Paraxial Eikonal Equations and Applications

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Agenda

Basics: rays, traveltimes, eikonal,...

The Paraxial Eikonal: how to specify data

Numerical Aspects: high order schemes, adpative gridding

Extension 1 - beyond isotropy: quasi-P arrival times in elasticity

Extension 2 - beyond paraxial: full traveltime field by post-sweeping

Extension 3 - beyond viscosity: multiple arrivals by slowness matching

Basics

(i) $\Omega \subset \mathbf{R}^n$ open, bounded

(ii) *velocity* $v \in C^K(\Omega)$, $K \geq 3$, $0 < v_{\min} \leq v(\mathbf{x}) \leq v_{\max}$ for all $\mathbf{x} \in \Omega$

(iii) *slowness* $s \equiv v^{-1}$.

(iv) *Rays* $\mathbf{x}(t)$ from *source point* $\mathbf{x}_s \in \Omega$: first component of solutions of *Hamilton's equations*

$$\frac{d\mathbf{x}}{dt} = \frac{\partial H}{\partial \mathbf{p}}, \;\; \frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{x}} \qquad (1)$$

where $H(\mathbf{x},\mathbf{p}) = \frac{1}{2}v^2(\mathbf{x})|\mathbf{p}|^2$ is the *Hamiltonian*.

Constraints on initial conditions of rays from $\mathbf{x}_s$:

$$\mathbf{x}(0) = \mathbf{x}_s,$$

$$\|\mathbf{p}(0)\| = s(\mathbf{x}_s)$$

$\Rightarrow$ rays from $\mathbf{x}_s$ parametrized by *takeoff direction* $v(\mathbf{x}_s)\mathbf{p}(0) \in S^{n-1}$.

(v) $t \geq 0$ is a *traveltime* from $\mathbf{x}_s$ to $\mathbf{x}$ iff $\mathbf{x} = \mathbf{x}(t)$ for some ray $\mathbf{x}$ from $\mathbf{x}_s$.

(vi) Traveltimes generally not unique - *but* each $\mathbf{x}_s$ there is an open nbhd $\Omega(\mathbf{x}_s)$ of $\mathbf{x}_s$ so that a unique ray from $\mathbf{x}_s$ to $\mathbf{x}$ exists, lying entirely within $\Omega(\mathbf{x}_s)$, for each $\mathbf{x} \in \Omega(\mathbf{x}_s)$ (eg. Lemma 10.2, Milnor 1973).

(vii) $\Rightarrow$ traveltime is well-defined function τ of x $\in \Omega(\mathbf{x}_s)$, via $\tau(\mathbf{x}(t), \mathbf{x}_s) = t$

also $\mathbf{p(t)} = \nabla_{\mathbf{x}} \tau(\mathbf{x}, \mathbf{x}_s)$, whence τ satisfies the *eikonal equation*

$$|\nabla_{\mathbf{x}} \tau(\mathbf{x_s}, \mathbf{x})| = \frac{1}{v(\mathbf{x})}. \tag{2}$$

with the *point source initial condition*

$$\lim_{\mathbf{x} \to \mathbf{x}_s} \frac{\tau(\mathbf{x}, \mathbf{x}_s)}{\|\mathbf{x} - \mathbf{x}_s\|} = s(\mathbf{x}_s),\ \tau \geq 0. \tag{3}$$

(eg. Courant & Hilbert, 1962).

Paraxial Traveltimes

Point source problem for eikonal appears to be BVP. In some applications a *distinguished direction of propagation* exists - interested energy/information propagating in this direction, which should solve IVP.

Examples:

- reflection seismology (Gray & May 1994, WWS) - cf. Lambaré talk

- axisymmetric models of laser/plasma interation (Benamou et al., Solliec thesis 2002)

The 2D case: write $\mathbf{x} = (x, z), \mathbf{p} = (p, q)$ and $\mathbf{x}_s = (x_s, z_s)$, distinguished direction $= z$.

Interested in rays oriented in z direction. Along such rays, $\partial\tau/\partial z > 0$, so solve (2) for z-derv.:

$$\frac{\partial \tau}{\partial z} = \sqrt{s^2 - \left(\frac{\partial \tau}{\partial x}\right)^2}$$

and treat as evolution equation in z.

Big Trouble: This problem is not well-posed - RHS not even well-defined for arbitrary smooth τ. Also - what initial data?

Q: can one transform the stationary eikonal (2) into a well-posed evolution problem in the distinguished direction?

A: Yes! Features of *paraxial eikonal*:

- produces paraxial traveltime = actual traveltime at well-defined and computable subset of Ω, viscosity solution beyond Ω
- use standard ENO/WENO technology (also in applied lit: many interesting ad-hoc schemes)
- *post-sweeping* modification gives solution of original point-source problem, optimal complexity ($O(N)$)
- extensions to other GO quantities (eg. amplitudes), anisotropic elasticity, non-viscosity solutions

Seek H-J problem for traveltime along rays oriented in the positive z direction, making an angle $\leq \theta_{\text{max}} < \frac{\pi}{2}$ with vertical:

$$\frac{\partial \tau}{\partial z} \;\geq\; s \cos \theta_{\text{max}} > 0, \tag{4}$$

Claim: such times solve *paraxial eikonal* (Gray & May, 1994):

$$\frac{\partial \tau}{\partial z} = H\left(\frac{\partial \tau}{\partial x}\right) \;=\; \sqrt{\phi\left(s^2 - \left(\frac{\partial \tau}{\partial x}\right)^2, s^2 \cos^2 \theta_{\text{max}}\right)}, \tag{5}$$

where ϕ suff. smooth, > 0, and

$$\phi(x, a) = x, \; x \geq a$$

Example: quintic spline $\phi \in C^3$ for $a > 0$:

$$\phi(x,a) = \begin{cases} \frac{1}{2}a & \text{if } x < 0, \\ \frac{1}{2}a + 2\frac{x^4}{a^3}(1 - \frac{4}{5}\frac{x}{a}) & \text{if } 0 \le x < \frac{a}{2}, \\ x + 2\frac{(x-a)^4}{a^3}(1 + \frac{4}{5}\frac{x-a}{a}) & \text{if } \frac{a}{2} \le x < a, \\ x & \text{if } x \ge a, \end{cases}$$

