A DIRECT METHOD FOR COMPUTING THE EFFECTIVE HAMILTONIAN IN THE MAJDA-SOUGANIDIS MODEL OF TURBULENT COMBUSTION

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ABSTRACT. We propose a simple and direct method to compute the normal speed of propagation of the flame front in the Majda-Souganidis model of turbulent combustion. We describe our approximation and show some numerical results.

1 Introduction In the Majda-Souganidis model describing the turbulent combustion of premixed flames, one can estimate the enhancement of the speed of the flame front due to the turbulence by computing the so-called effective (or averaged) Hamiltonian \( \bar{H}(P) \) which solves a nonlinear eigenvalue problem often called “the cell problem”:

\[
|P + D_{(x,y)}w|^2 - V(x,y) \cdot (P + D_{(x,y)}w) = \bar{H}(P) \quad \text{for } (x,y) \in [0,1]^2.
\]

In the above equation, \( P \) is a constant vector in \( \mathbb{R}^2 \) and \( V \) is a given velocity field, periodic in \( x \) and \( y \); the unknown eigenfunction \( (x,y) \to w(x,y) \) associated with the eigenvalue \( \bar{H}(P) \), is a continuous and real-valued periodic function defined on \([0,1]^2\).

The cell problem is a stationary Hamilton-Jacobi equation (HJ in short) derived from a reaction-diffusion-advection equation through a homogenization procedure. For a detailed presentation of this model, we refer to [11] and [17]. Homogenization theory for Hamilton-Jacobi equations has been initiated by Lions, Papanicolaou and Varadhan in [16] (see also [12]).

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Next, the flame front evolves with normal velocity $F$

\begin{equation}
F(n) = \min_{r > 0} \frac{H(rn) + \frac{1}{r}}{
\end{equation}

where $n = (\cos(\theta), \sin(\theta))$ denotes the unit exterior normal to the flame front. Here we propose a new and simple method for approximating the effective Hamiltonian and thus computing $F$. At first, this question seems rather difficult, not only because the equation involved is nonlinear (there are actually many good solvers available for this type of nonlinear operator), but also because there is no general method for solving numerically a nonlinear eigenvalue problem and last, but not least, $H(rn)$ must be determined for a large number of values of $r$ in the minimization problem (1) and one also wishes to estimate $F$ for a large number of vectors $n$.

To our knowledge, this particular HJ equation has never been solved directly. The effective Hamiltonian has been previously obtained by Bourlioux and Khouider in [6] by solving instead a system of Conservation Laws derived from the cell problem.

Recent results concerning the behaviour of Hamilton-Jacobi equations for a large time obtained by Barles and Souganidis in [5] suggest that the eigenvalue is actually given by the time derivative of the solution of a time-dependent HJ equation for a large time. In practice, we approximate this Cauchy problem using a monotone first-order finite difference scheme whose convergence can be proven by applying the result of Barles and Souganidis in [4]. A higher order extension of this approximation called Essentially Non Oscillatory scheme (ENO in short) is also implemented. ENO schemes have been developed by Osher and Shu in [18]. No proof of convergence is available for such schemes. As pointed out in [17] and [6], one can compute a solution in closed form in some cases; this helps us validate our algorithms. We also compare our results with those in [6].

In [14], Gomes and Oberman propose an alternate method for this type of problem based on a representation formula for the effective Hamiltonian. Finally, in [19], Qian uses a similar approach as ours to solve various cell problems but he does not consider the application that we are studying here.

In Section 2, we describe our numerical approximation and in Section 3, we present our experimental results.
2 Numerical approximation

Our goal is to compute numerically the effective Hamiltonian \( \overline{H}(P) \) appearing in the cell problem

\[
|P + D_{(x,y)} w|^2 - V(x,y) \cdot (P + D_{(x,y)} w) = \overline{H}(P) \quad \text{for } (x,y) \in [0,1]^2.
\]

In the above equation, the unknown is a pair \((\overline{H}(P), w)\) where \( \overline{H}(P) \), the averaged Hamiltonian, is a real number parametrized by the vector \( P \) and \( w \) is a continuous and periodic real-valued function defined on \([0,1]^2\). Here, \( D_{(x,y)} w \) stands for the spatial gradient of \( w \), \(| \cdot |\) denotes the standard Euclidian norm in \( \mathbb{R}^2 \) and \( \cdot \) represents the Euclidian inner product in \( \mathbb{R}^2 \).

