Computing the Effective Hamiltonian using a Variational Approach

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***Abstract*— A numerical method for homogenization of Hamilton-Jacobi equations is presented and implemented as an L^∞ calculus of variations problem. Solutions are found by solving a nonlinear convex optimization problem. The numerical method is shown to be convergent and error estimates are provided. Several examples are worked in detail, including the cases of non-strictly convex Hamiltonians and Hamiltonians for which the cell problem has no solution.**

I. Introduction

Given the Hamiltonian $H(p,x)$ which is smooth, convex in p, and periodic in the second variable x, we consider, for a given $P \in \mathbb{R}^n$, periodic solutions of the Hamilton-Jacobi equation

$$H(P + D_x u, x) = \bar{H}(P). \tag{HB}$$

For each fixed P the problem (HB) can be regarded as a nonlinear eigenvalue problem for the function function $u(x)$ and the number $\bar{H}(P)$, the *effective Hamiltonian*.

In this paper, we reduce the problem of finding the (approximate) effective Hamiltonian to a finite dimensional convex optimization problem, which may solved numerically using standard methods.

Numerical computations of effective Hamiltonians have been done by [EMS95], [KBM01], with applications to front propagation and combustion, and in [Qia01], both of them using partial differential equations methods.

In this work we circumvent the difficulties of solving (HB) by computing $\bar{H}(P)$ without finding the solution u. Our methods are based on the representation formula

$$\bar{H}(P) = \inf_{\phi \in C^1_{per}} \sup_x H(P + D_x\phi, x) \tag{1}$$

due, for strictly convex Hamiltonians, to [CIPP98].

In this paper we always assume that H to be convex but not necessarily strictly convex. This assumption has implications for the existence and smoothness of solutions of (HB). If strict convexity fails, solutions may (see §IV-B) or may not (see §IV-C) exist, and the degree of smoothness will depend on the Hamiltonian in question.

Computing the effective Hamiltonian is relevant in several problems, as we describe briefly next.

In *homogenization problems* [LPV88], [Con95], if w^ϵ solves

$$-w^\epsilon_t + H(D_x w^\epsilon, \frac{x}{\epsilon}) = 0,$$

then as ϵ goes to 0, the solution w^ϵ converges to w^0 which is a solution of the limiting problem

$$-w^0_t + \bar{H}(D_x w^0) = 0.$$

In the study of *long time limits of viscosity solutions of Hamilton-Jacobi equations*

$$-w_t + H(P + D_x w, x) = 0,$$

the difference $w(x,t) - \bar{H}(P)\,t$ converges as $t \to -\infty$ to a stationary solution of (HB) [Fat98b], [BS00]. See also [AI01], [CDI01].

In *classical mechanics* smooth solutions u of (HB) yield a canonical change of coordinates $X(p,x)$ and $P(p,x)$: ($p = P + D_x u,\ X = x + D_P u$), which simplifies the Hamiltonian dynamics

$$\dot{x} = -D_p H(p,x) \qquad \dot{p} = D_x H(p,x) \tag{2}$$

into the trivial dynamics

$$\dot{P} = 0 \qquad \dot{X} = -D_P \bar{H}(P).$$

In *Aubry-Mather theory* [Mat89], [Mat91], one looks for probability measures μ on $\mathbb{T}^n \times \mathbb{R}^n$ that minimize

$$\int L(x,v) + P \cdot v d\mu, \tag{3}$$

where $L(x,v)$ is the Legendre transform of $H(p,x)$, and satisfy a holonomy condition:

$$\int v D_x \phi \, d\mu = 0, \text{ for all } \phi(x) \in C^1(\mathbb{T}^n).$$

The supports of these measures are called the Aubry-Mather sets, [E99], [Fat97a], [Fat97b], [Fat98a], [Fat98b], [CIPP98], [EG01a], [EG01b], [Gom01b]. Viscosity solutions of (HB) encode important properties of the Aubry-Mather sets. In particular,

$$\int L(x,v) + P \cdot v d\mu = -\bar{H}(P),$$

the support of the Mather measure is a subset of the graph

$$(x, -D_p H(P + D_x u, x)),$$

for any viscosity solution of (HB), and if (x,p) belongs to any Mather, and $(x(t), p(t))$ is its orbit under (2) then

$$\frac{x(T)}{T} \to -D_P \bar{H}(P),$$

for some P, if $\bar{H}$ is differentiable.