(use with difference schemes of up to 3rd order accuracy)

Theorem: There exist $\delta > 0$, $z_p > z_s + \delta$, and smooth $\tau_0^p(x, x_s, z_s)$ so that the smooth solution $\tau^p(x, z, x_s, z_s)$ of (5) with initial data $\tau^p(x, z_s + \delta, x_s, z_s) = \tau_0^p(x, x_s, z_s)$ in

$$\Omega^p(x_s, z_s) = \Omega(x_s, z_s) \bigcap \{(x, z) : z_s + \delta \leq z \leq z_p\}$$

satisfies:

(i) Suppose that unique ray from (x_s, z_s) to $(x, z) \in \Omega^p(x_s, z_s)$ makes an angle $\leq \theta_{\text{max}} < \frac{\pi}{2}$ with the vertical *at every point*. Then $\tau(x, z, x_s, z_s) = \tau^p(x, z, x_s, z_s)$.

(ii) $(x, z) \in \Omega^p(x_s, z_s)$, characteristic = *paraxial ray* for (5) with initial cond. $\tau_0^p(x, x_s, z_s)$ through (x, z) makes an angle $\leq \theta_{\text{max}}$ with vertical throughout $\Rightarrow$ it is a ray from x_s, z_s to x, z.

Proof: Step 1, construction of initial data

Parametrize rays satisfying (4) by z rather than t, also *takeoff angle* θ_0 ($p_s = s(x_s, z_s)\sin\theta_0$ etc.). Then hor. coord. $x(z, \theta_0)$, angle w. vertical $\theta(x, \theta_0)$ satisfy

$$\frac{dx}{dz} = \tan\theta \tag{6}$$

$$\frac{d\theta}{dz} = \frac{1}{s}\left(\frac{\partial s}{\partial z} - \frac{\partial s}{\partial x}\sin\theta\right) \tag{7}$$

with initial conditions

$$x(z_s, \theta_0) = x_s, \tag{8}$$

$$\theta(z_s, \theta_0) = \theta_0 \tag{9}$$

To understand behaviour at $z = z_s$, suppose w.l.o.g. $x_s = 0, z_s = 0$ and examine *scaled trajectory*

$$x_\delta(z,\theta_0) = \frac{1}{\delta}x(\delta z,\theta_0),\ \theta_\delta(z,\theta_0) = \theta(\delta z,\theta_0)$$

Calculation: scaled trajectory satisfies (7) w. $s(x,z)$ replaced by scaled slowness $s_\delta(x,z) = s(\delta x,\delta z)$, same initial conditions.

As $\delta \to 0$, $s_\delta \to s(0,0)$ in C^k, any $k \leq K$, sim. for RHS of (7). So scaled trajectory converges to const. slowness trajectory

$$x_c(z,\theta_0) = z\tan\theta_0,\ \theta_c(z,\theta_0) = \theta_0$$

uniformly in compact sets of parameters.

Note that $x_c(1, \theta_0)$ is monotone as a function of θ_0. Define

$$\theta^1_{\mathsf{max}} = \frac{\pi}{4} + \frac{\theta_{\mathsf{max}}}{2}$$

For sufficiently small δ, $x_\delta(1, \theta_0)$ is monotone in $\theta_0 \in [-\theta^1_{\mathsf{max}}, \theta^1_{\mathsf{max}}]$. Fix such δ, and set

$$\begin{aligned}
x_- &= \delta x_\delta(1, -\theta_{\mathsf{max}}) \\
x_+ &= \delta x_\delta(1, \theta_{\mathsf{max}}) \\
x^1_- &= \delta x_\delta(1, -\theta^1_{\mathsf{max}}) \\
x^1_+ &= \delta x_\delta(1, \theta^1_{\mathsf{max}})
\end{aligned}$$

It follows that

$$\theta_0 \mapsto x(\delta, \theta_0) \text{ is monotone on } [-\theta^1_{\mathsf{max}}, \theta^1_{\mathsf{max}}] \tag{10}$$

Reintroduce general x_s, z_s

Choose $\psi \in C^\infty(\mathbf{R})$ with (1) $\psi(x) = 1,\ x_- \le x \le x_+$, (2) $\psi(x) = 0,\ x \le x_-^1$ or $x \ge x_+^1$, and (3) $\psi'(x) \le 0, x_+ \le x \le x_+^1$ and $\psi'(x) \ge 0, x_-^1 \le x \le x_-$.

Choose positive $A > \sup_{(x,z)\in\Omega} s(x,z)$ and set

$$\tau_0^p(x, x_s, z_s) = \psi(x, x_s)\tau(x, z_s + \delta, x_s, z_s) + A(1 - \psi(x, x_s))|x - x_s| \tag{11}$$

Check that

$$\left|\frac{\partial \tau_0^p(x, x_s, z_s)}{\partial x}\right| > s(x, z_s + \delta)\sin\theta_{\max} \text{ if } x > x_+ \text{ or } x < x_- \tag{12}$$

Define $\tau^p =$ solution of (5) with initial data τ_0^p on $\{(x,z) : z = z_s + \delta\} \bigcap \Omega(x_s, z_s)$.

