Aubry-Mather Theory for PDEs

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CNA Seminar
Carnegie Mellon University

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Outline

1. Background Material
2. Comparison for the Sobolev Gradient
3. Numerical Method
4. Asymptotic Analysis

Energy Functionals and Minimizers

- A function $u \in H^1(\mathbb{R}^d, \mathbb{R})$ is a minimizer for a formal energy

$$S(u) = \int_{\mathbb{R}^d} F(x, u, \nabla u)\, dx$$

if for all compactly supported $\varphi \in H^1(\mathbb{R}^d, \mathbb{R})$

$$\int_{\text{supp}(\varphi)} F(x, u + \varphi, \nabla(u + \varphi)) - F(x, u, \nabla u)\, dx \geq 0.$$

- Assumptions: F is smooth, $F(x + k, y + l, p) = F(x, y, p)$ for all $(k, l) \in Z^{d+1}$, and satisfies growth and convexity requirements in p, so that the Euler-Lagrange equation for S is elliptic.

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Birkhoff Minimizers and Average Slope

- A continuous $u : \mathbb{R}^d \to \mathbb{R}$ is a *Birkhoff* function if

$$u(x-k)+j-u(x) \leq 0 \quad \text{or} \quad \geq 0$$

depending on $(k,j) \in \mathbb{Z}^{d+1}$ but independent of x.

- If u is a Birkhoff minimizer, then there is a $\omega \in \mathbb{R}^d$ such that

$$\sup_{x \in \mathbb{R}^d} |u(x) - \omega \cdot x| < \infty$$

Theorem (Moser, '86)

For each $\omega \in \mathbb{R}^d$ there is a Birkhoff minimizer u with slope ω.

$$\mathcal{M}_\omega = \{u \,|\, u \textit{ is Birkhoff minimizer of } S \textit{ with slope } \omega\} \neq \emptyset$$

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Minimal Average Energy and Crystal Shape

- The average energy of Birkhoff minimizers depends only on the slope:

$$E(\omega) = \lim_{r\to\infty} \frac{1}{|B_r|}\int_{B_r} F(x,u,\nabla u)\,dx, \quad u \in \mathcal{M}_\omega$$

  - The differentiability of $E(\omega)$ depends on the structure of $\mathcal{M}_\omega$.

- A crystal $W \subset \mathbb{R}^3$ can be modeled as a set that minimizes surface energy, ϕ, for a fixed volume:

$$\min_W \int_{\partial W} \phi(\nu(x))dx, \quad \mathrm{vol}(W) = const,$$

where

$$\phi(\nu) = \frac{1}{|\nu|}E(\omega), \quad \nu = (\omega, -1).$$

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Specific Form of S

- $Au = -\text{div}(a(x)\nabla u)$

$$S(u) = \int_{\mathbb{R}^d} \frac{1}{2}(Au)u + V(x,u)\,dx = \int_{\mathbb{R}^d} \frac{1}{2}\,(a(x)\nabla u)\cdot\nabla u + V(x,u)\,dx$$

  V is $\mathbb{Z}^{d+1}$-periodic, and $a(x)$ is symmetric, positive definite and Z^d-periodic.

- Minimizing surfaces satisfy the elliptic PDE

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The Reduced Functional

- Fix $\omega \in \frac{1}{N}\mathbb{Z}^d$ and look for N-periodic Birkhoff minimizers of S of the form $u(x) = \omega \cdot x + z(x)$.

- This reduces to minimizing

$$S_N(u) = \int_{[0,N]^d} \frac{1}{2}(Au)u + V(x, u(x))\, dx$$

where $u(x) = \omega \cdot x + z(x)$ and $z(x+k) = z(x)$ for all $k \in N\mathbb{Z}^d$.

- S_N is called a *reduced functional*, and minimizers satisfy

$$\operatorname{div}(a(x)\nabla u) = V_u(x,u), \quad z(x+k) = z(x)\ \forall\ k \in N\mathbb{Z}^d.$$

This is a cell problem for $z(x)$.