Equation (HB) and related stationary first and second order Hamilton-Jacobi equations are also important to the *ergodic control problem* [Ari98], [Ari97]. Effective Hamiltonians also arise in the study of *propagation of flame fronts in combustion*: in this case, solving a homogenization problem gives the effective or averaged front speed [EMS95], [KBM01].

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II. CONVERGENCE RESULTS

We start this section by reviewing two results concerning the function $\bar{H}(P)$:

Proposition 1 (Lions, Papanicolao, Varadhan): There is at most one value $\bar{H}$ for which (HB) has a periodic viscosity solution.

Proposition 2 (Contreras, Iturriaga, Paternain, Paternain): Suppose H is periodic in x and convex in p. Assume that there exists a viscosity solution u of (HB). Then

$$\bar{H} = \inf_{\psi \in C^1(\mathbb{T}^n)} \sup_{x \in \mathbb{T}^n} H(D_x\psi, x), \tag{4}$$

in which the infimum is taken over the space $C^1(\mathbb{T}^n)$ of periodic functions.

We should note that the original proof required strict convexity, but a simple viscosity solution argument overcomes this problem.

The next issue is the approximation of the problem (1). To this effect, consider a triangulation of $\mathbb{T}^n$ with cells of diameter smaller than h. Let $C(T_h)$ be the collection of piecewise linear finite elements which interpolate given nodal values.

Proposition 3: Suppose $H(p,x)$ is convex in p. Then

$$\inf_{\psi \in C^1(\mathbb{T}^n)} \sup_x H(D_x\psi, x) = \lim_{h \to 0} \inf_{\phi \in C(T_h)} \operatorname*{esssup}_x H(D_x\phi, x).$$

Proof: Fix $\epsilon > 0$. Let ψ be a C^1 function for which

$$\sup_{x \in \mathbb{T}^n} H(D_x\psi, x) \le \inf_{\psi \in C^1(\mathbb{T}^n)} \sup_{x \in \mathbb{T}^n} H(D_x\psi, x) + \epsilon.$$

Because ψ is C^1, $D_x\psi$ is uniformly continuous. Thus, for h sufficiently small, there is $\phi \in C(T_h)$ such that $\operatorname*{esssup}_{x \in \mathbb{T}^n} |D_x\phi - D_x\psi| \le \epsilon$. This implies

$$\operatorname*{esssup}_{x \in \mathbb{T}^n} H(D_x\phi, x) \le \sup_{x \in \mathbb{T}^n} H(D_x\psi, x) + O(\epsilon),$$

by Lipschitz continuity of H in p. Thus, taking first $\lim_{h\to 0}\inf_{\phi \in C(T_h)}$, then $\inf_{\psi \in C^1(\mathbb{T}^n)}$, and finally $\epsilon \to 0$, we obtain the first inequality.

To prove the converse inequality observe that if $\phi \in C(T_h)$, η_ϵ is a smooth mollifier, and $\psi = \eta_\epsilon * \phi$, then convexity yields

$$H(D_x\psi(x), x) \le \int H(D_x\phi(y), y)\eta_\epsilon(x-y)dy + O(\epsilon),$$

every x, and so the result follows from

$$H(D_x\psi(x), x) \le \operatorname*{esssup}_{x \in \mathbb{T}^n} H(D_x\phi(x), x) + O(\epsilon),$$

taking first $\inf_{\psi \in C^1}$, then $\lim_{h \to 0}\inf_{\phi \in C(T_h)}$, and finally $\epsilon \to 0$. ■

First observe that

$$\mathcal{H}(\phi) = \sup_{x \in \mathbb{T}^n} H(D_x\phi, x),$$

is a convex, but not strictly convex, functional. Therefore local minima are global minima.

Proposition 4: The approximate Hamiltonian

$$\bar{H}_h(P) = \inf_{\phi \in C(T_h)} \operatorname*{esssup}_{x \in \mathbb{T}^n} H(P + D_x\phi, x)$$

is convex in P.