Next, the periodic velocity field \( V(x,y) : [0,1]^2 \to \mathbb{R}^2 \) is given by

\[
V(x,y) = \overline{\nu} + \lambda v = \overline{\lambda}(\cos \overline{\theta}, \sin \overline{\theta}) + \lambda(v_1(x,y), v_2(x,y))
\]

where \( \overline{\nu} \) is the mean flow speed, \( \overline{\lambda} \) is the amplitude of the mean flow and \( \overline{\theta} \) is its direction; the intermediate scale velocity field is modeled by \( v \), a periodic function in \( x \) and \( y \) and \( \lambda \) is its magnitude or turbulence intensity. We refer to \([11], [17], [6]\) for a more detailed presentation of this model. Since, in general, \( (2) \) does not possess any classical solution, we interpret it in the viscosity sense. For an introduction to the theory of viscosity solutions, see \([1], [7], [8], [9], [10], [15]\).

Furthermore, it has been proven in \([16]\), that since our Hamiltonian is strictly convex, there exists for any given \( P \), a unique number \( \overline{H}(P) \) such that there is a least one periodic viscosity solution \( w \) of \( (2) \). In addition, \( P \to \overline{H}(P) \) is convex and coercive, i.e.,

\[
\frac{\overline{H}(P)}{|P|} \to +\infty \quad \text{as } |P| \to +\infty.
\]

The effective Hamiltonian then leads to \( F_e \), the enhancement in the normal speed of propagation due to the turbulence

\[
F_e(n) = F + \overline{\lambda} \cdot n - 1 = \min_{r>0} \frac{\overline{H}(rn) + \frac{1}{r}}{r} + \overline{\lambda} \cdot n - 1.
\]

Indeed, when there is no turbulence, \( v \) is equal to 0 and the normal velocity of the front is then simply \( 1 - \overline{\lambda} \cdot n \) (see \([11]\) for more details).

The goal of this article is to compute numerically the quantity \( F_e \).

Next, we describe our method: Instead of solving \( (2) \), we consider the Cauchy problem

\[
u_t + |P + D_{(x,y)} u|^2 - V(x,y) \cdot (P + D_{(x,y)} u) = 0 \quad \text{for } (x,y) \in [0,1]^2.
\]
Barles and Souganidis proved in [5] the following asymptotic result: If \( u \) denotes a periodic solution of the Cauchy problem (3), then

\[
u + \mathcal{H}(P)t \to w \quad \text{as} \quad t \to +\infty\]

where \( w \) is a periodic solution of the cell problem (2). It is also shown in [5] that \( u \) grows at most linearly in time. Besides, it is a well established fact that there is a unique periodic solution in the viscosity sense of (3) given any continuous initial condition in the closure of the square (see for instance [2]). Note that, given a periodic velocity field, the solution \( u \) of (3) is necessarily periodic.

Next, we set \( P = rn \) where \( r \) is a positive real number. Then, If \( u_{i,j}^k \) denotes an approximation of \( u \) at the point \((i\Delta x, j\Delta y, k\Delta t)\) with \( i, j \in \{0, 1, ..., N\} \), \( \Delta x = \Delta y = 1/N \) and \( k \in \{0, 1, \ldots\} \), an estimate for \( \mathcal{H}(rn) \) is provided by:

\[
\mathcal{H}(rn) \approx -\frac{u_{i,j}^{k+1} - u_{i,j}^k}{\Delta t} \quad \text{for} \quad k \text{ large}.
\]

Note that since \( u \) grows linearly in time, this method will perform well only if the time derivative converges substantially faster than linearly.

We continue with the description of our scheme. We let

\[
v_{i,j} = v(i\Delta x, j\Delta y), \quad v_{1,i,j} = v_1(i\Delta x, j\Delta y), \quad v_{2,i,j} = v_2(i\Delta x, j\Delta y).
\]

We also use the standard definitions

\[
D_x^+ u_{i,j}^k = \frac{u_{i+1,j}^k - u_{i,j}^k}{\Delta x}, \quad D_x^- u_{i,j}^k = \frac{u_{i,j}^k - u_{i-1,j}^k}{\Delta x},
\]

\[
D_y^+ u_{i,j}^k = \frac{u_{i,j+1}^k - u_{i,j}^k}{\Delta y}, \quad D_y^- u_{i,j}^k = \frac{u_{i,j}^k - u_{i,j-1}^k}{\Delta y},
\]

and

\[
f^+ = \max(f, 0), \quad f^- = \max(-f, 0).
\]