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The Sobolev Spaces $H^{\beta}_{\gamma,A}$

- For $\gamma > 0$, fractional powers of $\gamma I + A$ are defined as

$$(\gamma I + A)^{-\beta} = C_\beta \int_0^\infty t^{\beta-1} e^{-t(\gamma I + A)} dt$$

- $H^{\beta}_{\gamma,A}$ is defined as

$$H^{\beta}_{\gamma,A}(N\mathbb{T}^d) = \{u \in H^0(N\mathbb{T}^d) : \langle (\gamma I + A)^{\beta} u, u \rangle_0 < \infty\}$$

with the inner product

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Gradient Descent and $H^{\beta}_{\gamma,A}$

$$\begin{aligned}
DS_N(u)\eta &= \langle \nabla_0 S_N(u), \eta\rangle_0 \\
&= \langle Au + V_u(x,u), \eta\rangle_0 \\
&= \langle (\gamma I + A)^{\beta}(\gamma I + A)^{-\beta}(Au + V_u(x,u)), \eta\rangle_0 \\
&= \langle (\gamma I + A)^{-\beta}(\gamma u + Au - \gamma u + V_u(x,u)), \eta\rangle_\beta \\
&= \langle (\gamma I + A)^{1-\beta} u - (\gamma I + A)^{-\beta}(\gamma u - V_u(x,u)), \eta\rangle_\beta \\
&= \langle \nabla_\beta S_N(u), \eta\rangle_\beta
\end{aligned}$$

The descent equation $\partial_t u = -\nabla_\beta S_N(u)$ is

$$\partial_t u = -(\gamma I + A)^{1-\beta} u + (\gamma I + A)^{-\beta}(\gamma u - V_u(x,u))$$

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The Descent Equation: $\partial_t u = -\nabla_\beta S_N(u)$

Theorem (B., de la Llave, Valdinoci)

If $u(t,x)$ and $w(t,x)$ are solutions to the gradient descent equation

$$\partial_t u = -(\gamma + A)^{1-\beta} u + (\gamma + A)^{-\beta}(\gamma u - V_u(x,u))$$

for initial conditions $u_0, w_0 \in L^\infty(N\mathbb{T}^d)$, with $\beta \in [0,1]$, $\gamma > \sup |V_{uu}|$, $V \in C^3$, $u_0(x) \geq w_0(x)$ for a.e. x, then $u(t,x) \geq w(t,x)$ for all $t > 0$ and a.e. $x \in N\mathbb{T}^d$. In particular, if $u_0(x) = \omega \cdot x + z_0(x)$ is a Birkhoff function, then $u(t,x) = \omega \cdot x + z(t,x)$ is Birkhoff for each $t > 0$.

Sketch of Proof: Semigroup Theory

We rewrite gradient as $-\nabla_\beta S(u) = Lu + X(u)$

$$L := -(\gamma I + A)^{1-\beta}, \quad X(u) := (\gamma I + A)^{-\beta}\left(\gamma u - V_u(x,u)\right).$$

Mild solutions of $\partial_t u = Lu + X(u)$ satisfy

$$u(t,x) = e^{tL}u_0(x) + \int_0^t e^{(t-\tau)L}X(u(\tau,x))d\tau.$$

Smoothing estimates for e^{tL}, X and Moser estimates show that solutions exist for bounded initial data and gain regularity.

$$\|e^{tL}\|_{\mathcal{L}(H^s,H^{s+2\alpha(1-\beta)})} \leq c_\alpha t^{-\alpha}, \quad \|V(x,u)\|_{H^r} \leq c_r|V|_{C^r}(1+\|u\|_{H^r}).$$

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Sketch of Proof: Comparison

If $u \geq w$ and $\gamma > \sup |V_{uu}|$ then $\gamma u - V_u(x,u) \geq \gamma w - V_u(x,w)$.

$$(\gamma I + A)^{-\beta} = C_\beta \int_0^\infty \tau^{\beta-1} e^{-\tau(\gamma I + A)} d\tau$$

implies $(\gamma I + A)^{-\beta} u \geq (\gamma I + A)^{-\beta} w$ when $u \geq w$, and $X(u) \geq X(w)$ follows.

The Bochner identity

$$e^{tL} = \int_0^\infty \phi(t,\beta,\tau) e^{-\tau(\gamma I + A)} d\tau, \quad \phi(t,\beta,\tau) > 0 \ \forall \ \tau > 0$$

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Sketch of Proof: Iteration and Extension

If $u \geq w$ then $e^{(t-\tau)L}X(u(\tau,x)) \geq e^{(t-\tau)L}X(w(\tau,x))$.

