The Phase Flow Method

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Agenda

- The phase flow method
- Applications in computational high frequency wave propagation
  - Wave front propagation
  - Amplitude computations
  - Multiple arrival times computations
- Numerical results
- Epilogue

Problem Statement

- Nonlinear autonomous ODE

$$\frac{\mathrm{d}y}{\mathrm{d}t} = F(y), \quad t > 0,$$

where $y : \mathbf{R} \longrightarrow \mathbf{R}^d$ and $F : \mathbf{R}^d \longrightarrow \mathbf{R}^d$ is smooth.

- Compute $y(T) = y(T, y_0)$ for many initial conditions y_0.
- Standard approach: time step τ and local integration rule for each y_0.
- Not very efficient.

Terminology

- *Phase map*: $g_t : \mathbf{R}^d \longrightarrow \mathbf{R}^d$ defined by $g_t(y_0) = y(t, y_0)$.
- *Phase flow*: collection of all phase maps $\{g_t, t \in \mathbf{R}\}$.
- A manifold $M \subset \mathbf{R}^d$ is *invariant* if $g_t(M) \subset M$.

Example: Bicharacteristic Flow

Ray equations in phase space $\mathbf{R}^d \times \mathbf{R}^d$, $d = 2, 3$

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \nabla_p H(x,p), \quad \frac{\mathrm{d}p}{\mathrm{d}t} = -\nabla_x H(x,p),$$

with Hamiltonian $H(x,p)$

$$H(x,p) = c(x)|p|,$$

- Autonomous
- Wish to integrate for each $y_0 = (x_0, p_0) \in \Sigma_0$ (initial wave front)
- Invariant manifold M:
  - $\mathbf{R}^d \times \mathbf{R}^d$
  - $\mathbf{R}^d \times S^{d-1}$
  - $[0,1]^3 \times S^{d-1}$

Key Structure

Rapid construction of the complete phase map g_T at time T.

1. Discretization. Start with a uniform or quasi-uniform grid M_h on M.
2. Initialization. Fix a small time step τ and compute an approximation of g_τ.
   - For each $y_0 \in M_h$, $g_\tau(y_0)$ is computed by a standard ODE integration rule
   - The value of g_τ at any other point is defined via local interpolation.
3. Loop. Construct $g_{2^k\tau}$ from $g_{2^{k-1}\tau}$
   - For each $y_0 \in M_h$, $g_\tau(y_0)$

     $$g_{2^k\tau}(y_0) = g_{2^{k-1}\tau}(g_{2^{k-1}\tau}(y_0))$$

   - Otherwise, local interpolation.

Key point: Systematic use of already computed information

Peek at the results

- Very efficient
- Surprisingly accurate

Algorithm 1 (Basic Version)

- Parameter selection. Select a grid size $h > 0$, a time step $\tau > 0$, and an integer constant $S \geq 1$ such that $B = (T/\tau)^{1/S}$ is an integer power of 2.
- Discretization. Select a uniform or quasi-uniform grid $M_h \subset M$ of size h.
- Burn-in. Compute $\tilde{g}_\tau$.
  - For a gridpoint y_0, $\tilde{g}_\tau(y_0)$ is calculated by applying the ODE integrator.
  - Construct an interpolant and compute $\tilde{g}_\tau(y_0)$ by evaluating the interpolant outside of the grid.
- Loop. For $k = 1, \ldots, S$, evaluate $\tilde{g}_{B^k\tau}$.
  - $\tilde{g}_{B^k\tau}(y_0) = (\tilde{g}_{B^{k-1}\tau})^{(B)}(y_0)$ for each y_0 on the grid.
  - Construct an interpolant which and use it for out-of-grid evaluation.
- Terminate. When $k = S$, we hold $\tilde{g}_t$, for $t = \tau, 2\tau, 4\tau, 8\tau, \ldots, T$ and more.

Main Result

- ODE integrator is of order α.
- Local interpolation scheme is of order $\beta \geq 2$.
- Size of grid is $O(h^{-d_M})$

Approximation error at time t

$$\varepsilon_t = \max_{b \in M} |g_t(b) - \tilde{g}_t(b)|.$$

(i) The approximation error obeys

$$\varepsilon_T \leq C \cdot (\tau^\alpha + h^\beta)$$

(ii) The complexity is $O(\tau^{-1/S} \cdot h^{-d_M})$.

(iii) For each $y \in M$, $\tilde{g}_T(y)$ can be computed in $O(1)$ operations.

(iv) For any intermediate time $t = m\tau \leq T$ and $y \in M$, $\tilde{g}_t(y)$ is evaluated in $O(\log(1/\tau))$ operations.