Proof: Let $P_1, P_2 \in \mathbb{R}^n$ and let $\phi_1, \phi_2 \in C(T_h)$ be the corresponding minimizers. Let $0 \le \lambda \le 1$, and set $P = \lambda P_1 + (1-\lambda)P_2$, and $\phi = \lambda\phi_1 + (1-\lambda)\phi_2$. Then, for any x we have

$$\begin{aligned} &H(P + D_x\phi, x) \\ &\quad \le \lambda H(P_1 + D_x\phi_1, x) + (1-\lambda)H(P_2 + D_x\phi_2, x), \end{aligned}$$

and so

$$\begin{aligned} \bar{H}_h(P) &= \inf_{\phi \in C(T_h)} \operatorname*{esssup}_{x \in \mathbb{T}^n} H(P + D_x\phi, x) \\ &\le \lambda\bar{H}_h(P_1) + (1-\lambda)\bar{H}_h(P_2). \end{aligned}$$

■

Theorem 1: For any convex Hamiltonian $H(p,x)$ for which (HB) has a viscosity solution

$$\bar{H} \le \inf_{\phi \in C(T_h)} \operatorname*{esssup}_x H(D_x\phi, x).$$

If there exists a globally C^2 solution of (HB) then

$$\inf_{\phi \in C(T_h)} \operatorname*{esssup}_x H(D_x\phi, x) = \bar{H} + O(h).$$

If (HB) has a Lipschitz solution (for instance if $H(p,x)$ is strictly convex in p) we have

$$\inf_{\phi \in C(T_h)} \operatorname*{esssup}_x H(D_x\phi, x) = \bar{H} + O(h^{1/2}).$$

If H is convex but not strictly convex and (HB) has a viscosity solution then

$$\inf_{\phi \in C(T_h)} \operatorname*{esssup}_x H(D_x\phi, x) = \bar{H} + o(1).$$

Proof: Observe that

$$\bar{H} = \inf_{\psi \in C^1(\mathbb{T}^n)} \sup_x H(D_x\psi, x) \le \inf_{\phi \in C(T_h)} \operatorname*{esssup}_x H(D_x\phi, x),$$

because by convexity we can associate to each $\phi \in C(T_h)$ a function $\psi = \phi * \eta_\epsilon \in C^1(\mathbb{T}^n)$ such that $\sup_x H(D_x\psi, x) \le \operatorname*{esssup}_x H(D_x\phi, x) + O(\epsilon)$, for arbitrary $\epsilon > 0$.

To prove the second assertion suppose u is a C^2 viscosity solution of (HB). Fix h and construct a function $\phi_u \in C(T_h)$ by interpolating linearly the values of u at the nodal points. In each triangle T^i, the oscillation of the derivative of u is $O(h)$, since u is C^2. Thus, we obtain

$$D_x\phi_u(x) = D_xu(x) + O(h),$$

for any x. Since $H(D_xu, x) = \bar{H}$, at every point $x \in T^i$ we have $H(D_x\phi_u, x) \le \bar{H} + O(h)$, which implies

$$\inf_{\phi \in C(T_h)} \operatorname*{esssup}_{x \in \mathbb{T}^n} H(D_x\phi, x) \le \bar{H} + O(h).$$

If u is a Lipschitz viscosity solution, let $\tilde{u} = \eta_{h^{1/2}} * u$. Observe that $|D^2_{xx}\tilde{u}| \le \frac{C}{h^{1/2}}$, and

$$H(D_x\tilde{u}, x) \le \bar{H} + O(h^{1/2}).$$

Construct a function $\phi_u \in C(T_h)$ by interpolating linearly the values of $\tilde{u}$ at the nodal points. In each triangle T^i, the oscillation of the derivative of $\tilde{u}$ is $O(h^{1/2})$.

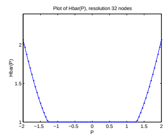

Fig. 1: $\bar{H}(P)$ for the one-dimensional pendulum.

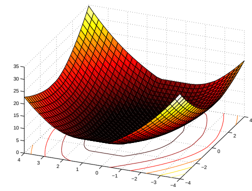

Fig. 2: $\bar{H}(P)$ for the double pendulum

Thus $D_x\phi_u(x) = D_x\tilde{u}(x) + O(h^{1/2})$, for any x. Since $H(D_x\tilde{u}, x) \leq \bar{H} + O(h^{1/2})$, for every point $x \in T^i$ we have $H(D_x\phi_u, x) \leq \bar{H} + O(h^{1/2})$. This implies

$$\inf_{\phi \in C(T_h)} \operatorname*{esssup}_{x \in \mathbb{T}^n} H(D_x\phi, x) \leq \bar{H} + O(h^{1/2}).$$

