Remarks on the Lagrangian stucture of the Eikonal Equation and its impact on Eulerian numerics

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N° ????

Juillet 2007

Thème NUM

Rapport de recherche

ISSN 0249-6399 ISRN INRIA/RR--????--FR+ENG

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Thème NUM — Systèmes numériques
Projets Otto

Rapport de recherche n° ???? — Juillet 2007 — 33 pages

Abstract: We make use of the *Lagangian structure* of the Eikonal equation obtained by considering its gradient to

1. observe a superconvergence phenomena on the Rouy-Tourin first order algorithm .
2. propose a second order pure upwind extension of the Rouy Tourin algorithm.

We also discuss the exension of this second order algorithm to the Transport equation.

Key-words: Eikonal equation, upwind scheme, transport equation, Hamilton-Jacobi, Hamiltonian System, Ray Tracing, Viscosity Solution, Level Set method, méthode de Sweeping

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Quelques remarques sur la structure Lagrangienne de l'équation Eikonale et son impact sur sa résolution numérique par des méthodes Eulériennes

Résumé : Nous utilisaons la *structure Lagrangienne* de l'équation Eikonale pour

1. observer un phénomène de superconvergence sur le schéma du premier ordre à la Rouy-Tourin.
2. proposer une extension du second ordre purement décentrée au schéma Rouy Tourin.

Nous discutons également de l'extension de cet algorithme à l'equation de Transport linéaire associée.

Mots-clés : équation Eikonale , schéma décentré, équation de transport, Hamilton-Jacobi, système Hamiltonien, Lancer de rayons, solutions de Viscosité , méthode Level Set, Sweeping Method

Notations and conventions

- We will work in 2D.
- upercase letters will always be vectors.
- lowercase are scalars or scalar functions
- $. \cdot .$ or $< ., . >$ unconsistently represent either scalar product of vectors or matrix vector multiplications. My lousy mathematical education is to blame for this but I really like using both ... and in different context ... I find the result more readable ... I am sorry.
- Numerical results are best viewed in color.

1 Introduction

The Eikonal equation and its companion the Transport equation arise from WKB (high frequency) asymptotics of various Linear and Non-linear wave equations (see [1] for a nice review of WKB methods). As a natural front propagator, it also has a strong relationship with *the level set methods* with many applications, in particular in image processing ([2] [3]...) I think this probably is the shortest motivation section I ever wrote ...

Locally, the Eikonal equation simply prescribes the gradient of the unknown scalar function ϕ to be on the sphere of radius $n(X)$ at each point X.

$$\|\nabla\phi(X)\| = n(X). \tag{1}$$

Obviously, this equation makes sense for positive right hand side and local classical solutions only exist for strictly positive smooth ($C^1 \cup W^{2,\infty}$) given functions n, an assumption we will stick to in this paper. Assuming that the gradient (or *a* gradient) exists and has at least Lipschitz derivatives on some open set, one can construct a solution by the method of characteristics : let us define the integral curves of the gradient $Y(s)$ (also called "rays")

$$\frac{d}{ds}Y(s) = \nabla\phi(Y(s)) \tag{2}$$

and set $P = \nabla\phi(Y)$. We easily eliminate ϕ using (1)

$$\frac{dP}{ds} = D^2\phi \cdot \frac{d}{ds}Y = D^2\phi \cdot \nabla\phi(Y) = \frac{1}{2}\nabla n^2(Y(s)) \tag{3}$$

The ODE system (2) (3) can be solved independently from (1) and the "phase" function ϕ can be computed along the *Lagrangian* coordinate Y using a third ODE

$$\frac{d}{ds}\phi(Y(s)) = \frac{dY}{ds} \cdot \nabla\phi(Y(s)) = \|P(s)\|^2 = n^2(Y(s)) \tag{4}$$

It gets more complicated when it comes to global solutions, for instance : solving (1) in some domain Ω or Ω^c (exterior problem, Ω can be just a source point) with Dirichlet boundary conditions

$$\phi = \phi_0, \ \ on\ \partial\Omega. \tag{5}$$

The existence of a unique smooth gradient field compatible with the boundary conditions (even if there are themselves also smooth) is not garanteed. Even worse : it is fairly easy to construct many weak solutions by patching local solutions obtained by the method of characteristics. In this paper we will focus on the so called *viscosity solution* of this equation wich ensures that (1)(5) is well posed. The viscosity solution ϕ_v can conveniently be characterized as minimization over all paths Y of the *optical length* (this is in essence Fermat principle) :

$$\phi_v(X) = \inf_{\begin{cases} Y_0,\, Y \in \mathcal{W}^{1,\infty}(0,t) \\ Y(t) = X \\ Y(0) = Y_0 \end{cases}} \left\{ \phi_0(Y_0) + \int_0^t n(Y(s)) \|\dot{Y}(s)\| ds \right\} \tag{6}$$

Mathematically the solutions of (2)(3) (with ad-hoc initial conditions) are the Euler Lagrange equations of (6). The viscosity solution is therefore the minimum "phase" value out of all possible solutions given by (4). This produces bounded uniformly continuous solutions that are generally $C1$ except possibly along curves (or surfaces on 3D) called *kinks* where the gradient is discontinuous. This *minimum property* contributes to the well posedness of (1) in this class of solution and also helps making upwind finite difference aproximations convergent. This is further discussed in section 2 and 3 where the widely used Rouy Tourin (RT) Finite Difference Scheme [4] is reviewed and analysed in terms of *Lagrangian characteristics*.

As made explicit in the computations above, the method of characteristics, a classics for linear hyperbolic problems, can only be applied to the non-linear Eikonal equation (1) because of its *Lagrangian structure* :

1. As already mentionned (1) constrains the gradient to be on a sphere and solving locally the Eikonal equation reduces to find an angle.

2. Assuming the second order derivatives exists, (1) also yields

$$D^2\phi \cdot \nabla\phi = \frac{1}{2}\nabla n^2 \tag{7}$$

   which express that the derivatives of n prescribe the second derivatives of ϕ in the Lagrangian trajectory direction.

This paper is a discussion on the impact of this Lagrangian structure in the understanding and the design of Eulerian numerical methods for the Eikonal equation. In particular we uncover a superconvergence phenomena of RT algorithm which was not apparently known and also derive an elegant compact upwind second order scheme.

Readers interested in the theory of viscosity solutions can find more details in [14] [5] Let us quickly mention that this theory was originally develloped for a general class of first order Hamilton-Jacobi equations

$$H(X, \nabla\phi(X)) = 0 \tag{8}$$

where the Hamiltonian function $H(X, P)$ is convex (or concave) and coercive in P, thus retaining the essential features the *Lagrangian structure.* in particular (7) becomes

$$H_x(X, \nabla\phi) + D^2\phi \cdot H_p(X, \nabla\phi) = 0 \tag{9}$$

where H_p is strictly monotonic and thus invertible. We have not written all the details but we believe that most of the discussion carried out in this paper apply to (8).

2 The Rouy-Tourin (RT) Algorithm

We briefly review the RT first order Finite Difference scheme [4] from a *Lagrangian* view point.

The first step consist in a rewrite of (1) as a pointwise optimization problem :

$$\|\nabla\phi(X)\| = n(X) \Leftrightarrow \sup_{\|Q\|\leq 1} \{\nabla\phi(X) \cdot Q - n(X)\} = 0. \tag{10}$$

This is easily proven by writing both $\nabla\phi$ and Q in polar coordinates. The optimal Q is given by $Q_{opt} = \frac{\nabla\phi}{\|\nabla\phi\|}$.

Then, discretize the directional derivative by introducing a fictitious "time" :

$$\sup_{\|Q\|\leq 1}\{\frac{\phi(X - dt\,Q) - \phi(X)}{-dt} - n(X)\} = 0 \Leftrightarrow \phi(X) = \inf_{\|Q\|\leq 1} \phi(X - dt\,Q) + dt\,n(X) \tag{11}$$

Remark that we have slightly manipulated the expression to make it appear consistent with (6). Indeed remember that

1. $Q_{opt} = \frac{\nabla\phi}{\|\nabla\phi\|}$ is the direction of a ray passing through X, see (2).
2. $dt\,n(X)$ is a local approximation of the *optical length.*

Only by minimizing the phase over locally over "portions of rays" can we recover the minimum over global rays initialized on the boundary, i.e. the *viscosity solution.* Conversely only an absolute minimum can be computed by local minimization steps. This unfortunately makes plain viscosity solutions irrelevant for the multivalued traveltime problem, for more

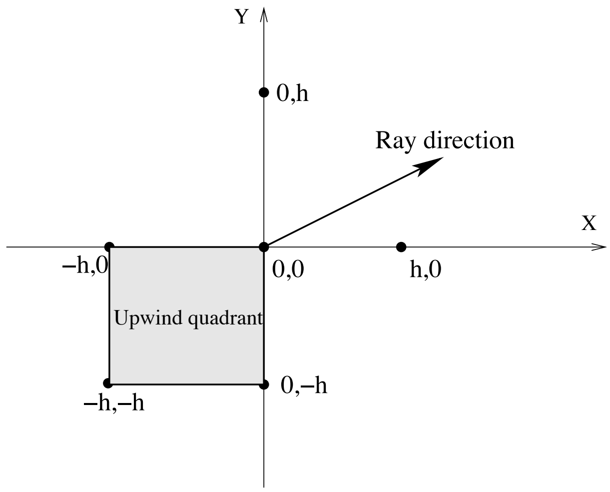

Figure 1: Stencil and upwind quadrant

on this topic see [11] [9]).