For some $z_p > z_s + \delta$, method of characteristics gives smooth solution of IVP (5), (11) in $\Omega^p(x_s, z_s) \equiv \Omega(x_s, z_s) \bigcap \{(x,z) : z_s + \delta \leq z \leq z_p\}$.

Step 2, identification of rays

(i) (x,z) on ray through (x_s, z_s), angle $< \theta_{\text{max}}$ w. vertical $\Rightarrow$ $|\theta_0| \leq \theta_{\text{max}}$, so (10) implies that ray crosses $z = z_s + \delta$ at $x = x_c$ with $x_- < x_c < x_+$ and is also paraxial ray. Data on $z = z_s + \delta$ same as for traveltime field near x_c $\Rightarrow$ meth. of char. gives $\tau^p(x, z, x_s, z_s) = \tau(x, z, x_s, z_s)$.

Proof of (ii) similar. **Q. E. D.**

Remarks

1. Consequence of (ii): since direction of characteristic is computed, can monitor (4) during solution of (5) hence approx. Ω^p.

2. Practical definition of initial data: specify tolerance ϵ, use constant solution locally near source,

$$\tau_0^p(x, x_s, z_s) = \psi(x, x_s)\tau_c(x, z_s + \delta, x_s, z_s) + A(1 - \psi(x, x_s))|x - x_s| \tag{13}$$

where $\tau_c(x, z, x_s, z_s) = s(x_s, z_s)\sqrt{(x - x_s)^2 + (z - z_s)^2}$ and choose δ so that

$$|\tau(x, z_s + \delta, x_s, z_s) - \tau_c(x, z_s + \delta, x_s, z_s)| \le \epsilon, \;\; x_-^1 \le x \le x_+^1 \tag{14}$$

M. of C. $\Rightarrow$ consequent error in $\Omega(x_s, z_s)$ is $O(\epsilon)$.

Numerical Aspects

Issue of scheme order:

- local truncation error in scheme of order p is $O(\delta^{p+1}\max_{|\alpha|=p+1}|\nabla^\alpha \tau|)$
- $\tau \sim s(\mathbf{x}_s)|\mathbf{x}|$ near $\mathbf{x} = \mathbf{x}_s$,
- so $|\nabla^\alpha \tau(\mathbf{x}, \mathbf{x}_s)| = O(|\mathbf{x} - \mathbf{x}_s|^{-|\alpha|+1})$
- Upshot: at distance $O(\delta)$ to source, truncation error is $O(\delta^2)$ independent of scheme order, and error propagates$\Rightarrow$ al-l schemes are effectively first order!

Way out: take results about paraxial eikonal seriously, adapt grid.

- *a priori* estimate for δ based on $\|\log s\|_{C^1}$ - use to determine initial data surface $z = z_s + \delta$, "practical" init. data.

- use standard adaptive heuristics based on pair of schemes, *a posteriori* local error estimation as in production RK codes. Our choice: 2nd/3rd order WENO.

- Nested grids: adjust Δz by factors of two. Use fixed global CFL ratio to det. Δx from Δz.

- Output times on user specified fixed grid *via* interpolation of approp. order - user never sees comp. grid!

Details J.-L. Qian and WWS, *Geophysics* 2002.

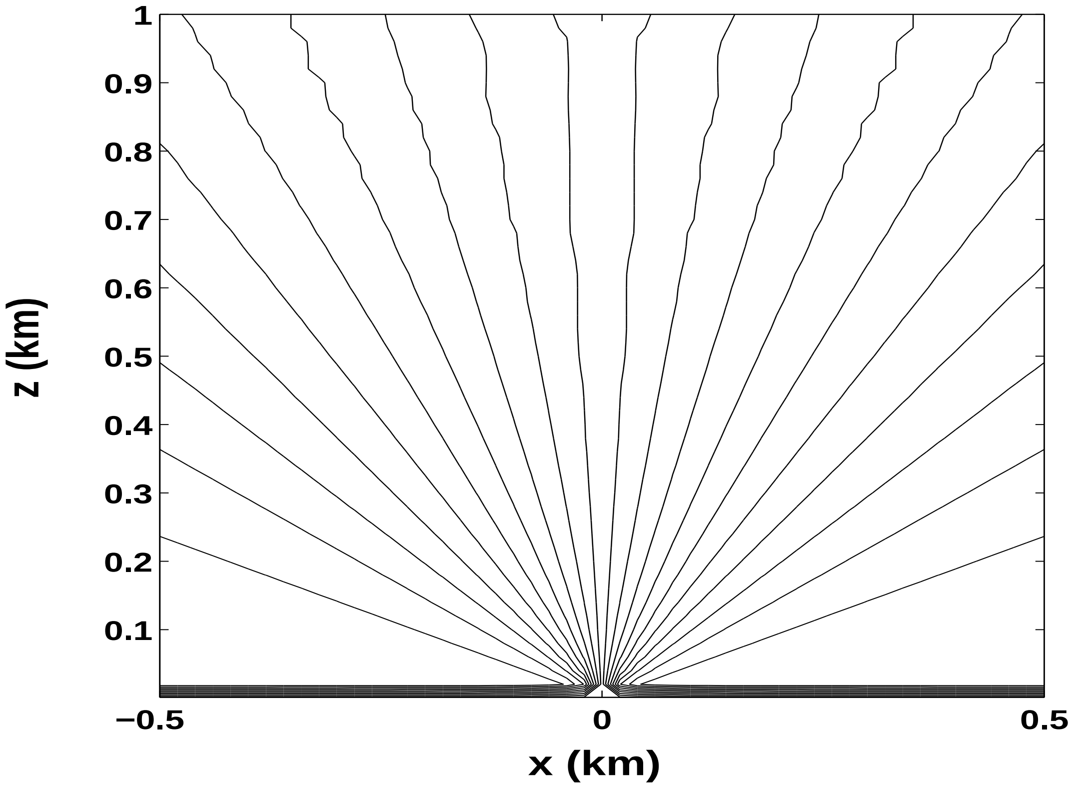
Basic example: $s = $ const, so $\tau = \tau_c$ in unit square, $x_s = 0, z_s = 0$ midpoint of top, treated as IVP for (5).