Asymptopia

Balancing of errors $h^\beta \sim \tau^\alpha$

- Accuracy $O(\tau^\alpha)$
- Complexity $O(\tau^{-r})$, $r = d_M \alpha/\beta + 1/S$.

Suppose that M and F are sufficiently smooth, and choose β and S s.t. $r < 1$.

In an asymptotic sense, one can compute an approximation to the entire phase map g_T much faster than one computes—with the same order of accuracy—a single solution with the standard ODE integration rule.

Variation I: Time-doubling

Select $B = 2$, and construct $g_{2^k\tau}$ from $g_{2^{k-1}\tau}$ via

$$g_{2^k\tau}(y_0) = g_{2^{k-1}\tau}(g_{2^{k-1}\tau}(y_0))$$

- Complexity is lower $O(h^{-d_M}\log(1/\tau))$
- Accuracy is reduced $O((\tau^\alpha + h^\beta)/\tau)$

Variation II: Algorithm 2 (Practical Version)

For large times, g_T may become quite oscillatory, and one would need a very fine initial spatial resolution.

(a) Choose $T_0 = O(1)$, $T = mT_0$, such that g_{T_0} remains non-oscillatory and pick h so that the grid is sufficiently dense to approximate g_{T_0} accurately.

(b) Construct $\tilde{g}_{T_0}$ using Algorithm 1.

(c) For any y_0, define $\tilde{g}_T(y_0)$ by $\tilde{g}_T(y_0) = (\tilde{g}_{T_0})^{(m)}(y_0)$.

Problem specific components

- Discretization of M
- ODE integration rule
- Local interpolation scheme

Geometrical Optics

- Inhomogeneous scalar wave equation in 2D and 3D:

$$u_{tt} - c^2(x)\Delta u = 0, \quad t > 0.$$

- High-frequency expansion (WKB)

$$u(t,x) = e^{i\lambda\Phi(t,x)} \sum_{n\geq 0} A_n(t,x)(i\lambda)^{-n}$$

  where Φ and A_n are smooth.

- Eikonal equations

$$\Phi_t \pm c(x)|\nabla\Phi| = 0.$$

- Bicharacteristics equations:

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}\boldsymbol{t}} = \boldsymbol{c}(\boldsymbol{x})\frac{\boldsymbol{p}}{|\boldsymbol{p}|}, \quad \frac{\mathrm{d}\boldsymbol{p}}{\mathrm{d}\boldsymbol{t}} = -\boldsymbol{\nabla}\boldsymbol{c}(\boldsymbol{x})|\boldsymbol{p}|$$

- Reduced Hamiltonian flow, $\boldsymbol{p} = |\boldsymbol{p}|\boldsymbol{\nu}$

$$\frac{\mathrm{d}\boldsymbol{x}}{\mathrm{d}\boldsymbol{t}} = \boldsymbol{c}(\boldsymbol{x})\boldsymbol{\nu}, \quad \frac{\mathrm{d}\boldsymbol{\nu}}{\mathrm{d}\boldsymbol{t}} = -\boldsymbol{\nabla}\boldsymbol{c}(\boldsymbol{x}) + (\boldsymbol{\nabla}\boldsymbol{c}(\boldsymbol{x}) \cdot \boldsymbol{\nu})\boldsymbol{\nu}$$

  or compactly $\mathrm{d}\boldsymbol{y}/\mathrm{d}\boldsymbol{t} = \boldsymbol{F}(\boldsymbol{y})$.

- Assume $\boldsymbol{c}(\boldsymbol{x})$ is periodic on $[\mathbf{0}, \mathbf{1}]^{\boldsymbol{d}}$ (can be relaxed).

- $\boldsymbol{M} = \{(\boldsymbol{x}, \boldsymbol{\nu}) \in [\mathbf{0}, \mathbf{1}]^{\boldsymbol{d}} \times \boldsymbol{S}^{\boldsymbol{d}-\mathbf{1}}\}$ compact and smooth.

The Phase Flow Method for HFWP (2D)

- $M = [0,1]^2 \times [0, 2\pi]$

$$\frac{\mathrm{d}x}{\mathrm{d}t} = c(x,y)\cos\theta, \quad \frac{\mathrm{d}y}{\mathrm{d}t} = c(x,y)\sin\theta, \quad \frac{\mathrm{d}\theta}{\mathrm{d}t} = c_x \sin\theta - c_y \cos\theta$$

- ODE integrator: 4th order Runge-Kutta
- Cartesian uniform grid on $M = [0,1]^2 \times [0, 2\pi]$
- Local interpolation:
  - Interpolate the periodic shift $g_t(y) - y$ instead of $g_t(y)$.
  - Interpolation of a periodic function on a Cartesian grid.
  - Solution: tensor-product Cardinal B-spline (interpolant is constructed by means of FFT's).