In the next section we show that RT algorithm can indeed be linked to ray tracing but let us first finish the derivation of the algorithm. We follow a slightly different technique which we find simpler than the presentation in [4]. Let h be a discretization step in x and y the cartesian coordinates $X = \{x, y\}$, $(\{0,0\}, \{h,0\}, \{0,h\}, \{-h,0\}, \{0,-h\})$ are the coordinates of the usual regular grid five point stencil around the origin (figure 1) and $(\phi_{0,0}, \phi_{h,0}, \phi_{0,h}, \phi_{-h,0}, \phi_{0,-h})$ are the unknown values of the phase at these grid points. We first assume that the direction of the "optimal" ray passing through $\{0,0\}$ points in the $x \geq 0, y \geq 0$ quadrant (figure 1) . This means that the point $X - dt\, Q_{opt}$ should be chosen in the $x \leq 0, y \leq 0$ quadrant, this is know as *upwinding*.

We focus on one this quadrant, denote $\nabla\phi = (a, b)$ and Taylor expand

$$\begin{cases} \phi_{0,-h} = \phi_{0,0} - ha + O(h^2) \\ \phi_{-h,0} = \phi_{0,0} - hb + O(h^2) \end{cases}$$

As usual we make a linear approximation by neglecting the second order error terms, the Eikonal equation becomes

$$\sqrt{a^2 + b^2} = \sqrt{(\frac{\phi_{0,0} - \phi_{0,-h}}{h})^2 + (\frac{\phi_{0,0} - \phi_{-h,0}}{h})^2} = n_{0,0}$$

Note that the assumption that the ray points in the $x \geq 0, y \geq 0$ quadrant is equivalent to $\phi_{0,0} - \phi_{0,-h} \geq 0$ and $\phi_{0,0} - \phi_{-h,0} \geq 0$: the phase increases in the direction of the ray. This remark combined with the using the inf property of (11) leads to the four quadrant formula

$$\sqrt{\max(a_l^+, a_r^-)^2 + \max(b_l^+, b_r^-)^2} = n_{0,0} \tag{12}$$

where $a^+ = \max(0, a)$, $a^- = \max(0, -a)$ and

$$a_l = \frac{\phi_{0,0} - \phi_{-h,0}}{h} \quad a_r = \frac{\phi_{0,0} - \phi_{h,0}}{h}$$
$$b_l = \frac{\phi_{0,0} - \phi_{0,-h}}{h} \quad b_r = \frac{\phi_{0,0} - \phi_{0,h}}{h}$$

We end the discretization of (1)(5) by writing (12) at all interior grid points and using the Dirichlet boundary conditions. This yields a system of non-linear equations for $(\phi_{i,j})_{i,j}$, the phase at all grid points. This can more abstractly written as

$$g(\phi_{i,j}, \phi_{i+1,j}, \phi_{i-1,j}, \phi_{i,j+1}, \phi_{i,j-1}) = 0 \tag{13}$$

for all interior grid points (i, j), boundary point values are specified using the Dirichlet boundary condition. The function g is the called the numerical Hamiltonian and embodies formula (12). Existence and uniqueness of the discrete solution is proved in [4]. It theoretically is $O(\sqrt{h})$ accurate but it is also well know that the expected first order accuracy is the rule away from the kinks where the gradient is discontinous. The impact of the regularity of the boundary conditions (especially point sources) also needs attention (see [12]).

We finally adress the problem of solving this non-linear system. Once again the *Lagrangian* interpretation of scheme (11) is helpful. Information clearly propagate along the *Lagrangian wind* and the value at the center of the stencil is "down the local wind". It therefore makes sense to relax (13) and compute iteratively a sequence of solutions $(\phi^k_{i,j})_{i,j}$ as

$$g(\phi^{k+1}_{i,j}, \phi^k_{i+1,j}, \phi^k_{i-1,j}, \phi^k_{i,j+1}, \phi^k_{i,j-1}) = 0 \tag{14}$$

for all interior grid points (i, j). Getting back to our simple one quadrant description this is easily solved using

$$\begin{array}{l} \phi^{k+1}_{0,0} = 0.5\,(\phi^k_{0,-h} + \phi^k_{-h,0}) + 0.5\,\sqrt{2\,h^2\,n^2_{0,0} - (\phi^k_{0,-h} - \phi^k_{-h,0})^2} \\ \mathit{Assuming}\,(\phi^k_{0,-h} - \phi^k_{-h,0})^2 < h^2\,n^2_{0,0} \\ \phi_{0,0} = \min(\phi^k_{-h,0}, \phi^k_{0,-h}) + h\,n_{0,0} \quad \mathit{else} \end{array}$$

Once again we can generalized to the four quadrant using the inf property

$$\begin{array}{l} \alpha = \min(\phi^k_{0,-h}, \phi^k_{0,h}) \\ \beta = \min(\phi^k_{-h,0}, \phi^k_{h,0}) \\ \phi^{k+1}_{0,0} = 0.5\,(\alpha + \beta) + 0.5\,\sqrt{2\,h^2\,n^2_{0,0} - (\alpha - \beta)^2} \quad \mathit{Assuming}\,(\alpha - \beta)^2 < h^2\,n^2_{0,0} \\ \phi_{0,0} = \min(\alpha, \beta) + h\,n_{0,0} \quad \mathit{else} \end{array} \tag{15}$$

The first minimization pick up the upwind quadrant, the last test is then just activated when the optimal direction is exactly on a grid line. This iterative process has been shown to produce a monotonicaly convergent sequence to the solution of (13). The grid point ordering of the update (14) for each iteration k has been much studied and has a very important impact on the speed of convergence, i.e. the number of iterations needed for (14) to converge to (13). An "optimal" strategy clearly needs to take into account some kind of Lagrangian information. The famous fast marching method [13] achieves a $O(N\,logN)$ complexity , N beeing the number of grid points. at the expense of a sophisticated sorting algorithm. Group marching algorithm [16] is elegant even though it does not seem to be as simple and efficient of the Sweeping algorithm [15] [16] which is in essence just Gauss-Seidel combined with the inf property and alternate choice of "sweeping" direction $\{x > 0, x < 0, y > 0, y < 0\}$. Sweeping seems in most cases to be of complexity $O(N)$ and was proven to be so for $n \equiv 1$ [15]. We rediscuss sweeping as a motivation in the next section and also in section 6 where we propose our own implementation of the Sweeping method.

3 Eulerian based Ray tracing (EBRT)

As explained in the introduction, the method of characteristics (ray tracing) can be considered as the fundamental method of resolution of the Eikonal equation. It also plays a role through upwinding (see 11) in designing Eulerian numerical methods such as the RT algorithm. In this section we try to walk our way backward from the discrete viscosity solution $(\phi_{i,j})_{i,j}$ of the preceding section to the rays underlying the solution, that is the optimal paths of problem (6). The starting motivation was, other than mere curiosity, linked to the Sweeping method for which there are no rigorous estimate on the number sweep needed to converge. One possible understanding of sweeping method is that it picks portions of correct rays along the direction is propagates and that it therefore takes as many iterations of sweeps in all directions than 45^o turns in the underlying exact rays to propagate the correct phase from portions to portions. So it seems that a reasonable first step towards a convergence speed theory is to make sure that we can really interpret locally the discrete solution as local ray tracing : we want to check that (11) is really a local discrete version of (6).

So we propose to construct "discrete rays" from RT discrete Eulerian solution by the following EBRT procedure :

1. Compute the viscosity solution $\phi_{i,j}$ on a regular grid.
2. Build ϕ_h a continuous P1 linear interpolant of $\phi_{i,j}$.
3. From any point X do a gradient descent on the surface.

Note that step 2. is not uniquely determined as for each group of four neighbors points we can split the cell quadrangle along either diagonal to build ϕ_h. Numerical experiment do not seems to be sensitive to this issue which however raises a technical difficulty (discussed

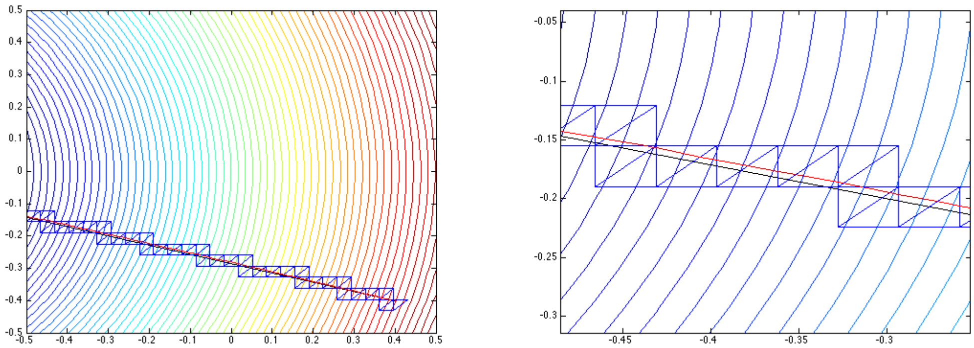

Figure 2: Homogeneous index of refraction : EBRT : red, Exact ray : black -

below). Upwinding offers a way out as in each such cell only three points are linked by the scheme (12) the remaining point is attached to another neighboring cell. In order to make the discussion as simple as possible we choose the diagonal which is consistent with the scheme. Steps 1. to 3. produce $Y_h(s)$ a polygonal path solution of $\dot{Y_h} = -\nabla\phi_h$ for all $(\tau_i)_{i\in I}$, I being the set of indices of triangles crossed by Y_h. Because there are no sinks ($\phi_{i,j}$ cannot be strictly smaller than all its neighbors) and no plateau in the ϕ_h surface (n_h is strictly positive), Y_h must exit the domain in a finite number of triangles, say at Y_0. There is however no garantee of uniqueness for Y_h in particular if it hits a grid point where branching could occur. We resort once again to the inf property and choose the steepest descent direction in that case. Figure 2 and 3 show this algorithm in action both for $n \equiv 1$ (homogenous index of refraction) and n as a Gaussian, thus bending the rays (heterogeneous). A zoom details the ϕ_h triangles used. We also plotted the contour lines of the phase.