Fixed grid 3rd order WENO, IC $p_0(x) = A|x|$ on $z = 0$:

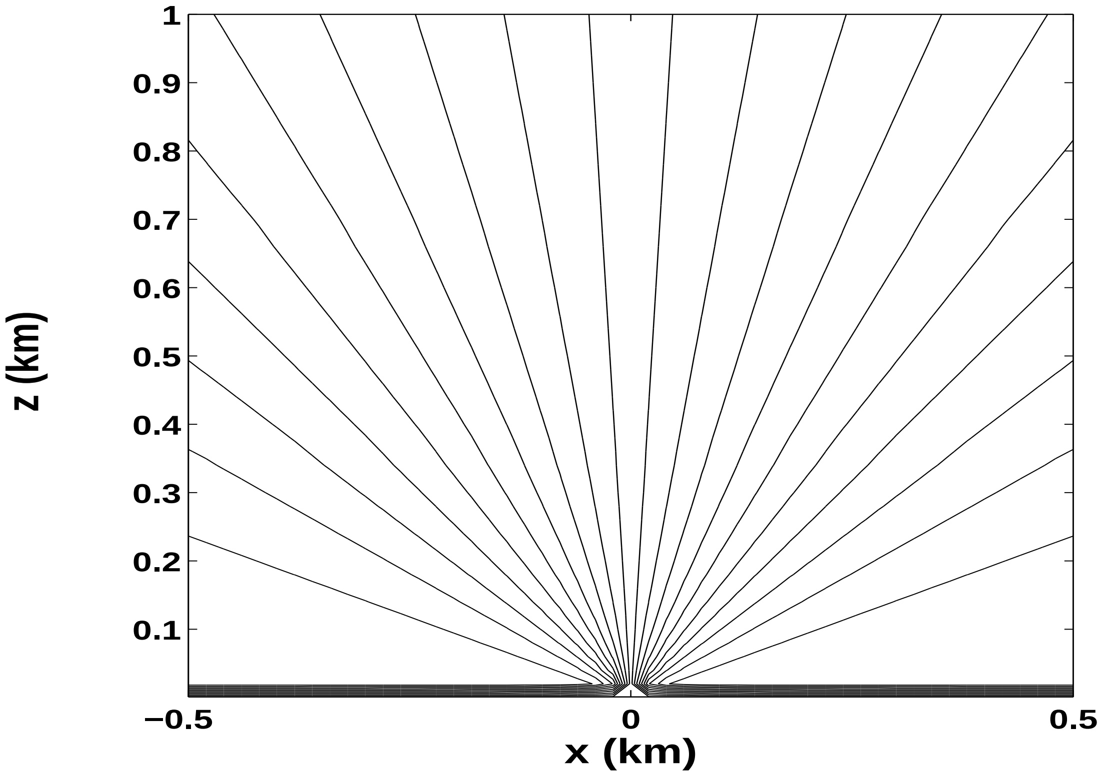
Δx	abserr	flops
1.00×10^{-2}	1.23×10^{-3}	2.6×10^5
1.25×10^{-3}	2.19×10^{-4}	1.7×10^7

Adaptive Grid 2nd/3rd order WENO, paraxial IC (13):

ϵ	abserr	flops
2.5×10^{-5}	1.04×10^{-3}	4.0×10^4
1.7×10^{-6}	1.60×10^{-4}	9.3×10^5



Isocontours, Fixed grid computation of $\partial\tau/\partial x$, $\Delta x = 0.005$.
Note wiggles in contours: they don't go away.



Isocontours, Adaptive grid computation of $\partial\tau/\partial x$,
$\epsilon = 1.0 \times 10^{-5}$ - much cheaper!

Auxiliary quantities needed in geometric optics computations: all computable from *takeoff angle* $\phi(x, z) = \theta_0$, for $x = x(z, \theta_0)$, and its derivatives.