If $u_0(x) \geq w_0(x)$ then $u^j(t,x) \geq w^j(t,x)$, where

$$u^{j+1}(t,x) = e^{tL}u_0(x) + \int_0^t e^{(t-\tau)L}X(u^j(\tau,x))d\tau, \quad u^0(t,x) = e^{tL}u_0(x).$$

$u^{j+1}(t,x)$ converges to solution of $\partial_t u = Lu + X(u)$.

The method generalizes to energies of the form

$$S(u) = \int_{\mathbb{R}^d} \frac{1}{2}(A^\alpha u)u + V(x,u)\,dx, \quad \alpha \in (0,1)$$

where equilibrium solutions solve

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The Numerical Method, $d = 2$

Constant coefficients case: $u(x) = \omega \cdot x + z(x)$

$$\partial_t z = -(\gamma I - \Delta)^{1-\beta} z + (\gamma I - \Delta)^{-\beta}(\gamma z - V(x, \omega \cdot x + z))$$

In Fourier space the descent equation is

$$\partial_t \widehat{z} = -\left(\gamma + \frac{4\pi^2}{N^2}|k|^2\right)^{1-\beta} \widehat{z} + \left(\gamma + \frac{4\pi^2}{N^2}|k|^2\right)^{-\beta} (\gamma \widehat{z} - \mathcal{F}[V_u(x, \omega \cdot x + z)])$$

- If n^2 Fourier modes are used, the number of operations for one step is on the order of $n^2 \log(n)$.
- If $\beta \approx 1$, the stiffness of the equation is greatly reduced.

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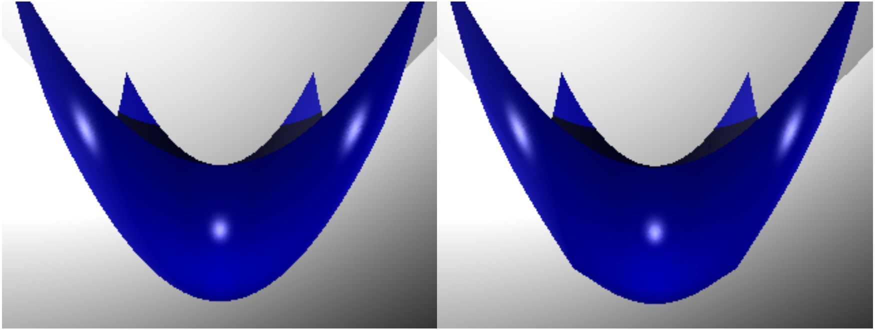
Example: $\varepsilon = 0$ compared with $\varepsilon > 0$

$$E_\varepsilon(\omega) = \frac{1}{N^2}\int_{[0,N]^2} \frac{1}{2}|\nabla u|^2 + \varepsilon \sin(2\pi k_1 x_1)\sin(2\pi k_2 x_2)\cos(2\pi u)\, dx$$



(a) $\varepsilon = 0$ (b) $\varepsilon > 0$

Computed from $u(x) = \omega \cdot x + z(x)$ for $\omega \in [-2,2]^2$ and $k = (1,1)$

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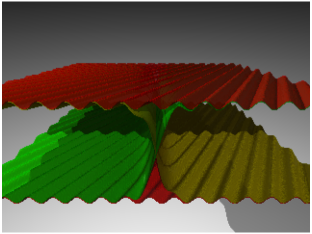
Senn's Formula

- Minimizing surfaces define a set of gaps G.
- Senn's Formula for the derivative:

$$D_{e_j}A_\varepsilon(\omega)+D_{-e_j}A_\varepsilon(\omega)=\sum_G\int_0^\infty\int_0^1 F_\varepsilon(x,u_T,\nabla u_T)-F_\varepsilon(x,u_B,\nabla u_B)dx_idx_j$$



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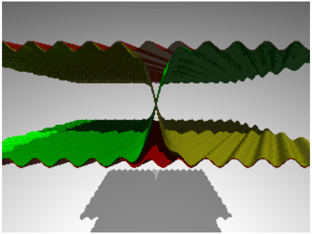