We now want to check that as h goes to 0 our EBRT solution converges to the actual piece of ray yielding the viscosity solution. Let's focus on one triangle τ_i, ϕ_h is built to satisfy $\|\nabla\phi_h\| = n_h$ where n_h is the value at the center grid point of the scheme (this is not true on all triangles as discussed below). Let $Y_h : Y_{in} \to Y_{out}$ be the piece of path going through our triangle The phase difference satisfy

$$\delta\phi_i = \phi_h(Y_{in}) - \phi_h(Y_{out}) = n_h \|Y_{out} - Y_{in}\| = \int_{Y_{out}}^{Y_{in}} n_h(Y_h(s))ds \tag{16}$$

and as n_h is a piecewise constant approximation of n

$$\delta\phi_i = \int_{Y_{out}}^{Y_{in}} n(Y_h(s)) + O(h)ds = \int_{Y_{out}}^{Y_{in}} n(Y_h(s))ds + O(h^2)$$

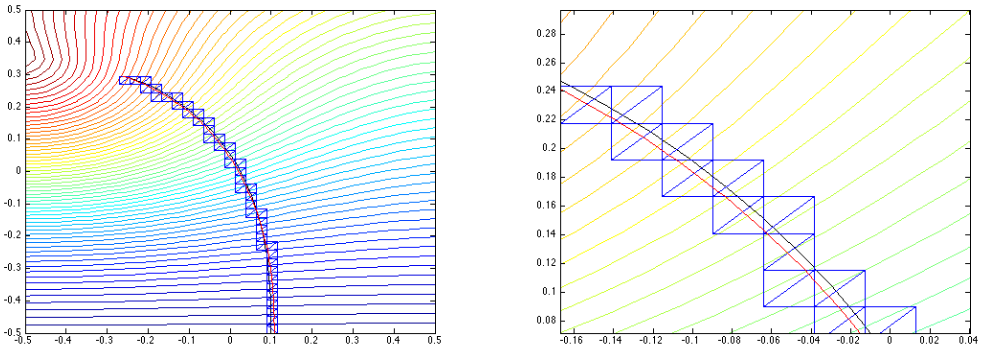

Figure 3: Heterogeneous index of refraction : EBRT : red, Exact ray : black -

Summing over all triangles we have

$$\phi_h(X) = \phi_0(Y_0) + \sum_{i \in I} \delta\phi_i = \phi_0(Y_0) + \int_{Y_0}^{X} n(Y_h(s))ds + O(h)$$

We now recall that $\phi_h \to \phi_v$ uniformly (standard convergence results are not established for the $P1$ interpolant but ϕ_h can be bounded by convergent sub and super solutions) and $(Y_h)_h$ is uniformly bounded in $\mathcal{C}^0 \cup \mathcal{W}^{1,\infty}$. So, for any convergent subsequence $Y_{h'} \to Y'$:

$$\phi_v(X) = \phi_0(Y_0) + \int_{Y_0}^{X} n(Y'(s))ds$$

We conclude using the inf property in (6). The optimal path is necessarily a ray, uniquely determined by intial and end points.

There is a technical issue linked to step 2. of our EBRT procedure : $\|\nabla\phi_h\| = n_h$ may not be satisfied exactly on all (τ_i)s.

We then distinguish two cases :

1. $\|\nabla\phi_h\| < n_h$. Then, it is fine because

$$\delta\phi_i = \phi_h(Y_{in}) - \phi_h(Y_{out}) < n_h \, \|Y_{out} - Y_{in}\| = \int_{Y_{out}}^{Y_{in}} n_h(Y_h(s))ds$$

2. $\|\nabla\phi_h\| > n_h$. Then, instead of gradient descent choose Y_{out} as $Y_{out} = Y_{in} + \vec{e}_\theta \, \|Y_{out} - Y_{in}\|$ note that Y_{out} depends on the angle θ. Then

$$\delta\phi_i = \phi_h(Y_{in}) - \phi_h(Y_{out}) = (\vec{e}_\theta \cdot \frac{\nabla\phi_h}{\|\nabla\phi_h\|}) \, \|\nabla\phi_h\| \, \|Y_{out} - Y_{in}\|$$

If $\|\nabla\phi_h\|$ is not too far from n_h (looks likely) then we can pick θ such that $(\vec{e}_\theta \cdot \frac{\nabla\phi_h}{\|\nabla\phi_h\|})\|\nabla\phi_h\| = n_h$. There is two possible angle on each side. Use again inf principle to make this step uniquely determined and we recover (16).

Summing again and passing to the limit we get this time

$$\phi_v(X) \geq \phi_h(Y_0) + \int_{Y_0}^{X} n(Y'(s))ds$$

and can conclude exactly as before as the inf property (6) actually gives us equality in the above relation.

We now check the convergence numerically. We give in the tables below both the phase error at the starting point (line Phi) the error on the exit point between the exact ray and the EBRT (line EBRT) output as a function of N the number of points used along one dimension ($h = \frac{1}{N}$). Errors are given in thousandth unit (x10^{-3})

Homogeneous index :

N	20	40	80	160
Phi	8.342164822988	4.183548796327	2.096150358148	1.049334449310
EBRT	7.634700799533	3.671886961461	1.746799748012	0.910111940347

Heteogeneous index :

N	20	40	80	160
Phi	10.141212310403	5.280400011813	2.940170090754	1.485838444092
EBRT	20.805149751783	8.463070495399	1.555524315021	0.914009038344

Both tables show the expected first order convergence on the phase function and a similar convergence for the EBRT procedure.

4 Superconvergence of upwind schemes

Section 3 leaves us with a paradox. If RT algorithm is first order and our EBRT procedures consists in solving $\frac{d}{ds}Y(s) = \nabla\phi_h(Y(s))$. How is possible to get convergence ? Indeed $\nabla\phi_h$

should be $O(1)$ with respect to h and not convergent.

It is worth noticing that the gradient does not really appear in the convergence arguments of section 3. An indeed a simple numerical study corroborates that the gradient is first order : We computed the max error for a smooth solution (homogeneous space experiment figure 2) both for the phase (line Phi) and the x derivative of the phase (line Phi_x). The table below indicated these values for different discretization N ($h = \frac{1}{N}$) in thousands unit (x10^{-3})

N	20	40	80	160
Phi	15.234247606216	7.759428468247	3.921528965098	1.972101681897
Phi_x	51.928505018272	26.039665569648	13.012745981813	6.502472321552

First order convergence ($O(h)$) can be observed both for the phase and its derivatives.

We make two remarks we think are relevant to understand this superconvergence phenomena.

First we recall that we made a first order approximation in (11)

$$\sup_{\|Q\|\le 1} \{ \frac{\phi(X - dt\,Q) - \phi(X)}{-dt} - n(X) \} = O(dt^2)$$

If we instead use a second order Taylor expansion we get

$$\sup_{\|Q\|\le 1} \{ \frac{\phi(X - dt\,Q) - \phi(X)}{-dt} + \frac{dt}{2} < Q, D^2\phi(X) \cdot Q > -n(X) \} = O(dt^3)$$

Remembering $Q_{opt} = \frac{\nabla\phi}{\|\nabla\phi\|} = \frac{\nabla\phi}{n}$. We obtain

$$\left\{ \frac{\phi(X - dt\,\frac{\nabla\phi(X)}{n(X)}) - \phi(X)}{-dt} + \frac{dt}{2} < \frac{\nabla\phi(X)}{n(X}, D^2\phi(X) \cdot \frac{\nabla\phi(X)}{n(X)} > \right\} - n(X) = O(dt^3)$$

But (7) : $D^2\phi(X) \cdot \nabla\phi(X) = \frac{1}{2}\nabla(n^2(X)) = n(X)\nabla n(X)$. So we can rearrange to recover a formula similar to (11) where a trapezoidal rule is used to approximate the local optical length :

$$\begin{aligned} \phi(X) &= \phi(X - dt\,\tfrac{\nabla\phi(X)}{n(X)}) - dt \left\{ \tfrac{dt}{2} < \tfrac{\nabla\phi(X)}{n(X)}, \nabla n(X) > -n(X) \right\} + O(dt^2) \\ &\phi(X - dt\,\tfrac{\nabla\phi(X)}{n(X)}) - dt\,\tfrac{1}{2} \left\{ < dt\,\tfrac{\nabla\phi(X)}{n(X)}, \nabla n(X) > -n(X) \right\} + O(dt^2) \\ &\phi(X - dt\,\tfrac{\nabla\phi(X)}{n(X)}) + dt\,\tfrac{1}{2} \left\{ n(X) + n(X - dt\,\tfrac{\nabla\phi(X)}{n(X)}) \right\} + O(dt^2) \end{aligned}$$

Apparently second order *upwinding* only requires a better approximation n and this is in particular alway true for constant indices of refraction. Of course, in deriving RT, we still have the piecewise linear approximation of $\phi(X - dt\, Q_{opt})$ which produces a first order error.

5 A second Order Scheme

The most popular high order schemes for Hamilton-Jacobi equation are based on the ENO (Essentially Non Oscillatory) technique [7] which automatically moves the second order stencil around a grid point to fetch the smoother (kink free) approximation. The approach followed here is different. Using the *Lagrangian structure* of the Eikonal equation we propose a pure upwind second order extension of R-T scheme that needs only one more point added to the stencil.