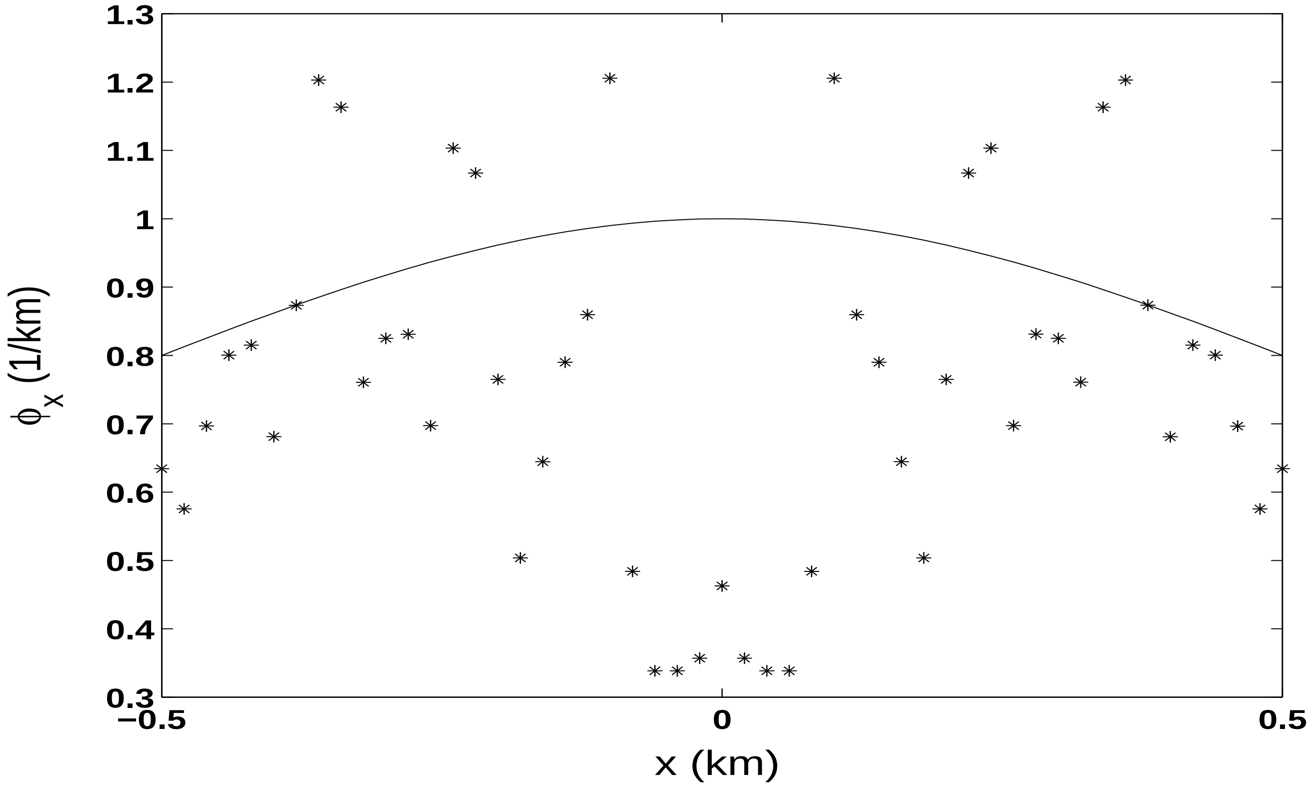
Transport equation for ϕ:

$$\nabla\tau \cdot \nabla\phi = 0$$

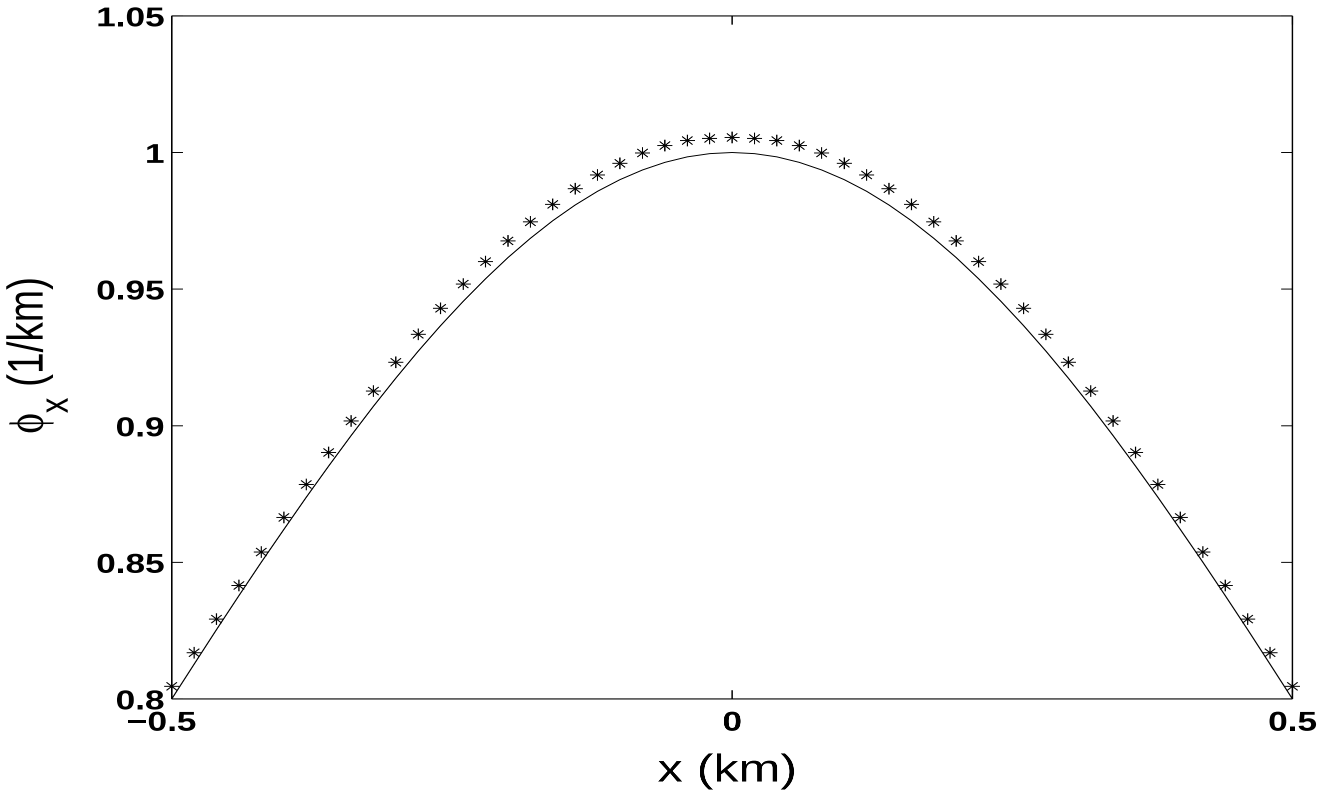
(this is obvious!!!)

Numerics: use WENO 2nd order piggyback scheme, using grid of τ computation. Accuracy is limited by accuracy of computed τ.