The Phase Flow Method for HFWP (3D)

- $M = [0,1]^3 \times S^2$
- ODE integrator: 4th order Runge-Kutta
- Discretization
  - Uniform Cartesian grid in $x \in [0,1]^3$
  - Spherical coordinates in $\nu \in S^2$

$$\nu(\theta, \phi) = (\cos\theta \sin\phi, \sin\theta \sin\phi, \cos\phi)$$

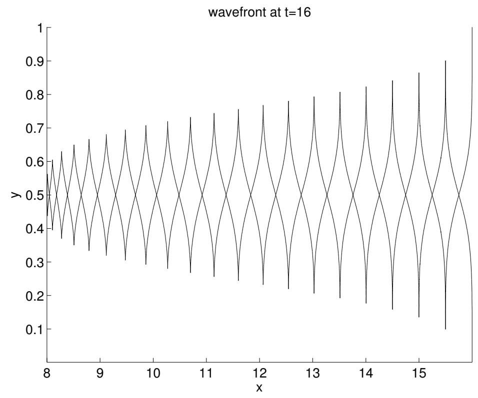
  with sample points $(0, h, \cdots, 2\pi - h) \times (h/2, \cdots, \pi - h/2)$.

- Local interpolation
  - Cardinal B-splines in x.
  - Cardinal B-splines in ν (after periodic extension trick)

$$f^e(\theta, \phi) = \begin{cases} f(\theta, \phi) & \phi \in [0, \pi) \\ f(\theta + \pi, -\phi) & \phi \in [-\pi, 0). \end{cases}$$

  f^e is periodic on $[0, 2\pi] \times [-\pi, \pi]$.

Wave Front Construction



Initial wave front $y_0(r) = (x_0(r), \nu_0(r))$ propogated up to time T. Basic algorithm:

- Choose T_0 and construct $\tilde{g}_{T_0}$.
- Discretize the wave front by sampling $y_0(r)$ at the points r_i.
- For each r_i, approximate $y(T, r_i)$ with $\tilde{y}(T, r_i) = (\tilde{g}_{T_0})^{(m)}(y_0(r_i))$ where $T = mT_0$.
- Connect $\tilde{x}(T, r_i)$ to construct the final wave front.

2D Adaptive Wave Front Construction

Choose a tolerance λ, and sample the initial wave front with $R = \{r_i\}$ s.t.

$$|y_0(r_i) - y_0(r_{i+1})| \leq \lambda$$

For $k = 1, \cdots, T/T_0$

- For any $r_i \in R$, $\tilde{y}(kT_0, r_i) = \tilde{g}_{T_0}(\tilde{y}((k-1)T_0, r_i))$.
- For any interval $I_i := [r_i, r_{i+1}]$ s.t. $|\tilde{y}(kT_0, r_i) - \tilde{y}(kT_0, r_{i+1})| > \lambda$:
  - Insert N_i new samples $\{r_\ell\}$ evenly distributed in I_i;

$$N_i = \lceil |\tilde{y}(kT_0, r_i) - \tilde{y}(kT_0, r_{i+1})| / \lambda \rceil.$$

  - The values $\tilde{y}(kT_0, r_\ell)$ at the new points are computed using

$$\tilde{y}(kT_0, r_\ell) = (\tilde{g}_{T_0})^{(k)}(y_0(r_\ell))$$

Inserting Rays

Standard Lagrange type methods insert new rays by interpolating nearby sampled values.

- Difficult (unstructured grid)
- Low accuracy

Effortless and accurate with the phase flow method.

Refinement condition.

- Standard methods need to use

$$|\tilde{y}(kT_0, r_i) - \tilde{y}(kT_0, r_j)| > \lambda.$$

- Here,

$$|x(kT_0, r_i) - x(kT_0, r_j)| > \lambda$$

  is sufficient since interpolation is not used. Increased efficiency.

Amplitude Computation, I

Squeezing and spreading of rays

$$\frac{A_0(x(t,r))}{A_0(x(0,r))} = \sqrt{\frac{|\partial_r x(0,r)|}{|\partial_r x(t,r)|} \cdot \frac{c(x(t,r))}{c(x(0,r))}} \qquad \text{(2D)}$$

$$\frac{A_0(x(t,r,s))}{A_0(x(0,r,s))} = \sqrt{\frac{|\partial_r x(0,r,s) \times \partial_s x(0,r,s)|}{|\partial_r x(t,r,s) \times \partial_s x(t,r,s)|} \cdot \frac{c(x(t,r,s))}{c(x(0,r,s))}} \qquad \text{(3D)}$$

- Additional information is needed: $\partial_r x(t,r)$ in 2D and $\partial_r x(t,r,s)$ and $\partial_s x(t,r,s)$ in 3D.
- It is sufficient to know $\nabla_b y(t,b)$.
- Approximate the gradient of the phase map along with the phase map.