We first write a second order Taylor expansion

$$\phi(X + \delta X) = \phi(X) + \delta X \cdot \nabla\phi(X) + \frac{1}{2} < \delta X, D^2\phi(X) \cdot \delta X > +O(\delta X^3) \qquad (17)$$

We want to take advantage of (7) : $D^2\phi(X) \cdot \nabla\phi(X) = n(X)\nabla n(X)$ and decompose the variation δ in the local coordinate system made of the Lagrangian direction and its orthogonal

$$\delta X = \frac{1}{n^2(X)} \left((\delta X \cdot \nabla\phi)\, \nabla\phi + (\delta X \cdot \nabla\phi^\perp)\, \nabla\phi^\perp \right)$$

Plugin this decomposition in the second order term of (17) yields

$$\begin{aligned} \tfrac{1}{2} < \delta X, D^2\phi(X) \cdot \delta X >= \; & \frac{1}{2\, n^4}(\delta X \cdot \nabla\phi)^2 < \nabla\phi, D^2\phi \cdot \nabla\phi > \\ & + \frac{1}{n^4}(\delta X \cdot \nabla\phi)(\delta X \cdot \nabla\phi^\perp) < \nabla\phi^\perp, D^2\phi \cdot \nabla\phi > \\ & + \frac{1}{2\, n^4}(\delta X \cdot \nabla\phi^\perp)^2 < \nabla\phi^\perp, D^2\phi \cdot \nabla\phi^\perp > \end{aligned} \qquad (18)$$

We first restrict to the simpler homogeneous case $n \equiv 1$. Derivatives of n vanish and (17) becomes

$$\phi(X + \delta X) = \phi(X) + \delta X \cdot \nabla\phi(X) + \frac{1}{2}(\delta X \cdot \nabla\phi^\perp)^2 < \nabla\phi^\perp, D^2\phi \cdot \nabla\phi^\perp > +O(\delta X^3) \quad (19)$$

For point sources solutions $\phi(X) = \|X - X_0\|$, $< \nabla\phi^\perp, D^2\phi \cdot \nabla\phi^\perp >$ is the curvature of the level sets of the phase (also called fronts). We will denote it C. Our new approximation of the phase (19) uses "shape function" of the form (denote $\nabla\phi = (a, b)$)

$$\phi(X + \delta X) = \phi(X) + \delta X \cdot (a, b) + \frac{C}{2\, n^4}(\delta X \cdot (-b, a))^2 + O(\delta X^3) \qquad (20)$$

This is a parabolic "local curvature" correction to RT piecewise linear interpolation (section 2).

We now proceed as in the RT scheme but using the second order approximation (20). We first restrict to a quadrant. To realize our approximation we need to determine the three coefficients (a, b, C). We therefore need three equation and we use the four grid points $(\{0,0\}, \{-h,0\}, \{0,-h\}, \{-h,-h\})$ to obtain

$$\begin{cases} \phi_{-h,0} = \phi_{0,0} - h\,a + \frac{C}{2}\,(-h\,b)^2 + O(h^3) \\ \\ \phi_{0,-h} = \phi_{0,0} - h\,b + \frac{C}{2}\,(h\,a)^2 + O(h^3) \\ \\ \phi_{-h,-h} = \phi_{0,0} - h\,(a+b) + \frac{C}{2}\,(h\,(b-a))^2 + O(h^3) \end{cases} \tag{21}$$

Truncating the third order error we can get a grid value approximation of the curvature C and eliminate the last equation for instance.

$$line\,1 + line\,2 - line\,3 \Leftrightarrow C = \frac{\phi_{0,-h} - \phi_{0,0} + \phi_{-h,0} - \phi_{-h,-h}}{h^2\,a\,b} \tag{22}$$

The next natural steps should be

1. to solve for (a, b) as a function of $(\phi_{0,0}, \phi_{-h,0}, \phi_{0,-h}, \phi_{-h,-h})$ and replace in the Eikonal equation to write the numerical Hamiltonian.
2. relax : compute $\phi_{0,0}$ as a function of the values at grid points $(\{-h,0\}, \{0,-h\}, \{-h,-h\})$.

This turn our to be a difficult non linear problem, involving the roots of a sixth order polynomial. Before explaining how to simplify this into a more tractable problem. We derive a natural and elegant interpretation of our scheme. Remembering the Eikonal equation can be recast locally as $\{a, b\} = \{n\,\cos(\theta), n\,\sin(\theta)\}$, we can use (21)(22) to write the a local weighted centered FD formula in the upwind quadrant

$$\begin{cases} a = (1 - \frac{1}{2}\,\tan(\theta))\,\frac{\phi_{0,0} - \phi_{-h,0}}{h} + \frac{1}{2}\,\tan(\theta)\,\frac{\phi_{0,-h} - \phi_{-h,-h}}{h} \\ b = (1 - \frac{1}{2}\,\tan^{-1}(\theta))\,\frac{\phi_{0,0} - \phi_{0,-h}}{h} + \frac{1}{2}\,\tan^{-1}(\theta)\,\frac{\phi_{-h,0} - \phi_{-h,-h}}{h} \end{cases} \tag{23}$$

This is not a practical solution formula as θ depends on (a, b) but it shows that we average the local first order finite difference (FD) according to the Lagrangian direction. For instance if the ray makes a $\frac{\pi}{4}$ angle with the x axis, i.e. exactly cuts in half the quadrant, then we use an arithmetic average of the FD derivatives of the four grid points of this quadrant. If the ray approaches an axis then the weight are non-linearly adjusted by the $\tan(\theta)$ functions.

In order to simplify our local solver we remember that RT scheme

1. determines the upwind quadrant.

2. does so with first order accuracy.

We will denote the first order gradient obtained from RT as (a_1, b_1) and assume the gradient points in the positive x and y direction. We can therefore work with the upwind quadrant $(\{0,0\},\{-h,0\},\{0,-h\},\{-h,-h\})$. This also means that

$$a1 = \frac{\phi^1_{0,0} - \phi_{-h,0}}{h} \quad b1 = \frac{\phi^1_{0,0} - \phi_{0,-h}}{h} \tag{24}$$

are given as a function of $\phi^1_{0,0}$ the first order RT solution. Using section 4 remark that $(a_1, b_1) = (a, b) + O(h)$, we notice that replacing in the quadratic term of the Taylor expansions (21) preserves second order accuracy

$$\begin{cases} \phi_{-h,0} = \phi_{0,0} - h\,a + \frac{C}{2}\,(-h\,b_1)^2 + O(h^3) \\ \phi_{0,-h} = \phi_{0,0} - h\,b + \frac{C}{2}\,(h\,a_1)^2 + O(h^3) \\ \phi_{-h,-h} = \phi_{0,0} - h\,(a+b) + \frac{C}{2}\,(h\,(b_1 - a_1))^2 + O(h^3) \end{cases} \tag{25}$$

We can again eliminate C with formula (22) where (a, b) is replaced by (a_1, b_1). Then, (23) simplifies to

$$\begin{cases} a = (1 - \frac{1}{2}\,\tan(\theta_1))\,\frac{\phi_{0,0} - \phi_{-h,0}}{h} + \frac{1}{2}\,\tan(\theta_1)\,\frac{\phi_{0,-h} - \phi_{-h,-h}}{h} \\ b = (1 - \frac{1}{2}\,\tan^{-1}(\theta_1))\,\frac{\phi_{0,0} - \phi_{0,-h}}{h} + \frac{1}{2}\,\tan^{-1}(\theta_1)\,\frac{\phi_{-h,0} - \phi_{-h,-h}}{h} \end{cases} \tag{26}$$

where θ_1 is the first order angle given by RT and therefore $\tan(\theta_1) = \frac{b1}{a1}$. We can now write our second order numerical Hamiltonian (restricted to the upwind quadrant)

$$g(\phi_{0,0}, \phi_{0,-h}, \phi_{-h,0}, \phi_{-h,-h}) = \sqrt{a^2 + b^2} - n_{0,0} = 0 \tag{27}$$

where a, b is given by (26).

About the properties of this numerical scheme :

1. Consistency of order 2.
2. Stability as long as θ_1 stays away from grid lines.
3. Monotonicity, as a second order scheme is of course non monotone (it is easily checked that g can not be simultaneously a decreasing function of $\phi_{0,-h}$ and $\phi_{-h,0}$ at the same time).

So the usual convergence theory [14] does not apply here. However a closer look (in the spirit of [6] th. 3.1[1] to the classic viscosity convergence shows that it is enough to be a $O(h)$ perturbation of a monotonic scheme to be convergent. We notice that (26) can also be written

$$\left\{ \begin{array}{l} a = a_1 - \frac{1}{2}\,\tan(\theta_1)\,\{\frac{\phi_{0,0} - \phi_{-h,0}}{h} - \frac{\phi_{0,-h} - \phi_{-h,-h}}{h}\} \\ b = b_1 - \frac{1}{2}\,\tan^{-1}(\theta_1)\,\{\frac{\phi_{0,0} - \phi_{0,-h}}{h} - \frac{\phi_{-h,0} - \phi_{-h,-h}}{h}\} \end{array} \right. \tag{31}$$

so as long as the $\tan(\theta_1)$ remains bounded above and from 0, and independently of h (which means that the ray direction should be away from an axis) any smooth grid sampled C^2 function ϕ will satisfy

$$g(\phi_{0,0}, \phi_{0,-h}, \phi_{-h,0}, \phi_{-h,-h}) = \sqrt{a_1^2 + b_1^2} - n_{0,0} + O(h) \tag{32}$$

and it is well known that $\sqrt{a_1^2 + b_1^2}$ leads up to a monotonic numerical Hamiltonian.

For the upper right quadrant, a condition like (see figure 4)

$$\frac{\pi}{2} - \epsilon > \theta_1 > \epsilon \tag{33}$$

where $\epsilon > 0$ is independent of h is sufficient to garrantee convergence of the second order scheme.