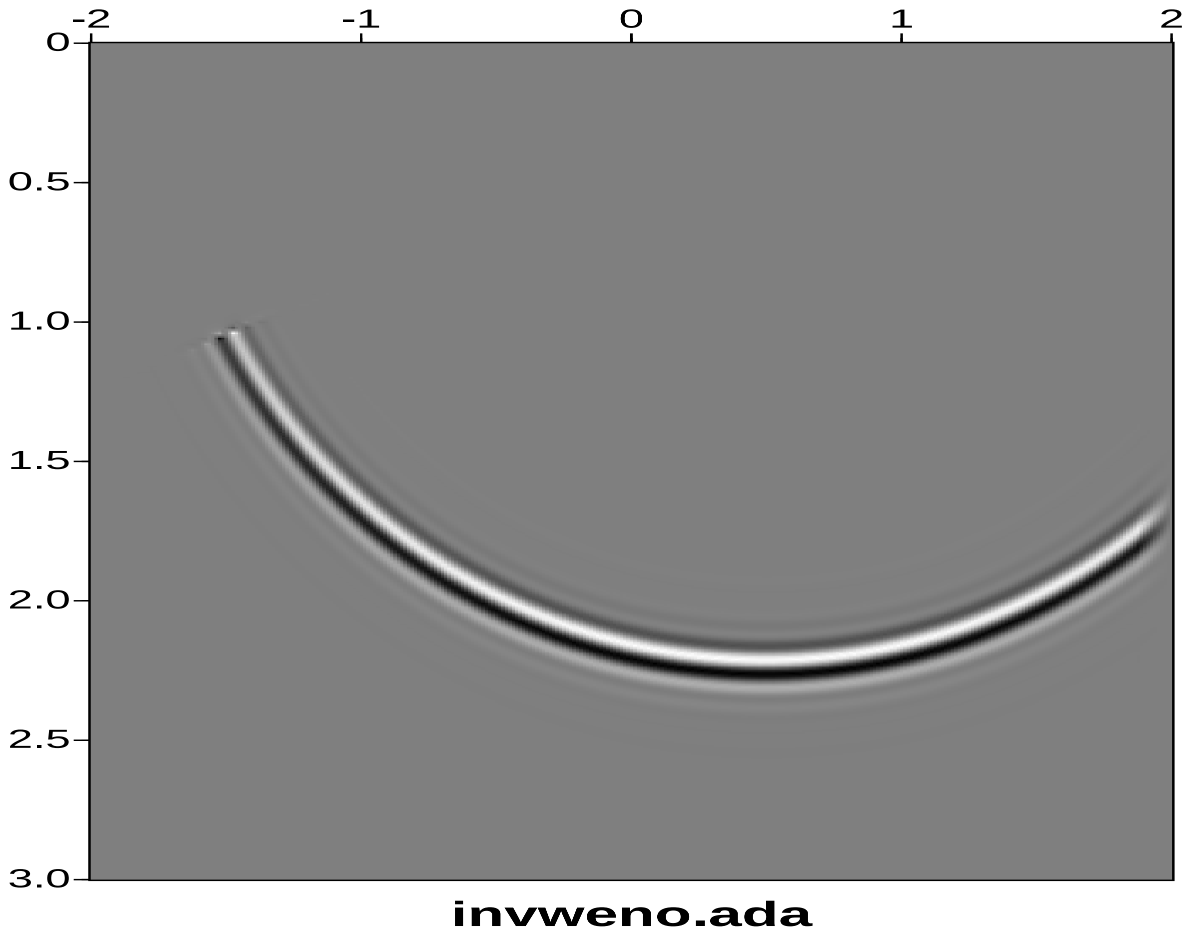
Display: x derivative of ϕ, key quantity in geometric optics amplitude, also *bandlimited impulse response of asymptotic inversion operator*, which uses extensive GO computations.



Solid = exact, stars = computed: Fixed grid computation of takeoff angle x-derivative $\partial\phi/\partial x$, 200×200 grid - not convergent as $\Delta x, \Delta z \to 0$!



Solid = exact, stars = computed: Adaptive grid computation of takeoff angle x-derivative $\partial\phi/\partial x$ - error is $O(\epsilon)$.



Impulse response of asymptotic inversion operator, some time delay.

Extensions

1. Elastic Anisotropy (Qian & S., *Geophysics* 2002)

Paraxial construction applies to any stationary H-J system with convex Hamiltonian. Example: qP Hamiltonian $H(\mathbf{x}, \mathbf{p}) =$ largest eigenvalue of *Christoffel Matrix*

$$\frac{1}{\rho(\mathbf{x})} \sum_{i,l} C_{ijkl}(\mathbf{x}) p_i p_l$$

Largest eigenvalue is simple $\Rightarrow H$ is convex in $\mathbf{p}$. *qP Slowness surface* $= \{\mathbf{p} : \lambda_{\text{max}}(\mathbf{p}) = 1\}$.

Computation of paraxial eikonal, construction of Godunov and ENO/WENO numerical Hamiltonians requires determination of *sonic points* = points where qP slowness surface is tangent to coordinate hyperplanes.