The last case, for not strictly convex Hamiltonians, the $\sup$ convolution yields a function $u_{h^{1/3}}$ that satisfies

$$H(D_x u_{h^{1/3}}, x) \leq \bar{H} + o(1),$$

almost everywhere and has Lipschitz constant bounded by $\frac{C}{h^{1/3}}$. Define $\tilde{u} = \eta_{h^{1/3}} * u_{h^{1/3}}$ which satisfies $H(D_x\tilde{u}, x) \leq \bar{H} + o(1)$ and has $|D^2_{xx}\tilde{u}| \leq \frac{C}{h^{2/3}}$. Since in each triangle the oscillation of the derivative is $O(h^{1/3})$ we have the result, since

$$H(D_x\phi_u, x) \leq \bar{H} + o(1).$$

■

A corollary to the previous theorem is the following:

Corollary 1: Suppose $\xi_h \in \mathbb{R}^n$ is a supporting plane for $\bar{H}_h(P)$ that converges as $h \to 0$ to ξ. Then ξ is a supporting hyperplane for $\bar{H}(P)$. As a consequence if $\bar{H}(P)$ is differentiable at P then ξ_h converges to the unique supporting hyperplane of $\bar{H}(P)$ at P.

III. Numerical implementation

We can make a further approximation, discretizing the spatial variable by computing the supremum only at the nodes x_i, which gives the minimax problem

$$\min_{\phi \in C(T_h)} \max_{x_i} H(D_x\phi, x_i), \tag{5}$$

for x_i at the nodal points of the finite element space.

The minimax problem (5) is a finite dimensional nonlinear optimization problem which can by solved using standard optimization routines. We carried out the implementation in MATLAB, using the Optimization Toolbox.

IV. Computational Results

A. Strictly convex Hamiltonians

We present two examples, the one-dimensional pendulum and the double pendulum.

Example 1 (one-dimensional pendulum): In this case the Hamiltonian is $H(p,x) = \frac{p^2}{2} - \cos 2\pi x$. the result is presented in Figure 1, and agrees with the explicit formula for $\bar{H}$, which is known in this case.

Example 2 (Double pendulum): The double pendulum is a well known non-integrable system for which the effective Hamiltonian is not known. The Hamiltonian for the double pendulum is

$$\frac{p_x^2 - 2p_xp_y\cos(2\pi(x-y)) + 2p_y^2}{2 - \cos^2(2\pi(x-y))} + +2\cos 2\pi x + \cos 2\pi y.$$

The result is presented in Figure 2.

B. Non strictly convex problems

In this section we study several examples in which H is convex, but not strictly convex, for which there is a viscosity solution of (HB).

Example 3 (Linear non-resonant): Consider the linear (nonresonant) Hamiltonian

$$H(p,x) = \omega \cdot p + V(x,y). \tag{6}$$

Suppose u is a smooth solution of (HB). Integrating the equation over $\mathbb{T}^n$ yields

$$\bar{H}(0) = \int_{\mathbb{T}^n} V, \tag{7}$$

and so $\bar{H}(P) = \bar{H}(0) + \omega \cdot P$.

For the example $u_x + \sqrt{2}u_y + \cos(2\pi x)$ we obtained $D_P\bar{H} = (1, \sqrt{2})$ and $\bar{H}(0,0) = 0$. In this (linear) case the optimization routine converged very quickly.

Example 4 (Vakonomic): Finally, we study an example of a non-strictly convex Hamiltonian which satisfies commutation relations related to vakonomic mechanics [AKN97],

$$H(p,x) = \frac{|f_1 \cdot Du|^2}{2} + \frac{|f_2 \cdot Du|^2}{2} + V(x,y)$$

in which the vector fields f_1, f_2 do not span $\mathbb{R}^2$ in every point but when we consider the commutator $[f_1, f_2]$ we have that

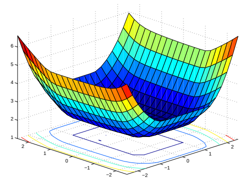

Fig. 3: $\bar{H}(P)$ for the Vakonomic Hamiltonian.

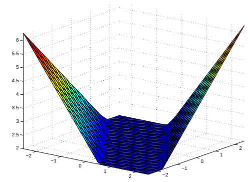

Fig. 4: $\bar{H}(P)$ for the quasi-periodic Hamiltonian.

$f_1, f_2, [f_1, f_2]$ span $\mathbb{R}^2$ in every point. In this situation (HB) has Hölder continuous viscosity solutions [EJ89], [Gom01a].