Of course, there is no way to systematically enforce (33) as it depends on the problem data. We must keep away from the second order scheme when (33) is not satisfied. In that case (assume for instance that $\theta_1 < \epsilon$) $b_1 = sin(\theta_1) = O(\epsilon)$, $a_1 = 1 - O(\epsilon)$, the upwind Taylor expansion along the x axis gives

$$\begin{array}{ll} \phi_{-h,0} & = \phi_{0,0} - h\,a + h\,O(\epsilon) + \frac{C}{2}\,(-h\,b_1)^2 + O(h^3) \\ & = \phi_{0,0} - h + h\,O(\epsilon) + O(h^2)\,O(\epsilon)^2 + O(h^3) \end{array} \tag{34}$$

[1] In the *classic proof* the key point is to consider sequences of approximations $h_n \to 0$, $X_n \to x_0$, $\phi_{h_n}(X_n) \to \underline{\phi}(X_0)$ and show that $\underline{\phi}$ is a viscosity super-solution of the Eikonal equation. To do so one assumes that X_0 is a point of local minimum for $\underline{\phi} - \psi$ and the above sequences are built such in such a way that X_n is a global minimum of $\phi_{h_n} - \psi$ in a neighborood of X_0 independent of h. Then one sets $\xi_n = \phi_{h_n}(X_n) - \psi(X_n)$ and gets $\xi_n \to 0$, $\phi_{h_n} \geq \psi + \xi_n$ near X_0. This is where monotonicity of the numerical Hamiltonian comes in. Replacing the ϕ_{h_n} values by $\psi + \xi_n$ we get (see (13)

$$H^{num}(\psi + \xi_n) = g(\psi_{i,j} + \xi_n, \psi_{i,j+1} + \xi_n, \psi_{i+1,j} + \xi_n, \psi_{i-1,j} + \xi_n, \psi_{i,j-1} + \xi_n) \geq 0 \tag{28}$$

Then pass to the limit (remark that in this first order equation the ξ_n cancel immediately) to get, using consistency (H is the Eikonal equation Hamiltonian).

$$H(X, \nabla\psi(X)) \geq 0 \tag{29}$$

which proves the viscosity super-solution of $\underline{\phi}$.

In [6] th. 3.1, the author uses a clever blending of first order monotonic and high order numerical Hamiltonians to satisfy approximately (28) and still get (29) at the limit. In our case this is much simpler as we get

$$H^{num}(\psi + \xi_n) + O(h_n) \geq 0 \tag{30}$$

where H^{num} is Rouy Tourin first order monotonic Hamiltonian, and can easily pass to the limit (29).

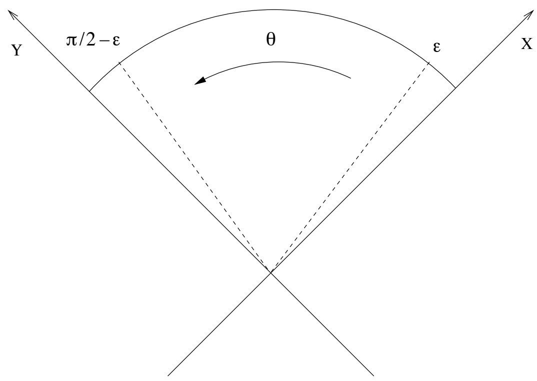

Figure 4: Authorized angles for the second order scheme

If we use this formula to update $\phi_{0,0}$ we get $hO(\epsilon)$ accuracy. In practice we just use the already computed first order value $\phi^1_{0,0}$.

Remark : Of course this treatment will only hold as long as $\epsilon = O(h)$ and ϵ need to fixed independent of h (see p.15 16 on the convergence of the scheme). So we will loose second order accuracy when h gets below a threshold depending on ϵ. The most reasonable treatment when $\theta_1 < \epsilon$ is to change the stencil, the ray direction is along the x axis. To get a better approximation of the curvature of the front we can add the point $(0, -2h)$ instead of $(-h, -h)$. This will change formulae (26) and eliminate the problematic division by $cos(\theta_1)$ in the coefficients. This is currently under investigation ... [10].

Before summarizing the complete scheme we need to adress the resolution of the discrete system. As for the RT algorithm we use relaxation. We need to be able to solve for $\phi^{k+1}_{0,0}$

$$g(\phi^{k+1}_{0,0}, \phi^k_{0,-h}, \phi^k_{-h,0}, \phi^k_{-h,-h}) = 0 \tag{35}$$

This boils down to finding the roots of a second order polynomial. For simplicity we omit the k upperscripts, the equation is

$$a^2 + b^2 = n^2_{0,0}$$

where (a, b) are given in (31). This can be rewritten (carefully) as

$$A\,\phi^2_{0,0} + B\,\phi_{0,0} + C = 0 \tag{36}$$

where (A, B, C) are easily computed and depend on the values at the other grid points and on (a_1, b_1). When (33) is satisified, we expect (it works numerically and I need to find the energy to do the computation) (36) to have at least a real root close to $\phi^1_{0,0}$.

We recapitulate the algorithm in the constant index of refaction case

1. Iterate the relaxed RT first order Algorithm (14).
2. Make the second order correction (36) in the relevant quadrant if (33) is satisfied.
3. Otherwise, stay with the first order solution (34) else.

The heterogeneous index of refraction works the same but the algebra is more complicated. We keep all the terms in (18) but use (7) to simplify, equation (19) becomes

$$\begin{aligned}\phi(X+\delta X) = \phi(X) + \delta X\cdot\nabla\phi(X) \quad & + \frac{C}{2\,n^4}(\delta X\cdot\nabla\phi^\perp)^2 \\ & + \frac{1}{n^3}(\delta X\cdot\nabla\phi)(\delta X\cdot\nabla\phi^\perp)(\nabla\phi^\perp\cdot\nabla n) \\ & + \frac{1}{2\,n^3}(\delta X\cdot\nabla\phi)^2(\nabla\phi\cdot\nabla n) \\ & + O(\delta X^3)\end{aligned} \tag{37}$$

and (21), with the same notations augmented with $n = n_{0,0}$, $n_x = \partial_x n_{0,0}$, $n_y = \partial_y n_{0,0}$ and $\nabla\phi^\perp = (-b, a)$ corresponds to

$$\begin{cases}\phi_{-h,0} = \phi_{0,0} - h\,a + \dfrac{h^2}{2\,n^4}\,(C\,b^2 + n\,a^2\,(a\,n_x + b\,n_y) - 2\,a\,b\,(-b\,n_x + a\,n_y)) \\ \phi_{0,-h} = \phi_{0,0} - h\,b + \dfrac{h^2}{2\,n^4}\,(C\,a^2 + n\,b^2\,(a\,n_x + b\,n_y) + 2\,a\,b\,(-b\,n_x + a\,n_y)) \\ \phi_{-h,-h} = \phi_{0,0} - h\,(a+b) + \dfrac{h^2}{2\,n^4}\,(C\,(a-b)^2 + n\,(a+b)^2\,(a\,n_x + b\,n_y) + 2\,(a^2-b^2)\,(-b\,n_x + a\,n_y))\end{cases} \tag{38}$$

Where we've truncated to third order accuracy. Again we can get a grid value approximation of the curvature C and eliminate the last equation for instance.

$$C = \frac{1}{a\,b}\left(\frac{n^4}{h^2}(\phi_{0,-h} - \phi_{0,0} + \phi_{-h,0} - \phi_{-h,-h}) + n\,n_x\,a^3 + n\,n_y\,b^3\right) \tag{39}$$

We can then eliminate C and the last equation, set $F = \phi_{0,-h} + \phi_{-h,0} - \phi_{-h,-h}$ ...

$$\begin{cases}\phi_{-h,0} = (1 - \dfrac{b}{2\,a})\,\phi_{0,0} - h\,a + \dfrac{b}{2\,a}\,F + \dfrac{h^2}{2\,n^4}\,n\,n_x\,(a^3 + 2\,a\,b^2 + \dfrac{b^4}{a})) \\ \phi_{0,-h} = (1 - \dfrac{a}{2\,b})\,\phi_{0,0} - h\,b + \dfrac{a}{2\,b}\,F + \dfrac{h^2}{2\,n^4}\,n\,n_y\,(b^3 + 2\,b\,a^2 + \dfrac{a^4}{b}))\end{cases} \tag{40}$$

Note that it can be simplified further into the remarkably simple

$$\begin{cases}\phi_{-h,0} = (1 - \dfrac{b}{2\,a})\,\phi_{0,0} - h\,a + \dfrac{b}{2\,a}\,F + \dfrac{h^2}{2\,a}\,n\,n_x \\ \phi_{0,-h} = (1 - \dfrac{a}{2\,b})\,\phi_{0,0} - h\,b + \dfrac{a}{2\,b}\,F + \dfrac{h^2}{2\,b}\,n\,n_y\end{cases} \tag{41}$$

We have not (yet ?) been able to use this formulation so we go back to (40) and as in the homogeneous case this system with the additional Eikonal equation ($\{a, b\} = n\,\{\cos(\theta), \sin(\theta)\}$) must be solved for $(a, b, \phi_{0,0})$. It is hopelessly non-linear. We thus propose as in the homogenous case to get back to a linear system in (a, b) by reverting to the first order quantities (a_1, b_1) in the high order terms

$$\begin{cases} \phi_{-h,0} = (1 - \frac{b_1}{2\,a_1})\,\phi_{0,0} - h\,a + \frac{b_1}{2\,a_1}\,F + \frac{h^2}{2\,n^4}\,n\,n_x\,(a\,a_1^2 + 2\,a_1\,b_1\,b + b\,\frac{b_1^3}{a_1})) \\ \phi_{0,-h} = (1 - \frac{a_1}{2\,b_1})\,\phi_{0,0} - h\,b + \frac{a_1}{2\,b_1}\,F + \frac{h^2}{2\,n^4}\,n\,n_y\,(b\,b_1^2 + 2\,b_1\,a_1\,a + a\,\frac{a_1^3}{b_1})) \end{cases} \quad (42)$$

The first remark is that again we obtain a first order perturbation of R-T numerical Hamiltonian as these formula only differ from (26) by a $O(h^2)$ perturbation. After relaxation the problem reduces to finding the roots of a second order polynomial. We pick up the root closest to the solution given by the first order scheme. We leave the courageous reader to the remainder of the algebra and turn to the numerical study.