2. Solution of point source problem by "post-sweeping"

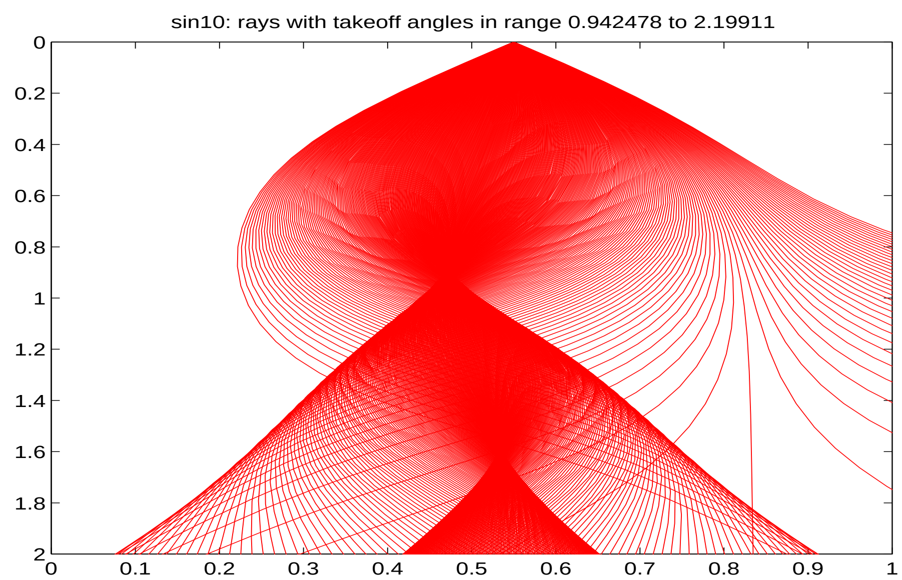
Idea: since paraxial eikonal computes times along ray segments propagating principally in one direction, could pick up times along ray segments propagating in other directions by solving paraxial eikonal in all coord directions successively $(+z, +x, -x, -z)$.

Introduced by Schneider et al, *Geophysics* 1992. Makes essential use of variational characterization of times: at each step, replace computed paraxial time by previously computed time from different direction if latter is smaller.

Kim and Cook, *Geophysics* 1992: 3D. Qian et al, SEG Abstract, 2001: anisotropy. Bounds on number of sweeps.

Upshot: method for point source problem with complexity $O(N)$. Claim (Kim, 2001): "faster than fast marching"!

3. Multivalued traveltimes - non-viscosity solutions



$\mathbf{x}, \mathbf{x}_s$ separated by suff. distance and $v(\mathbf{x})$ suff. heterogeneous $\Rightarrow$ connected by > 1 rays.

Lions, 1982: viscosity solution = selection of least traveltime ("first arrival"). Insufficient For applications to wave propagation! Later arrivals can carry considerably more energy, and therefore can be more important physically.

Lagrangian method, ie. solution of ray equations (1), computes all arrival times. Difficult to control sampling of domain - resolution via dynamic addition/removal of rays as computation proceeds = "wavefront construction method", cf. Lambaré this PM.

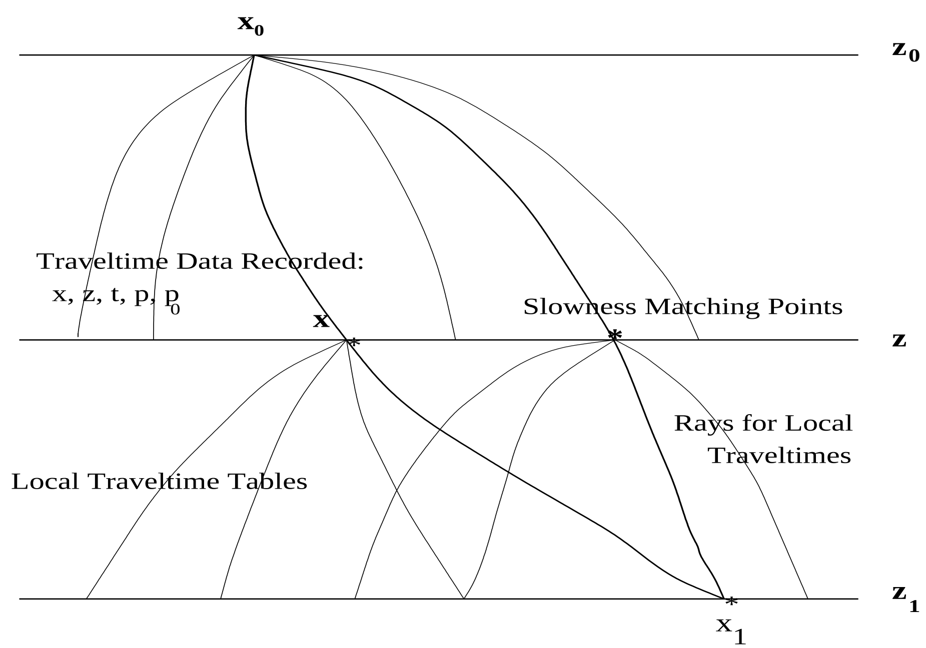
Eulerian methods (since early '90s): Big Rays, explicit caustic construction (Benamou), kinetic methods for multibranch entropy solutions (Brennier-Corrias, Gosse, rel. work by Engquist-Runborg), codim. 2 level set evolution (Osher et al.), dynamic surface extension (Steinhoff), Liouville equations for escape parameters (Sethian-Fomel),...

Slowness matching: Huyghen's principle to find all arrivals.

Paraxial version (WWS, 1996): compute only times along *paraxial rays* that propagate in $+z$ dir, making angle $< \theta_{\text{max}}$ with z axis.

For each z, there is $Z_d(z) > z$ so that times along such rays from (x, z) to $(X, Z_d(z))$ are single-valued.