The first numerical scheme we implement inside the square is a first-order monotone and explicit approximation. For simplicity, we assume here that \( \theta \in [0, \pi/2] \). In the case where both components of the velocity field are nonnegative, the iteration reads:
If \((i, j)\) is such that \(\overline{x} \cos \overline{y} + \lambda v_{1,i,j} \geq 0\) and \(\overline{x} \sin \overline{y} + \lambda v_{2,i,j} \geq 0\), then
\[ u_{i,j}^{k+1} = u_{i,j}^k + \Delta t \left\{ -\left( \max \{(D_x u_{i,j}^k)^+, (D_x^+ u_{i,j}^k)^-\} \right)^2 
- \left( \max \{(D_y u_{i,j}^k)^+, (D_y^+ u_{i,j}^k)^-\} \right)^2 
+ (\overline{\sigma} + \lambda v_{i,j}) \cdot ((D_x^+ u_{i,j}^k, D_y^+ u_{i,j}^k) + rn) 
- r^2 - 2rn \cdot (D_x^* u_{i,j}^k, D_y^* u_{i,j}^k) \right\}. \]

For the sake of completeness, we also include the three remaining cases. Note that \(\overline{\sigma} + \lambda v \cdot D_{(x,y)} u\) is the only term requiring a different approximation.

If \((i, j)\) is such that \(\overline{x} \cos \overline{y} + \lambda v_{1,i,j} < 0\) and \(\overline{x} \sin \overline{y} + \lambda v_{2,i,j} < 0\), then
\[ u_{i,j}^{k+1} = u_{i,j}^k + \Delta t \left\{ -\left( \max \{(D_x u_{i,j}^k)^+, (D_x^+ u_{i,j}^k)^-\} \right)^2 
- \left( \max \{(D_y u_{i,j}^k)^+, (D_y^+ u_{i,j}^k)^-\} \right)^2 
+ (\overline{\sigma} + \lambda v_{i,j}) \cdot ((D_x^+ u_{i,j}^k, D_y^+ u_{i,j}^k) + rn) 
- r^2 - 2rn \cdot (D_x^* u_{i,j}^k, D_y^* u_{i,j}^k) \right\}. \]

If \((i, j)\) is such that \(\overline{x} \cos \overline{y} + \lambda v_{1,i,j} \geq 0\) and \(\overline{x} \sin \overline{y} + \lambda v_{2,i,j} < 0\), then
\[ u_{i,j}^{k+1} = u_{i,j}^k + \Delta t \left\{ -\left( \max \{(D_x u_{i,j}^k)^+, (D_x^+ u_{i,j}^k)^-\} \right)^2 
- \left( \max \{(D_y u_{i,j}^k)^+, (D_y^+ u_{i,j}^k)^-\} \right)^2 
+ (\overline{\sigma} + \lambda v_{i,j}) \cdot ((D_x^+ u_{i,j}^k, D_y^+ u_{i,j}^k) + rn) 
- r^2 - 2rn \cdot (D_x^* u_{i,j}^k, D_y^* u_{i,j}^k) \right\}. \]

If \((i, j)\) is such that \(\overline{x} \cos \overline{y} + \lambda v_{1,i,j} < 0\) and \(\overline{x} \sin \overline{y} + \lambda v_{2,i,j} \geq 0\), then
\[ u_{i,j}^{k+1} = u_{i,j}^k + \Delta t \left\{ -\left( \max \{(D_x u_{i,j}^k)^+, (D_x^+ u_{i,j}^k)^-\} \right)^2 
- \left( \max \{(D_y u_{i,j}^k)^+, (D_y^+ u_{i,j}^k)^-\} \right)^2 
+ (\overline{\sigma} + \lambda v_{i,j}) \cdot ((D_x^+ u_{i,j}^k, D_y^+ u_{i,j}^k) + rn) 
- r^2 - 2rn \cdot (D_x^* u_{i,j}^k, D_y^* u_{i,j}^k) \right\}. \]