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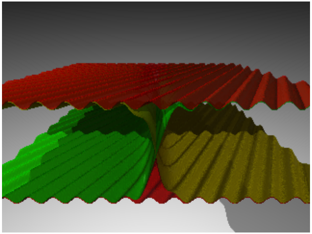

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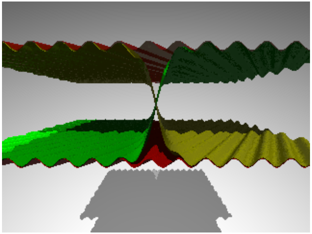

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Lindstedt Series

- Take $F_\varepsilon(x, u, \nabla u) = \frac{1}{2}|\nabla u|^2 + \varepsilon V(x, u)$
- For fixed $\omega \in \frac{1}{N}\mathbb{Z}^d$, find an expression for $u_\varepsilon(x)$ as a series in ε

$$u_\varepsilon(x) = \sum_{j=0}^{\infty} u_j(x)\varepsilon^j$$

with u_j N-periodic, and solving

$$-\Delta u_\varepsilon + \varepsilon V_u(x, u_\varepsilon) = 0, \quad \sup_x |u_\varepsilon(x) - \omega \cdot x| < \infty.$$

- Also find expression for the heteroclinic connections between the gaps.

Lindstedt Series

- Take $F_\varepsilon(x,u,\nabla u) = \frac{1}{2}|\nabla u|^2 + \varepsilon V(x,u)$
- For fixed $\omega \in \frac{1}{N}\mathbb{Z}^d$, find an expression for $u_\varepsilon(x)$ as a series in ε

$$u_\varepsilon(x) = \sum_{j=0}^{\infty} u_j(x)\varepsilon^j$$

with u_j N-periodic, and solving

$$-\Delta u_\varepsilon + \varepsilon V_u(x,u_\varepsilon) = 0, \quad \sup_x |u_\varepsilon(x) - \omega \cdot x| < \infty.$$

- Also find expression for the heteroclinic connections between the gaps.

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To solve $\Delta(u_0 + \varepsilon u_1 + \dots) = \varepsilon V_u(x, u_0 + \varepsilon u_1 + \dots)$ collect powers of ε:

$$\begin{aligned}
\Delta u_0 &= 0 \qquad \Longrightarrow \quad u_0 = \omega \cdot x + \alpha \\
\Delta u_1 &= V_u(x, u_0) \\
\Delta u_2 &= V_{uu}(x, u_0) u_1 \\
\Delta u_3 &= V_{uu}(x, u_0) u_2 + \frac{1}{2} V_{uuu}(x, u_0) u_1^2 \\
&\vdots \\
\Delta u_j &= \left[V_u(x, u^{<j})\right]_{j-1} = V_{uu}(x, u_0) u_{j-1} + \dots
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- Compatibility condition $\int_{N\mathbb{T}^d} \left[V_u(x, u^{<j})\right]_{j-1} dx = 0$.
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Solving to All Orders in ε

Theorem (B., de la Llave)

Let $u_0(x) = \omega \cdot x + \alpha$, $\omega \in \frac{1}{N}\mathbb{Z}^d$, *and* $\alpha \in [0,1)$. *If*

$$\int_{N\mathbb{T}^d} V_{uu}(x, u_0)\, dx \neq 0$$

then there are at least two choices of α *such that* $\Delta u_j = \left[V_u(x, u^{<j})\right]_{j-1}$ *has a periodic solution for all* $j \geq 1$.

Proof of Theorem

If $\Phi(\alpha) = \int_{N\mathbb{T}^d} V_u(x, \omega \cdot x + \alpha)\, dx$, then

$$\begin{aligned}
\int_0^1 \Phi(\alpha)\, d\alpha &= \int_0^1 \int_{N\mathbb{T}^d} V_u(x, \omega \cdot x + \alpha)\, dx\, d\alpha \\
&= \int_0^1 \int_{N\mathbb{T}^d} \frac{\partial}{\partial \alpha} V(x, \omega \cdot x + \alpha)\, dx\, d\alpha \\
&= \int_{N\mathbb{T}^d} V(x, \omega \cdot x + 1) - V(x, \omega \cdot x)\, dx = 0. \\
&\implies \Phi \text{ has a zero in } [0, 1)
\end{aligned}$$

- $\Phi(\alpha) = \Phi(\alpha + 1) \implies \Phi$ has at least two zeros.
- $\Delta u_1 = V_u(x, u_0)$ can be solved for $u_1 = u_1^* + \lambda_1$.