Idea: any paraxial ray can be broken into segments in depth intervals $\{z_i, Z_d(z_i) = z_{i+1}\}$, and time is sum of times along segments. Each segment time can be computed by local Eulerian solves of paraxial eikonal, and times to be summed identified by matching slownesses $= x$ derivatives of local traveltime fields along surfaces $z = z_i$.



x_0
z_0
Traveltime Data Recorded:
x, z, t, p, p_0
x
Slowness Matching Points
z
Rays for Local
Traveltimes
Local Traveltime Tables
z_1
x_1

Algorithm:

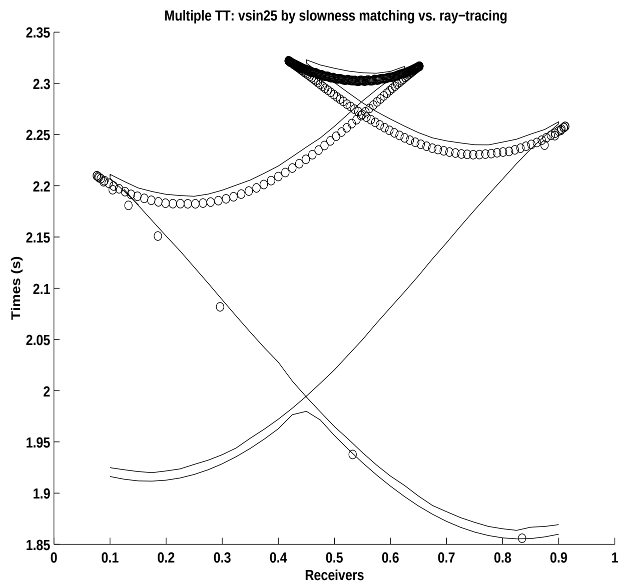
(i) identify (by *a priori* estimate, adaptive method, or guess) usable *layer thickness* $Z_l, Z_d(z) = z + Z_l$, pick Δx for traveltime output. Inizialize $z_0 = z_s$, use adaptive 2nd/3rd order WENO scheme to compute paraxial traveltimes for each $x_m = x_0 + m\Delta x$.

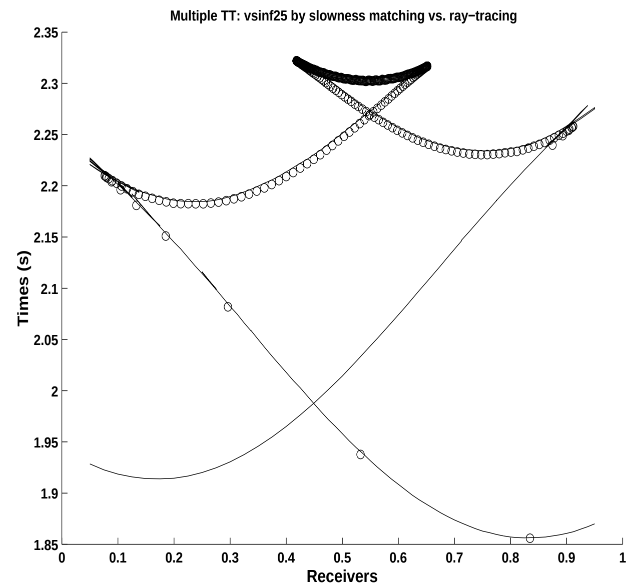
(ii) for $n = 1, ...$: compute paraxial times for sources on $z = z_i$, estimate takeoff slowness by divided difference in x, use linear interpolation to identify matches to arrival slowness from $z = z_{i-1}$ already recorded in data structure, append matches included incremented traveltimes.

Accuracy of adaptive parax. solver $\Rightarrow$ 2nd ord. accuracy of lin. interpolation preserved in computed times.

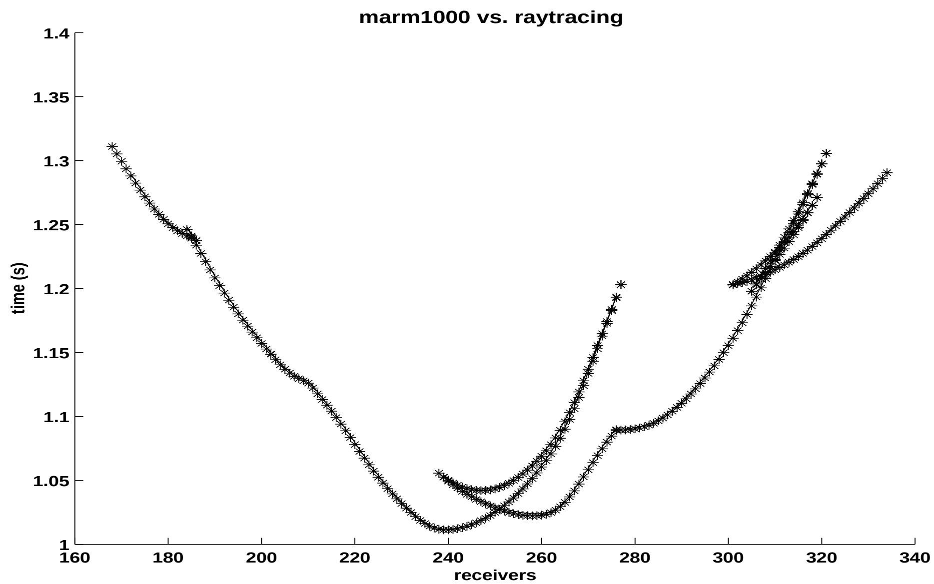
Re-use of local traveltimes $\Rightarrow$ economical when times are needed for dense grid of source points on $z = z_s$.

Details: Qian & WWS, J. Sci. Comp, in press.





Left: ray trace times (circles) vs. viscosity solution (lower curve) vs. slowness match solution with $\Delta x = 0.05$.
Right: ray trace times (circles) vs. slowness match solution with $\Delta x = 0.025$. Note apparent 2nd order convergence.



Slowness match times (solid) vs. raytrace times (stars, thanks L. Klimes) for Marmousi test set (see Benamou's traveltimes site).

Conclusions

- Paraxial eikonal permits accurate computation of traveltimes and related GO quantities at computable point set, provided initial condition, numerical issues properly addressed

- Post-sweeping extension removes paraxial limitation

- Anisotropic qP wave times also computable paraxially

- Slowness matching for multiple traveltimes - one of many Eulerian approaches for non-viscosity solutions.