Aubry-Mather Theory for PDEs

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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 \( (k, l) \in \mathbb{Z}^{d+1} \), and satisfies growth and convexity requirements in \( p \), so that the Euler-Lagrange equation for \( S \) is elliptic.
A function $u \in H^1(\mathbb{R}^d, \mathbb{R})$ is a minimizer for a formal energy

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

\[
\mathcal{M}_\omega = \{ u \mid u \text{ is Birkhoff minimizer of } S \text{ with slope } \omega \} \neq \emptyset
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Birkhoff Minimizers and Average Slope

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Theorem (Moser, ’86)

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

$$\mathcal{M}_\omega = \{u \mid u \text{ is Birkhoff minimizer of } S \text{ with slope } \omega\} \neq \emptyset$$
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, $\phi$, for a fixed volume:

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

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 $\mathbb{Z}^d$-periodic.

- Minimizing surfaces satisfy the elliptic PDE

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- Minimizing surfaces satisfy the elliptic PDE

$$-Au = V_u(x, u).$$
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

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

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

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The Reduced Functional

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This is a cell problem for $z(x)$.
For $\gamma > 0$, fractional powers of $\gamma I + A$ are defined as

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

$H_{\gamma,A}^{\beta}$ is defined as

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

with the inner product

$$ \langle u, v \rangle_\beta = \langle (\gamma I + A)^\beta u, v \rangle_0. $$
The Sobolev Spaces $H_{\gamma,A}^\beta$

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  \]

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  \[
  \langle u, v \rangle_\beta = \langle (\gamma I + A)^\beta u, v \rangle_0.
  \]
\[ DS_N(u)\eta = \langle \nabla_0 S_N(u), \eta \rangle_0 \]
\[ = \langle Au + V_u(x, u), \eta \rangle_0 \]
\[ = \langle (\gamma I + A)^\beta (\gamma I + A)^{-\beta} (Au + V_u(x, u)), \eta \rangle_0 \]
\[ = \langle (\gamma I + A)^{-\beta} (\gamma u + Au - \gamma u + V_u(x, u)), \eta \rangle_\beta \]
\[ = \langle (\gamma I + A)^{1-\beta} u - (\gamma I + A)^{-\beta} (\gamma u - V_u(x, u)), \eta \rangle_\beta \]
\[ = \langle \nabla_\beta S_N(u), \eta \rangle_\beta \]

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 $t > 0$. 
We rewrite gradient as $-\nabla_\beta S(u) = Lu + X(u)$

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

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.

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

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

gives \( e^{tL} u \geq e^{tL} w \) when \( u \geq w \).
Sketch of Proof: Comparison

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

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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

$$ -A^\alpha u = V_u(x, u). $$
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1. Background Material

2. Comparison for the Sobolev Gradient

3. Numerical Method

4. Asymptotic Analysis
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

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

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

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- 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.
Example: \( \varepsilon = 0 \) compared with \( \varepsilon > 0 \)

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

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

2 Comparison for the Sobolev Gradient

3 Numerical Method

4 Asymptotic Analysis
Senn’s Formula

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

$$D_{ej}A_{\varepsilon}(\omega) + D_{-ej}A_{\varepsilon}(\omega) = \sum_{G} \int_{0}^{1} \int_{0}^{\infty} F_{\varepsilon}(x, u_{T}, \nabla u_{T}) - F_{\varepsilon}(x, u_{B}, \nabla u_{B}) dx_{i} dx_{j}$$
Senn’s Formula

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

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

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

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 $\varepsilon$

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- For fixed $\omega \in \frac{1}{N} \mathbb{Z}^d$, find an expression for $u_\varepsilon(x)$ as a series in $\varepsilon$

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

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

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

\[
\begin{align*}
\Delta u_0 &= 0 \quad \implies \quad u_0 = \omega \cdot x + \alpha \\
\Delta u_1 &= V_u(x, u_0) \\
\Delta u_2 &= V_{uu}(x, u_0)u_1 \\
\Delta u_3 &= V_{uu}(x, u_0)u_2 + \frac{1}{2}V_{uuu}(x, u_0)u_1^2 \\
&\vdots \\
\Delta u_j &= [V_u(x, u^{<j})]_{j-1} = V_{uu}(x, u_0)u_{j-1} + \ldots
\end{align*}
\]

- Compatibility condition \( \int_{NTd} [V_u(x, u^{<j})]_{j-1} \, dx = 0 \).
- Will the series converge?
Lindstedt Series

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

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- Compatibility condition \( \int_{N_T^d} [V_u(x, u^{<j})]_{j-1} \, dx = 0. \)
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To solve $\Delta(u_0 + \varepsilon u_1 + \ldots) = \varepsilon V_u(x, u_0 + \varepsilon u_1 + \ldots)$ collect powers of $\varepsilon$:

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- Will the series converge?
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 \( \alpha \) such that \( \Delta u_j = [V_u(x, u^{<j})]_{j-1} \) has a periodic solution for all \( j \geq 1 \).
Proof of Theorem

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

$$
\int_0^1 \Phi(\alpha) \, d\alpha = \int_0^1 \int_{\mathbb{T}^d} V_u(x, \omega \cdot x + \alpha) \, dx \, d\alpha
$$

$$
= \int_0^1 \int_{\mathbb{T}^d} \frac{\partial}{\partial \alpha} V(x, \omega \cdot x + \alpha) \, dx \, d\alpha
$$

$$
= \int_{\mathbb{T}^d} V(x, \omega \cdot x + 1) - V(x, \omega \cdot x) \, dx = 0.
$$

$\implies$ $\Phi$ has a zero in $[0, 1)$

- $\Phi(\alpha) = \Phi(\alpha + 1) \implies \Phi$ 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 $\Delta u_j = [V_u(x, u^{<j})]_{j-1}$ for $u_j = u^*_j + \lambda_j$. Write $[V_u(x, u^{<j+1})]_j = V_{uu}(x, u_0)(u^*_j + \lambda_j) + R(u^{<j})$.

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

Then

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

and $\Delta u_{j+1} = [V_u(x, u^{<j+1})]_j$ 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 $u_\varepsilon$ with $G_\varepsilon(u_\varepsilon) = 0$.
- Find a zero of $G_\varepsilon$ via Newton Method:

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

with initial guess

$$U_0 = \omega \cdot x + \alpha + \varepsilon u_1 + \ldots + \varepsilon^M u_M.$$

Theorem (B., de la Llave)

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

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Aubry-Mather for PDE  
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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 $\alpha$.

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

$$\Delta \alpha = -\pi \cos(2\pi \alpha), \quad \alpha_+ = \frac{1}{4}, \quad \alpha_- = -\frac{3}{4}$$
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Log-Log Plots of $J(\omega, \varepsilon) = D_{e_1}A_{\varepsilon}(\omega) + D_{-e_1}A_{\varepsilon}(\omega)$

\[ (g) \quad J(\omega, \varepsilon) \approx \frac{4}{\pi} \sqrt{\varepsilon} \]

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

**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 $\omega = k$. 