Our first test case are cooked up to ensure that rays will propagate along the $x = y$ axis and never have angles over $\pm\frac{\pi}{4}$ with respect to this principal direction. The use of a staggered grid allows to consider always the same upwind quadrant (but one must be damn careful with the coordinate system in the implementation) see figure 5. Initial (boundary conditions) must be given on a 2 grid points layer.

Just one sweep of the grid in the direction of the rays is sufficient to compute the discrete solution. The table below show the max error at final depth for a constant index of refraction and a curved front (x10^{-4})

N	10	20	40	80
Phi	10.28491160694	2.383101764422690	0.5796556601644909	0.1739618008045341
Phi_x	60.08579687216	10.28491160694	2.957285321135705	0.4339775249684319

It indeed confirms second order convergence.

In the next experiment the index is formed of a convex/concave lense and given by ($(x, y) \in [-1, 1]^2$) $n(x, y) = 2.8$ if $\sqrt{x^2 + y^2} \geq 0.5$ $n(x, y) = 2.8 \pm 0.5\,\exp^{-30\,(x^2+y^2)}$ else. In figures 6 7 we plot the phase at final depth for

1. RT first order scheme using 40 (black solid line) and 1600 (red solid line) grid points (on each axis). The red line can be considered as the exact solution.

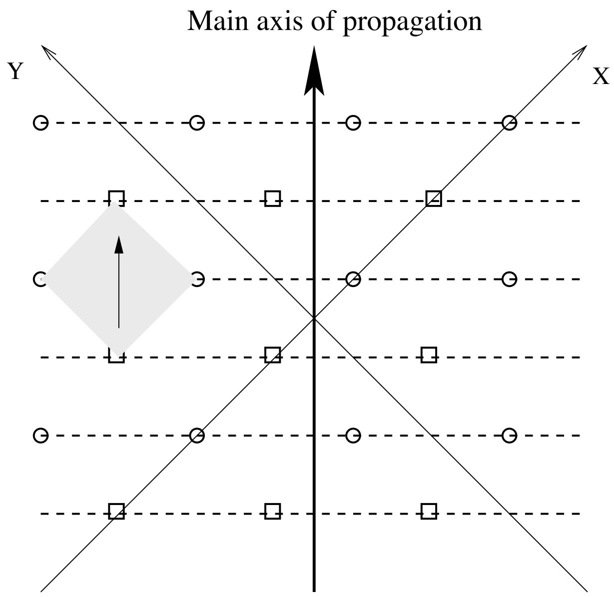

Figure 5: Staggered grid and upwind quadrant (shaded)

2. Our second order corrected scheme for or 10, 20, 40 points (stars : blue, red, black)

The second order convergence is obvious. Note how the kink is well resolved for the convex lense even with the second order scheme which stays purely upwind.

More numerical results in the next section.

6 Notes on a Sweeping implementation (staggered grid)

In order to be able to take into account any ray direction we alternate sweeps on our staggered grid as indicated in figure 8.

Sweeping for first order scheme usually update the value given by the current sweep only if it gives a *smaller value* than the previous sweep (the phase is initialized to a very large value except at sources and boundary conditions). This is an efficient want to iteratively take into account the minimization over the four quadrant in (15). Remark also that if the sweep determines the upwind quadrant it is not necessary to test for the upwind points. The second order algorithm first apply the RT first order algorithm. If the first order phase need to be updated, it means that the wind indeed follows the current sweeping direction and we can then apply the second order correction. It is not a good idea to try to accelerate by minimizing again between the first order and second order phase as this latter can indeed

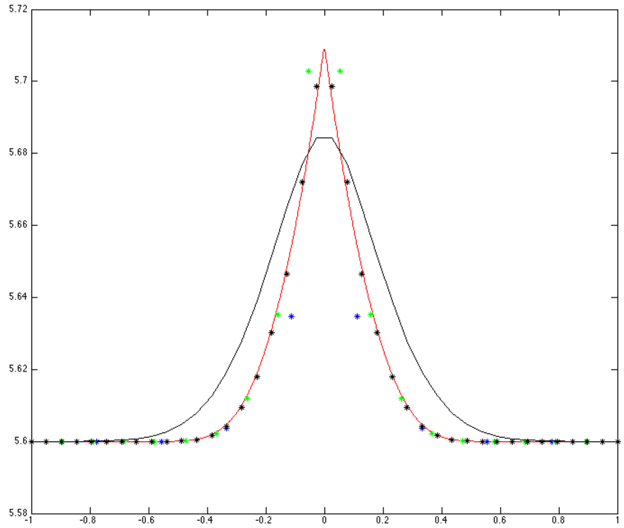

Figure 6: Convex lense

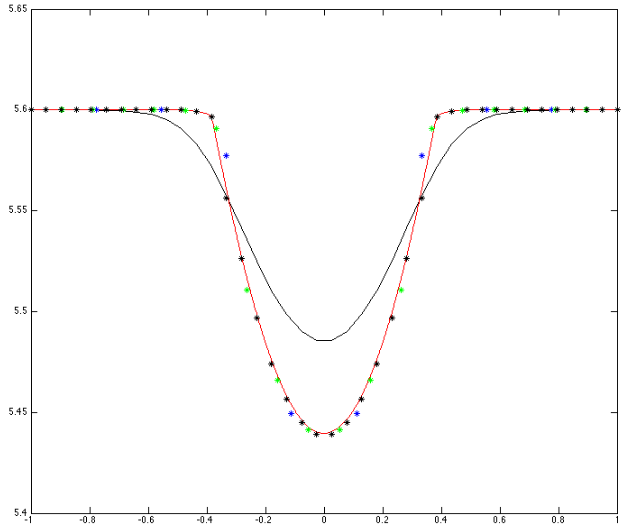

Figure 7: Concave lense

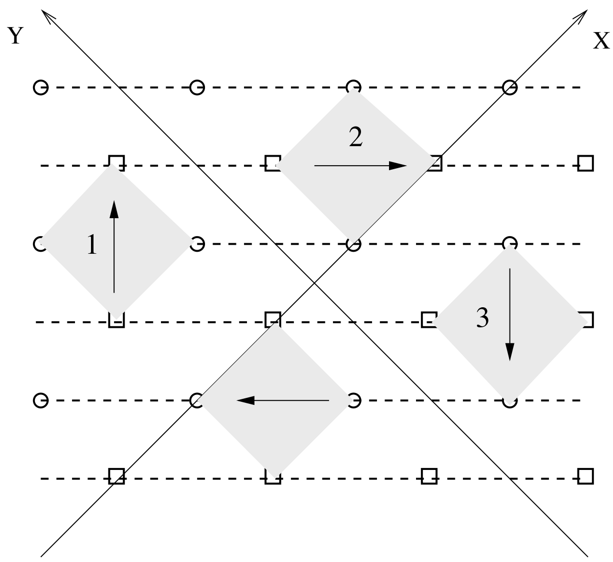

Figure 8: The whole grid is swept in the 4 (1,2,3,4) alternate directions and their quadrant

be slightly larger. So we just use the second order correction systematically when moving along the wind. There are several subtleties linked to the use of the staggered grid (axes tilted number of points ...). While implementing I significantly raised the number of bugs by insisting in having the same directionnal sweeping direction subroutine and rotating the phase and index of refraction unknown ....

We start with the standard homogeneous point sources cases. Phase is prescribed in neighborhood of the sources (several grid points). We use large values at the boundary to emulate outgoing boundary conditions (on a band 2 grid points wide of course ...).

Figure 9 and 10 show the contour line for the converged solution for 1 and 2 point sources for :

1. black : first order RT $h = \frac{2}{200}$ (10000 grid points). Can be considered as exact.
2. blue : first order RT $h = \frac{2}{20}$.
3. red : second order RT $h = \frac{2}{20}$.

As expected second order is much more accuracte and corrects well the anisotropy of the first order scheme along the vertical and horizontal. (linear approximation + curvature), remember we are staggered ... Also the remark that first order performs well along the axis is confirmed.

error study for two points source

L1 norm error (x 10^{-4}

N	20	40	80
error	6.959614404555503	2.523821530879525	1.335573687352103

We continue with an heterogeneous test case : $(x, y) \in [-1, 1]^2)$ $n(x, y) = 2.8$ if $\sqrt{x^2 + y^2} \geq 0.9$ $n(x, y) = 2.8 + 20 \exp^{-20\,(x^2+y^2)}$ else. It is similar to the heterogenous case of section 5 but the heterogenity is much stronger and rays turn significantly as shown in the contour line plot of figure 14. Initial (boundary) condition is a plane wave ($\phi = 0$) on $y = -1$. We use the exact boundary conditions $\phi = 2.8\,|y + 1|$ on $x = \pm 1$ and outgoing boundary condition on $y = 1$. On figures 15 and 16 We plot the phase at the final depth $y = 1$ for the first order and second order scheme respectively. We use different discretizations N $(h = 2/N)$.

The first order is clearly first order. The second order scheme converges much faster (it does extermely well when fronts are curved and smooth) except at the kink where it cannot be second order where it still converges without any spurious oscillations thanks to the upwind property of our scheme.