At the boundary of the square we use the fact that the solution \(u\) of (3) is periodic in \(x\) and \(y\) and incorporate in the above scheme the periodic boundary conditions:
\[ u_{i,j}^{k+1} = u_{i,j}^k, \quad u_{i,j+N}^k = u_{i,j}^k. \]
The derivation of the approximation on the boundary is straightforward. Furthermore, \( \Delta t \) satisfies the CFL condition:

\[
\Delta t \leq \min_{i,j} \left\{ \Delta x / \right. \\
2 \left( \max \{ (D_x u^k_{i,j})^+, (D_x^+ u^k_{i,j})^- \} + \max \{ (D_y^- u^k_{i,j})^+, (D_y^+ u^k_{i,j})^- \} \right) \\
+ |\lambda \cos \theta + \lambda v_{1,i,j}| + |\lambda \sin \theta + \lambda v_{2,i,j}| + 2r(\cos \theta + \sin \theta) \right\}
\]

ensuring the monotonicity and the stability of the scheme. In practice, we choose at every iteration an adaptive time step exactly equal to the above condition (4).

Let us make a few more comments on the above finite-difference scheme. The approximation of the quadratic term was derived previously by Rouy-Tourin in [20]. The linear term are replaced by the usual upwind finite differences. It is easy to verify that this approximation belongs to the class of schemes whose convergence to the (viscosity) solution has been proven by Barles and Souganidis in [4]. Indeed, it is clearly consistent with the Cauchy problem (3) and stable and monotone under the CFL condition (4) (for the definitions of monotonicity, consistency and stability, we refer to [4]). Each iteration yields a collection of eigenvalues \( \mathbf{P}(rn) \) indexed by \((i,j)\). We stop when the \( L^\infty \) norm of the difference between too successive eigenvalues falls below a given threshold. The eigenvalue is then taken to be the average over all pairs \((i,j)\). The algorithm is applied to a number of values of \( r \) and the minimization is then performed using a simple line search.

We also construct an ENO scheme of order 2 in space and time, based on the above first-order monotone approximation. This extension is straightforward and we refer to the original article [18] by Osher-Shu for a detailed description of this scheme. We only need to mention that we replaced the TVD limiter in [18] by a so-called min-mod limiter. It is a well-known fact that a solution \( w \) of the cell problem (2) is semiconcave (see for instance [13]), that is,

\[
w(x + h, y + k) - 2w(x, y) + w(x - h, y - k) \leq C(h^2 + k^2)
\]

for any \((x,y)\) and \( h, k \) sufficiently small. We hope that the semiconcavity of \( w \) will prevent the ENO scheme from undergoing large oscillations and experiments show that ENO schemes perform well when used for computing semiconcave functions (see for instance the numerical examples in [18]). Both algorithms have been implemented in Matlab on a single user workstation with Linux. Although the codes have not been
optimized, they are reasonably efficient. A typical single computation for a given value of $r$ with the ENO scheme on a $32 \times 32$ grid with $\delta = 1$ takes less than a second.

3 Experiments Concerning the experiments, we follow [6]: we first choose $\overline{A} = 0$, $\overline{B} = 0$ (no mean flow) and we always assume that $\theta = \pi/4$, i.e., $n = (\sqrt{2}/2, \sqrt{2}/2)$. The intermediate velocity scale $v$ is derived from the Childress-Soward stream function:

$$\Psi(x, y) = \sin(2\pi x) \sin(2\pi y) + \delta \cos(2\pi x) \cos(2\pi y).$$

We perform experiments for $\delta = 1, \delta = 0.5$ and $\delta = 0$. The turbulence intensity $\lambda$ is successively set to $\lambda = 0.4, 1.6$ and $6.4$.

As pointed out earlier, this method is stable if it converges long before $u$ reaches large values. In fact, in all our experiments, $u$ stays roughly of the same order of magnitude as the initial condition or about 10 times larger at most. First of all, in order to illustrate the convergence in time, we include below the approximation of the eigenvalue versus the number of iterations for both the first order monotone and the second order ENO schemes (Figures 1 and 2).

![Eigenvalue vs Number of Iterations (First order scheme)](image)

**FIGURE 1:** Eigenvalue vs number of iterations (first order scheme).
We have here $N = 16$, $\Delta t = 0.005$, $\lambda = 1.6$ and $r = 0.5$. Both schemes converge very fast to the eigenvalue. At 200 iterations, the time is equal to 1 and the $L^\infty$ norm of the difference between two successive derivatives is equal approximately to $6.7e^{-8}$. Also in most cases, the ENO algorithm converges as fast as the monotone scheme. However, in some rare instances, the ENO scheme undergoes some small amplitude oscillations for a much longer time before converging to the eigenvalue but it still does not affect the stability of the algorithm.