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Proof of Theorem

Assuming we have solved $\Delta u_j = \left[V_u(x, u^{<j})\right]_{j-1}$ for $u_j = u_j^* + \lambda_j$. Write $\left[V_u(x, u^{<j+1})\right]_j = V_{uu}(x, u_0)(u_j^* + \lambda_j) + R(u^{<j})$.

$$\text{Set} \quad \lambda_j = -\frac{\int V_{uu}(x, u_0)u_j^* + R(u^{<j})\, dx}{\int V_{uu}(x, u_0)\, dx}.$$

Then

$$\int_{N\mathbb{T}^d} \left[V_u(x, u^{<j+1})\right]_j dx = \int_{N\mathbb{T}^d} V_{uu}(x, u_0)(u_j^* + \lambda_j) + R(u^{<j})\, dx = 0$$

and $\Delta u_{j+1} = \left[V_u(x, u^{<j+1})\right]_j$ can be solved for $u_{j+1} = u_{j+1}^* + \lambda_{j+1}$. □

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Convergence via Newton Method

- Set $G_\varepsilon(u) = -\Delta u + \varepsilon V_u(x,u)$, find u_ε with $G_\varepsilon(u_\varepsilon) = 0$.
- Find a zero of G_ε via Newton Method:

$$U_\varepsilon^{n+1} = U_\varepsilon^n - DG_\varepsilon(U_\varepsilon^n)^{-1} G_\varepsilon(U_\varepsilon^n)$$

with initial guess

$$U_\varepsilon^0 = \omega \cdot x + \alpha + \varepsilon u_1 + \ldots + \varepsilon^M u_M.$$

Theorem (B., de la Llave)

Under non-degeneracy conditions on V, and if ε is small, and M is large, then $U_\varepsilon^n \to U_\varepsilon^\infty$, analytic in ε in a neighborhood of zero, and $G_\varepsilon(U_\varepsilon^\infty) = 0$.

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Connecting Surfaces in the Gaps

- If $\int V_{uu}(x, \omega \cdot x + \alpha)dx \neq 0$ then to solve $\Delta u_1 = V_u(x, \omega \cdot x + \alpha)$ we must make a choice of α.

- If we look for $u(x) = \omega \cdot x + \alpha(\sqrt{\varepsilon}x) + \varepsilon u_1(x) + \ldots$, we get a PDE of the form

$$\Delta\alpha = g_\omega(x, \alpha), \quad \alpha(x) \to \alpha_\pm \text{ as } x \cdot v \to \pm\infty.$$

- Example: $V(x, u) = \sin(2\pi kx)\cos(2\pi u)$, and $\omega = k \in \mathbb{Z}^2$

$$\Delta\alpha = -\pi\cos(2\pi\alpha), \quad \alpha_+ = \frac{1}{4}, \ \alpha_- = -\frac{3}{4}$$

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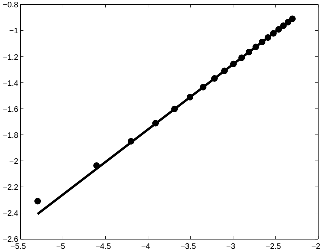
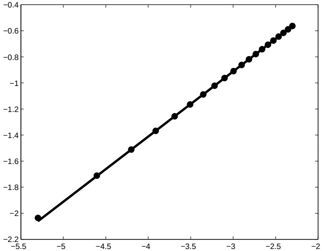
Log-Log Plots of $J(\omega,\varepsilon) = D_{e_1}A_\varepsilon(\omega) + D_{-e_1}A_\varepsilon(\omega)$



(g) $J(\omega,\varepsilon) \approx \frac{4}{\pi}\sqrt{\varepsilon}$



(h) $J(\omega,\varepsilon) \approx \frac{4\sqrt{2}}{\pi}\sqrt{\varepsilon}$

Figure: In 1(g) $V(x,u) = \sin(2\pi k_1 x_1)\sin(2\pi k_2 x_2)\cos(2\pi u)$, and in 1(h) $V(x,u) = \sin(2\pi k \cdot x)\cos(2\pi u)$. Both plots are for $\omega = k$.