We chose $f_1 = (0, 1)$, and $f_2 = (\cos 2\pi y, \sin 2\pi y)$, so that $f_1, f_2, [f_1, f_2]$ always span $\mathbb{R}^2$. Therefore there is a Hölder continuous viscosity solution. The potential is $V(x, y) = \cos 2\pi x + \sin 2\pi(x - y)$ The result is presented in Figure 3.

C. Non-existence of viscosity solutions

There are situations where there do not exist viscosity solutions to (HB), but $\bar{H}$ can still be defined by solving a more general problem, see [BS00], [BS01] and [LS03]. In some of these situations, the solution of the minimax problem (1) may exist and give a consistent result.

We work out two interesting examples and try to explain the results obtained numerically.

The problem

$$\alpha u^\alpha + H(P + D_x u^\alpha, x) = 0, \tag{8}$$

which (when $\alpha \neq 0$) has a unique solution is considered in [LS03]. Sending $\alpha \to 0$ gives the effective Hamiltonian

$$\bar{H}(P) \equiv \lim_{\alpha \to 0} \alpha u^\alpha. \tag{9}$$

Proposition 5: Let u^α be a solution of (8), and suppose αu^α converges uniformly to a constant number $\bar{H}(P)$. Then

$$\bar{H}(P) = \lim_{\alpha \to 0} \alpha u^\alpha = \inf_\phi \sup_{x \in \mathbb{T}^n} H(P + D_x \phi, x).$$

Proof: 1. Define $\bar{H}_\alpha \equiv -\alpha \min_x u^\alpha$ and

$$v^\alpha \equiv u^\alpha + \frac{\bar{H}_\alpha}{\alpha},$$

so that $\min_x v^\alpha = 0$. We will demonstrate $\bar{H}_\alpha \to \bar{H}$. We have

$$\begin{aligned} \bar{H} &= \lim_{\alpha \to 0} H(P + D_x u^\alpha, x) = \lim_{\alpha \to 0} -\alpha u^\alpha \\ &= \lim_{\alpha \to 0} \alpha(u^\alpha - \min_x u^\alpha) + \alpha \min_x u^\alpha = \bar{H}_\alpha \end{aligned}$$

2. Let v_α^ϵ denote the sup convolution of v_α and let $\phi = \eta_\epsilon * v_\alpha^\epsilon$. Then $H(D_x\phi, x) \leq \bar{H}_\alpha + O(\epsilon)$. Therefore $\inf_\phi \sup_{x \in \mathbb{T}^n} H(D_x \phi, x) \leq \bar{H}_\alpha \to \bar{H}$.

3. Now let $e_\alpha = \sup_x \alpha v_\alpha$, which converges to 0.

Let ϕ be any function. Then $v_\alpha - \phi$ has a local minimum at a point x_0. At this point

$$\alpha v_\alpha(x_0) + H(D_x \phi(x_0), x_0) \geq \bar{H}_\alpha,$$

and so $\sup_{x \in \mathbb{T}^n} H(D_x \phi, x) \geq \bar{H}_\alpha - e_\alpha \to \bar{H}$. Therefore $\inf_\phi \sup_{x \in \mathbb{T}^n} H(D_x\phi, x) \geq \bar{H}$. ■

Example 5 (Quasiperiodic Hamiltonians): We give an example from [LS03] where there is no viscosity solution to (HB), but where $\bar{H}(P)$ can be determined from (9). Let

$$H(p_x, p_y, x, y) = |p_x + \alpha p_y| + \sin(x) + \sin(y)$$

with α irrational.

We computed $\bar{H}(P)$ numerically from (1). The results are presented in Figure 4.

Example 6 (Linear resonant): Resonant linear Hamiltonians (6) may fail to have a viscosity solution. An example is

$$(0, 1) \cdot Du + \sin(2\pi x) = \bar{H}.$$

The formula (7) yields $\bar{H}(0) = 0$ if there were a solution of (HB). However, we have

$$\inf_\phi \sup_x H(D_x \phi, x) = 1.$$

In fact, let ϕ be an arbitrary periodic function. Set $x_0 = 1/4$, so that $\sin 2\pi x_0 = 1$. Then $\phi(x_0, y)$ is a periodic function of y and so $D_y \phi(x_0, y) = 0$ at some $y = y_0$. Thus

$$\sup_x H(D_x\phi, x) \geq H(D_x \phi(x_0, y_0), x_0, y_0) = 1.$$

Numerically we obtained $D_P \bar{H} = (0, 1)$ and $\bar{H}(0, 0) = 1$.

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