Furthermore, it turns out that the rate of convergence of the method is exponential. In Figure 3, we plot the logarithm of the $L^\infty$ norm of the difference between two successive time derivatives for $\delta = 1$, $\lambda = 1.6$, $N = 16$; also $r$ is set successively to $r = 0.1, 0.5, 0.7$. Note that the time interval is $[0.2, 1.5]$ and that, for $t = 1.5$, the $L^\infty$ norm of the difference between two successive time derivatives is equal to $1.75e^{-11}$.

We also plot the Hamiltonian $H(rn)$ as a function of the parameter $r$ when $\lambda = 1.6$ and $\delta = 1$ for 3 different numbers of grid points $N = 16, 32$ and 64 (Figure 4). As expected, it is convex and coercive.

Figure 5 represents the graph of the function to be minimized, i.e.,

$$G(r) = \frac{\Pi(rn) + 1/4}{r}$$
FIGURE 3: Plot in log scale of the test of convergence vs time.

FIGURE 4: Eigenvalue vs $r$. 
for the same set of parameters as in the previous graph. We check that the minimum point is at \( r = 0.5 \), as predicted by the explicit calculations in [17].

![Graph showing the function to be minimized vs \( r \).](image)

**FIGURE 5:** Plot of function to be minimized vs \( r \).

Finally, in the table that follows, we report the approximations obtained for \( F_e \) in the case \( \delta = 1 \), for different values of \( \lambda \), the turbulence intensity. Note that \( v \) is here given by:

\[
v(x, y) = \left( \frac{1}{\sqrt{2}} \sin 2\pi(x - y); \frac{1}{\sqrt{2}} \sin 2\pi(x - y) \right).
\]

We compare our results with the explicit solution \( F_e = \lambda \) and compute the error. For small values of \( \lambda \), the error is roughly of the same order as the truncation error. When the turbulence intensity is high, that is for \( \lambda = 6.4 \), the monotone scheme is slightly less accurate than for smaller values of \( \lambda \). Indeed, in this case, the accuracy of the monotone scheme falls somewhere between \( \sqrt{\Delta x} \) and \( \Delta x \) and the ENO scheme is slightly less accurate too but apparently, still of order 2. For the monotone schemes, these rates we obtain are better than the ones predicted by the theory for Hamilton-Jacobi-Bellman equations, at least when \( \lambda \) is not too big (see [3])!
Next, we perform a set of experiments for $\delta = 0.5$ and $\delta = 0$. Here $v$ is given respectively by:

$$v(x, y) = \frac{2}{\sqrt{5}} \left( \sin 2\pi x \cos 2\pi y - 0.5 \cos 2\pi x \sin 2\pi y \right)$$

and

$$v(x, y) = (\sin 2\pi x \cos 2\pi y; -\cos 2\pi x \sin 2\pi y).$$

In these cases, an explicit solution is no longer available. For $\delta = 0$, we show first the level curves of $w$, the solution of (2) that we computed, for 3 values of $\lambda$ (Figures 6, 7 and 8). The grid contains $64 \times 64$ points.

Secondly, we collected some results for both $\delta = 0.5$ and $\delta = 0$ in the tables below. We estimate $F_c$ by extrapolation based on the second-order results. For $\delta = 0.5$, we find $F_c = 1.50520$ for $\lambda = 1.6$ and $F_c = 5.95802$ for $\lambda = 6.4$ whereas, for $\delta = 0$, we obtain $F_c = 1.06683$ for $\lambda = 1.6$ and $F_c = 3.75604$ for $\lambda = 6.4$. We then compute the errors using these estimates. Note that for $\lambda = 1.6$, for both $\delta = 0.5$ and $\delta = 0$, the results for $F_c$ are consistent with those in [6].
Finally, we show one sample test in the presence of a nonzero mean flow. We choose $\delta = \pi/2$ and $\lambda = 0.1$. Here the estimated value for $F_e$, on which the computation of the error is based, is 1.59751.
FIGURE 7: Level curves of $w$, $\delta = 0$, $\lambda = 1.6$.

FIGURE 8: Level curves of $w$, $\delta = 0$, $\lambda = 6.4$. 
4 Conclusion  We showed that the averaged Hamiltonian arising in the Majda-Souganidis model can be computed directly (at least in the simple case considered in this article). Our results for the normal speed of propagation are consistent with those obtained in [6] by a different method.

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