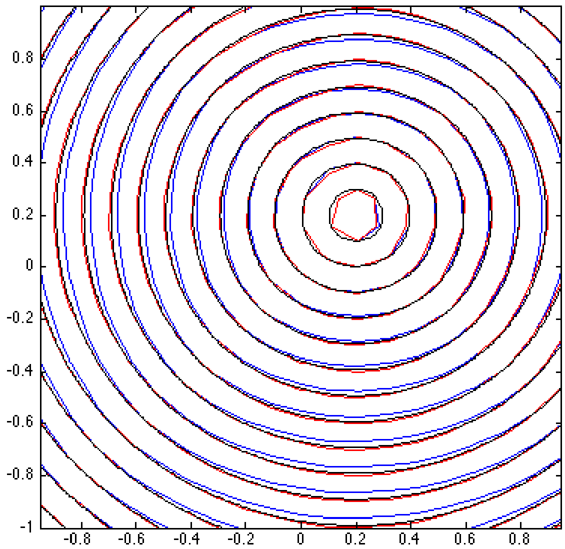

Figure 9: Homogeneous space : 1 point source

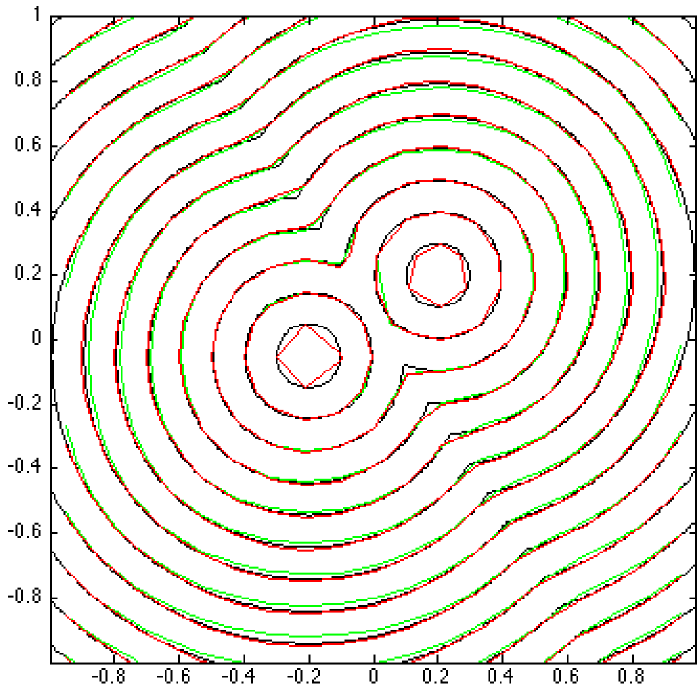

Figure 10: Homogeneous space : 2 point sources

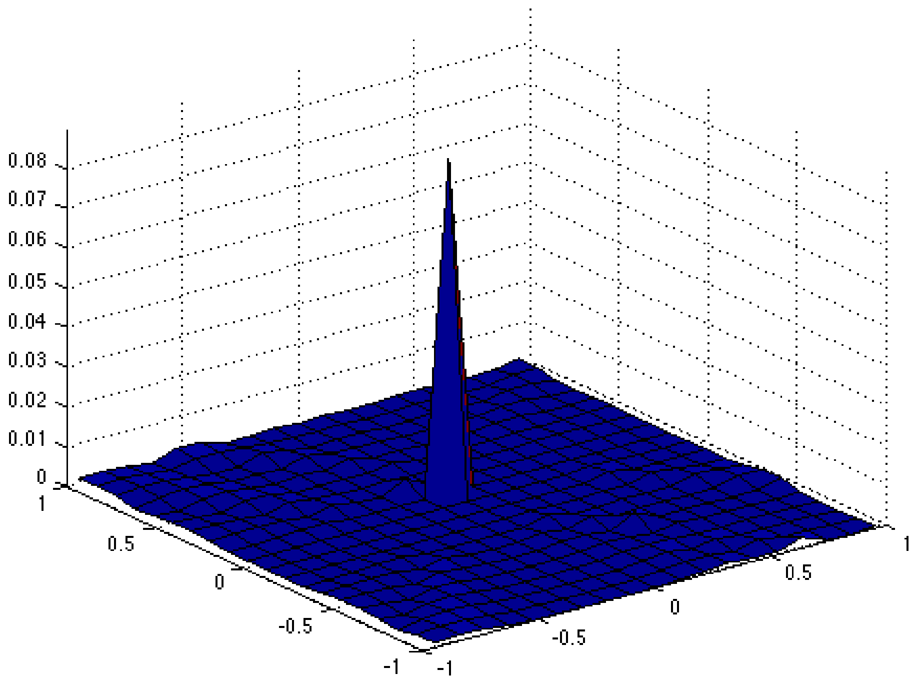

Figure 11: surface plot of the error. N=20

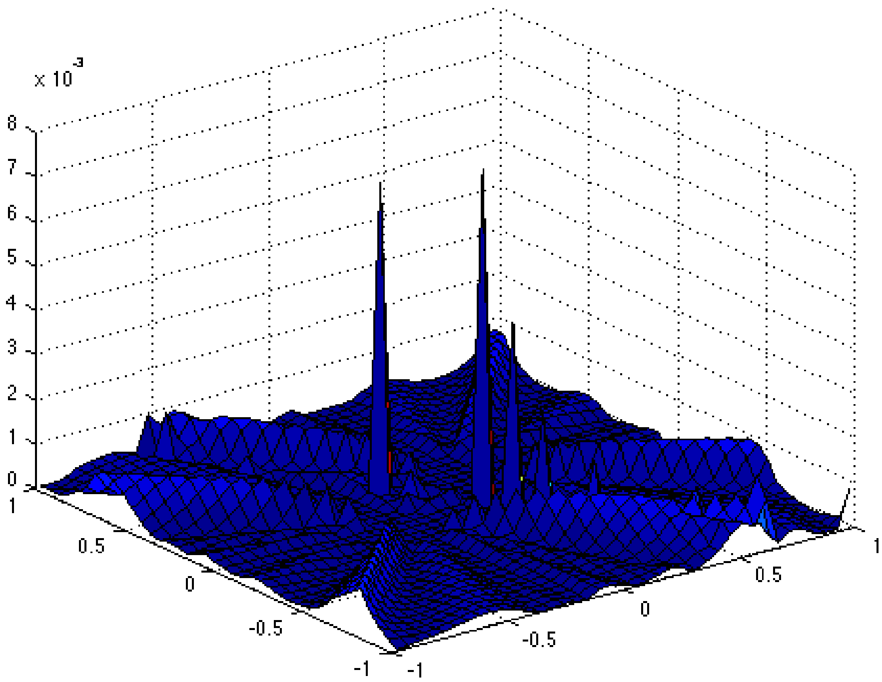

Figure 12: surface plot of the error. N=40

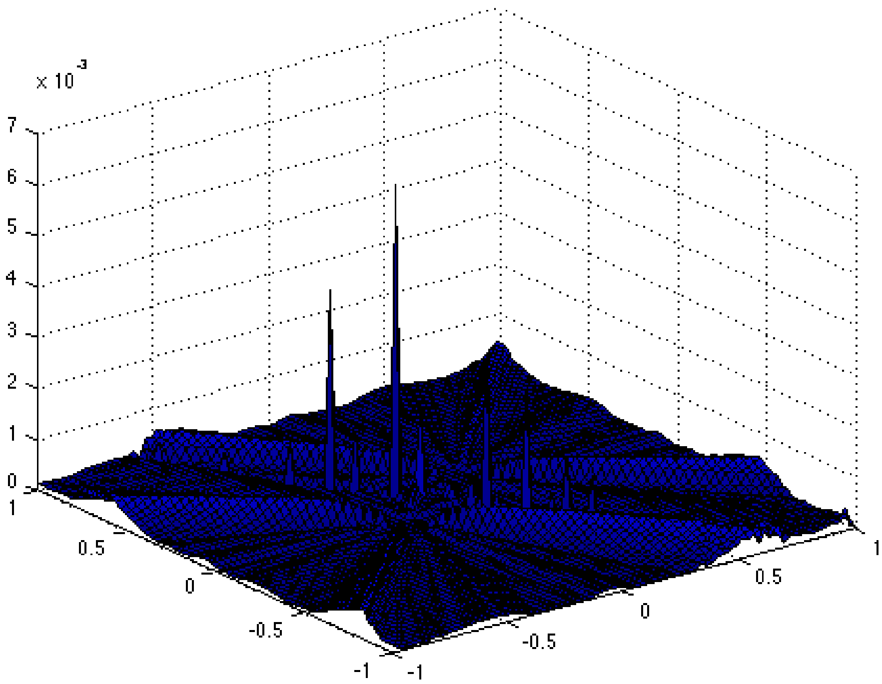

Figure 13: surface plot of the error. N=80

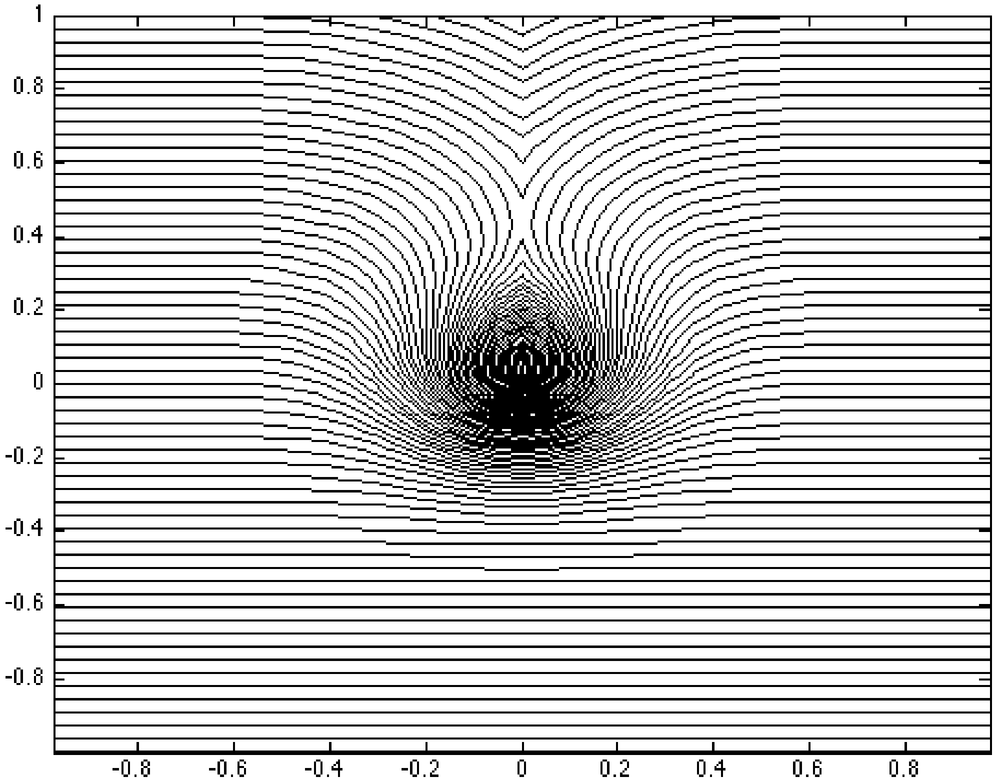

Figure 14: Heterogenous test case : contour lines

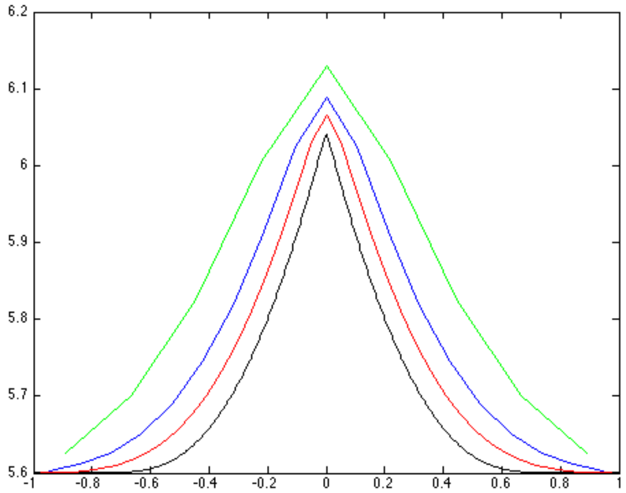

Figure 15: Heterogenous test case : first order scheme - N=10 (green), 20 (blue), 40 (red) - Black : exact solution (first order N=500)

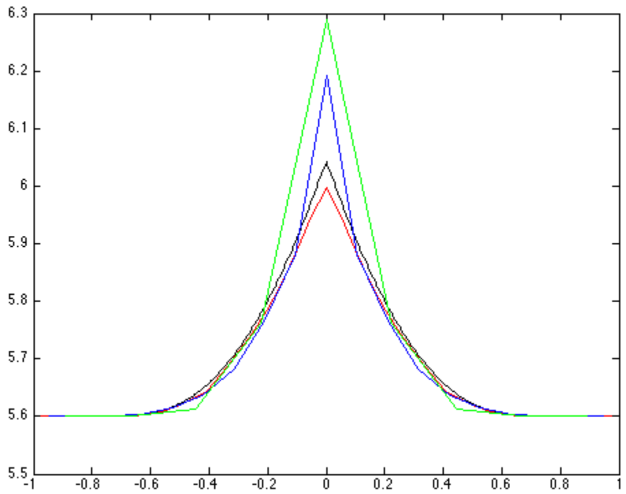

Figure 16: Heterogenous test case : second order scheme - N=10 (green), 20 (blue), 40 (red) - Black : exact solution (first order N=500)

7 Extension of the second order scheme to the Transport equation

The transport equation that comes with the Eikonal equation as part of the high frequency wave asymptotic model is usually written as

$$2\,\nabla\xi\cdot\nabla\phi+\xi\,\Delta\phi=0 \tag{43}$$

It is usually rewritten in conservation form

$$\nabla\cdot(\xi^2\,\nabla\phi)=0$$

and solved in Lagrangian terms : assuming initial conditions for the rays are prescribed on a curve Γ one can obtain

$$\frac{J(t,y_0)\,\xi^2(Y(t,y_0))}{n^2(Y(t,y_0)}=\frac{J(0,y_0)\,\xi^2(Y(0,y_0))}{n^2(Y(0,y_0)},\ \ \forall t \tag{44}$$

as long as $\frac{\partial Y}{\partial y_0}$ does not vanish, $Y(.,y_0)$ is the ray shot from $\Gamma(y_0)$ and $J=det(\frac{\partial Y}{\partial(t,y_0)})$ is the volume variation of the ray field around this ray. It is therefore necessary to compute J to solve (43). $\frac{\partial Y}{\partial t}=\nabla\phi(Y)$ is already a computed quantity, we also need $\frac{\partial Y}{\partial y_0}$. A simple Eulerian strategy strategy is to define a "label" variable ξ_0 such that $\xi_0(Y(.,y_0))=y_0$. Then, a_0 satisfies the even simplest transport equation

$$\nabla\xi_0\cdot\nabla\phi=0 \tag{45}$$

and $\nabla\xi_0(Y(.,y_0))=(\frac{\partial Y}{\partial y_0})^{-1}$.

As outlined by the above discussion, second order accuracy is pretty important both for ϕ as we use the gradient as advecting vector and also because the quantity we are generally interested in is the gradient of ξ_0. In this section we explain how to adapt the second order scheme of section 5 to solve (45). Extension to a non homogeneous right hand side is straightforward and arises in travel time based tomography [8].

The main idea is still the projection on the coordinate system made of the Lagrangian direction $\nabla\phi$ and its orthogonal $\nabla\phi^\perp$. We will again use the Lagrangian structure of the Eikonal equation but also the following two fundamental properties of the transport equation (45). First it can be rewritten with as new unknown scalar function α as

