+b} = f.} \qquad a > 0.\ b > 0.$$

Assume $a = 1$. $\beta = 1$. $D = 1$. (Just mathematics!)

$$\Delta v - v + \frac{1}{v+1} = f.$$

$$I[u] = \int \left[\frac{1}{2}|\nabla v|^2 + B(v) - f v\right] dv.$$

$$B'(v) = v - \frac{1}{v+1}, \quad B(v) = \frac{1}{2}v^2 - \log(v+1).$$

$B''(v) = 1 + \frac{1}{(v+1)^2} > 0$ convex!

So. The BVP has a unique solution.

⑤ $\begin{cases} D_1 \Delta u - \beta_1 u - k_1 u v = \alpha_1 \\ D_2 \Delta v - \beta_2 v - k_2 u v = \alpha_2 . \end{cases}$

$+$ B.C.

How to compute (u, v).

$$\begin{cases} (u_0, v_0): \text{ initial guess.} \\ k \geq 1: \quad D_1 \Delta u_{k+1} - \beta_1 u_{k+1} - k_1 u_{k+1} v_k = \alpha_1 \\ \qquad\qquad D_2 \Delta v_{k+1} - \beta_2 v_{k+1} - k_2 u_k v_{k+1} = \alpha_2 . \end{cases}$$

PDE: linear

$$D \Delta w - \beta w - k\, g(x)\, w = \alpha$$

$$\begin{cases} D \Delta w - G(x) w = \alpha \qquad G(x) \geq 0 . \ D > 0 . \\ \text{B.C.} \end{cases}$$

$$I[w] = \int_\Omega \left[\frac{D}{2} |\nabla w|^2 + \frac{1}{2} G(x) w^2 + \alpha w \right] dV .$$

Discussions on the existence and uniqueness of ~~the~~ minimizers of $I[u]$.

$$I[u] = \int_\Omega \left[\frac{\varepsilon(x)}{2} |\nabla u|^2 + B(u) - f u \right] dx .$$

$u = u_0$ on $\partial\Omega$.

For simplicity, assume $u_0 \equiv 0$.

Direct methods in the calculus of variations

Step 1. Bound: $I[u] \geq C_1 \|u\|^2_{H^1(\Omega)} - C_2 . \quad \forall u \in K .$

Need some assumptions on $B(\cdot)$.

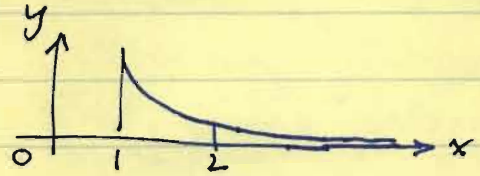
e.g. $B(u) = \frac{e^u + e^{-u}}{2}$. then, no such bound.

Some other cases: Sobolev ~~in~~ embedding inequality.

step 2 – step 3. similar to linear problems.

So there exists a minimizer of I over K.

Note: $y = \frac{1}{x}$ has a minimizer in $[1, 2]$
not in $[1, \infty)$.



The Euler-Lagrange equation

$$I[u] = \int_\Omega \left[\frac{\varepsilon(x)}{2}|\nabla u|^2 + B(u) - fu\right] dV$$

$$\delta I[u][v] = \frac{d}{dt}\Big|_{t} I[u+tv] = \frac{d}{dt}\Big|_{t=0} \int_\Omega \left[\frac{\varepsilon(x)}{2}|\nabla(u+tv)|^2 + B(u+tv) - f(u+tv)\right] dV$$

$$= \int_\Omega \frac{d}{dt}\Big|_{t=0} \left[\frac{\varepsilon(x)}{2}\left(|\nabla u|^2 + 2t\nabla u\cdot\nabla v + t^2|\nabla v|^2\right) + B(u+tv) - fu - tfv\right] dV$$

$$= \int_\Omega \left[\varepsilon(x)\nabla u\cdot\nabla v + B'(u)v - fv\right] dV$$

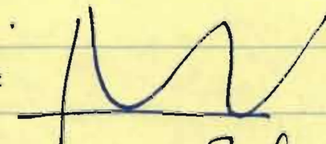
$$= \int_\Omega \left[-\nabla\cdot\varepsilon(x)\nabla u + B'(u) - f\right] v\, dV + \int_{\partial\Omega} \varepsilon \underset{\substack{\| \\ 0 \text{ on } \partial\Omega}}{\frac{\partial u}{\partial n}} v\, dS$$

$$\delta I[u] = -\nabla\cdot\varepsilon(x)\nabla u + B'(u) - f.$$

$$\delta I[u] = 0. \quad \boxed{-\nabla\cdot\varepsilon(x)\nabla u + B'(u) = f \quad \text{in } \Omega}$$

Example. $$I_\varepsilon[u] = \int_\Omega \left[\frac{\varepsilon}{2}|\nabla u|^2 + \frac{1}{\varepsilon} B(u)\right] dV + \frac{\lambda}{2}\left(\int_\Omega u\, dV - 1\right)^2.$$

$\lambda > 0$, $\varepsilon > 0$. (but very small). $B(u) =$



$$\delta I_\varepsilon[u][v] = \frac{d}{dt}\Big|_{t=0} \left\{ \int_\Omega \left[\frac{\varepsilon}{2}|\nabla u + t\nabla v|^2 + \frac{1}{\varepsilon} B(u+tv)\right] dV + \frac{\lambda}{2}\left(\int_\Omega (u+tv)\, dV - 1\right)^2 \right\}$$

$$= \int_\Omega \left[\varepsilon \nabla u \cdot \nabla v + \frac{1}{\varepsilon} B'(u) v\right] dV + \lambda\left(\int_\Omega u\, dV - 1\right)\int_\Omega v\, dV$$

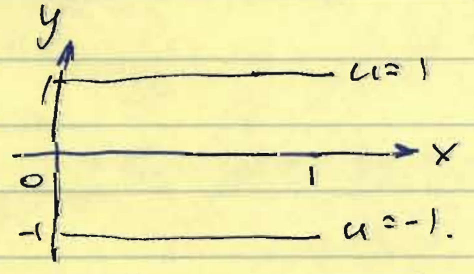
$$= \int_\Omega \left[-\varepsilon \Delta u + \frac{1}{\varepsilon} B'(u) + \lambda\left(\int_\Omega u\, dV - 1\right)\right] v\, dV$$

$$\delta I_\varepsilon[u] = -\varepsilon \Delta u + \frac{1}{\varepsilon} B'(u) + \lambda\left(\int_\Omega u\, dV - 1\right).$$

Note: $\frac{\lambda}{2}$: Lagrange multiplier for the constraint $$\int_\Omega u\, dV = 1.$$

What kind of functions $u = u(x)$ have very low energy $I[u] = \int_\Omega \left[\frac{\varepsilon}{2}|\nabla u|^2 + \frac{1}{\varepsilon} B(u)\right] dV$ for a fixed $\varepsilon > 0$ ($\varepsilon \ll 1$)? $\Omega = (0, 1)$ $\nabla u = u'(x)$.

$B(u) = (u^2 - 1)^2$



What if we require that $\int_0^1 u\, dx = 0$?