$$\nabla\xi_0=\alpha\,\nabla\phi^\perp \tag{46}$$

Then assuming second order derivative exists (which is necessary to derive a second order scheme anyway) we can take the gradient of (45) which yields

$$D^2\xi_0\cdot\nabla\phi=-D^2\phi\cdot\nabla\xi_0=-\alpha\,D^2\phi\cdot\nabla\phi^\perp \tag{47}$$

Using again the decomposition

$$\delta X = \frac{1}{n^2(X)}\left((\delta X \cdot \nabla\phi)\,\nabla\phi + (\delta X \cdot \nabla\phi^{\perp})\,\nabla\phi^{\perp}\right)$$

A taylor second order Taylor expansion gives (using (46) (47)

$$\begin{aligned} a_0(X+\delta X) = a_0(X) + \alpha\,(\delta X \cdot \nabla\phi^{\perp}(X)) \quad & -\frac{\alpha}{2\,n^4}(\delta X \cdot \nabla\phi^{\perp})^2 < \nabla\phi^{\perp}, D^2 a_0 \cdot \nabla\phi^{\perp} > \\ & -\frac{\alpha}{2\,n^4}(\delta X \cdot \nabla\phi)^2 (n\,\nabla n \cdot \nabla\phi^{\perp}) \\ & -\frac{\alpha}{n^4}(\delta X \cdot \nabla\phi^{\perp})(\delta X \cdot \nabla\phi) < \nabla\phi^{\perp}, D^2\phi \cdot \nabla\phi^{\perp} > \\ & + O(\delta X^3) \end{aligned} \tag{48}$$

In the above equation, the phase gradient $\nabla\phi = (a, b)$ ($\nabla\phi^{\perp} = (-b, a)$) is already given as well as $C =< \nabla\phi^{\perp}, D^2\phi \cdot \nabla\phi^{\perp} >$ the curvature term. They are in principle second order accurate computed quantity of the second order scheme. So the two unknown of our approximation are α and $D =< \nabla\phi^{\perp}, D^2 a_0 \cdot \nabla\phi^{\perp} >$. Let us write (48) on the same four point stencil $(\{0,0\}, \{-h,0\}, \{0,-h\}, \{-h,-h\})$, we revert to the simpler ξ notation instead of ξ_0

$$\begin{cases} \xi_{-h,0} = \xi_{0,0} + \alpha\,h\,b - \alpha\,\frac{h^2}{n^4}\,(\frac{b^2}{2}\,D + \frac{a^2}{2}\,n\,(n_y\,a - n_x\,b) - \,a\,b\,C) + O(h^3) \\ \xi_{0,-h} = \xi_{0,0} - \alpha\,h\,a - \alpha\,\frac{h^2}{n^4}\,(\frac{a^2}{2}\,D + \frac{b^2}{2}\,n\,(n_y\,a - n_x\,b) + \,a\,b\,C) + O(h^3) \\ \xi_{-h,-h} = \xi_{0,0} - \alpha\,h\,(a-b) - \alpha\,\frac{h^2}{n^4}\,(\frac{(a-b)^2}{2}\,D + \frac{(a+b)^2}{2}\,n\,(n_y\,a - n_x\,b) + \,(a^2 - b^2)\,C) + O(h^3) \end{cases} \tag{49}$$

Following the upwind relaxation strategy used for the Eikonal equation and after truncating the third order error, the above system must be solved for $(\xi_{0,0}, \alpha, D)$ with $(\xi_{0,-h}, \xi_{-h,0}, \xi_{-h,-h})$ given along with all the "phase" quantities (a, b, C). Looks doable to me ...

Acknowledgments : Many thanks to Jianlian Qian, Hong-Kai Zhao, Songtin Luo and Bill Symes for fruitful and helpful discussions. Part of this work was done while visiting Rice university and UC Irvine.

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ISSN 0249-6399