Amplitude Computation, II

- Linear equation for $\nabla_b y(t,b)$.

$$\frac{\mathrm{d}\nabla_b y(t,b)}{\mathrm{d}t} = \nabla_y F(y(t,b)) \cdot \nabla_b y(t,b), \quad \nabla_b y(0,b) = I.$$

with

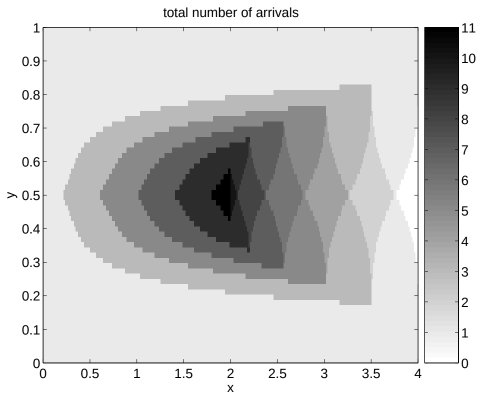
$$\nabla_y F(y) = \begin{pmatrix} \nu \nabla c^T & cI \\ -\nabla^2 c + \nu \nu^T \nabla^2 c & (\nabla c \cdot \nu) I + \nu \nabla c^T \end{pmatrix}$$

- Group property:

$$\nabla_b y(2t,b) = \nabla_b y(t, g_t(b)) \cdot \nabla_b y(t,b).$$

- Build the approximation to $\nabla_b y(t,b)$ along with $g_t(b)$ in Algorithms 1 & 2.

Multiple Arrival Times



- *Source*:
  - 2D: smooth curve in 3D phase space.
  - 3D: smooth surface in 5D phase space.
- *Target*: point in physical space.
- *Trace*: family of wave fronts from time index by $t \in [t_0, t_1]$.
  - 2D: smooth 2D surface in 3D phase space.
  - 3D: smooth 3D manifold in 5D phase space.

Problem: compute the number of arrivals and the arrival times (at the targets) up to time T.

Single Source / Multiple Targets

- Choose a time step ΔT and a tolerance $\lambda > 0$.
- Apply the adaptive wave front algorithm with time step ΔT to construct the final wave front at time T; the algorithm provides the values $\tilde{y}(k\Delta T, r_i)$ for $0 \leq k \leq T/\Delta T$.
- Approximate the trace by linear interpolation of the sampled values $\tilde{y}(k\Delta T, r_i)$—represented by a triangle mesh in phase space. The computed trace is piecewise linear.
- Project the approximate trace $\tilde{y}$ onto physical space (i.e. discard ν).
- For each target point, check whether it is covered by nearby projected triangles. If so, the arrival and arrival time are recorded.

Single Source and Single Target

Adaptive version

- Wasteful to compute the full trace
- Basic idea is to throw away large parts of the trace before construction
- Efficient algorithm

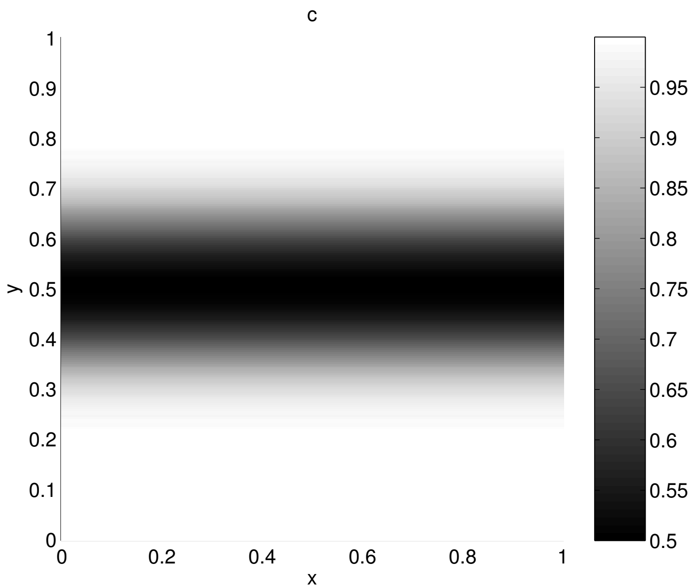
Details

- The nearby triangles can be collected efficiently using a bounding box test.
- Inside/outside test for each triangle is carried out using the determinant test (standard in computational geometry).
- The discretization of the source is not fixed and is refined as the wave front evolves.
- The parameters ΔT and λ control the accuracy.
  - ΔT and λ are of the order of $\sqrt{\varepsilon}$ suffice for an error tolerance of ε for the trace approximation.
  - Accuracy of arrival times is then $O(\varepsilon)$.

Example 1

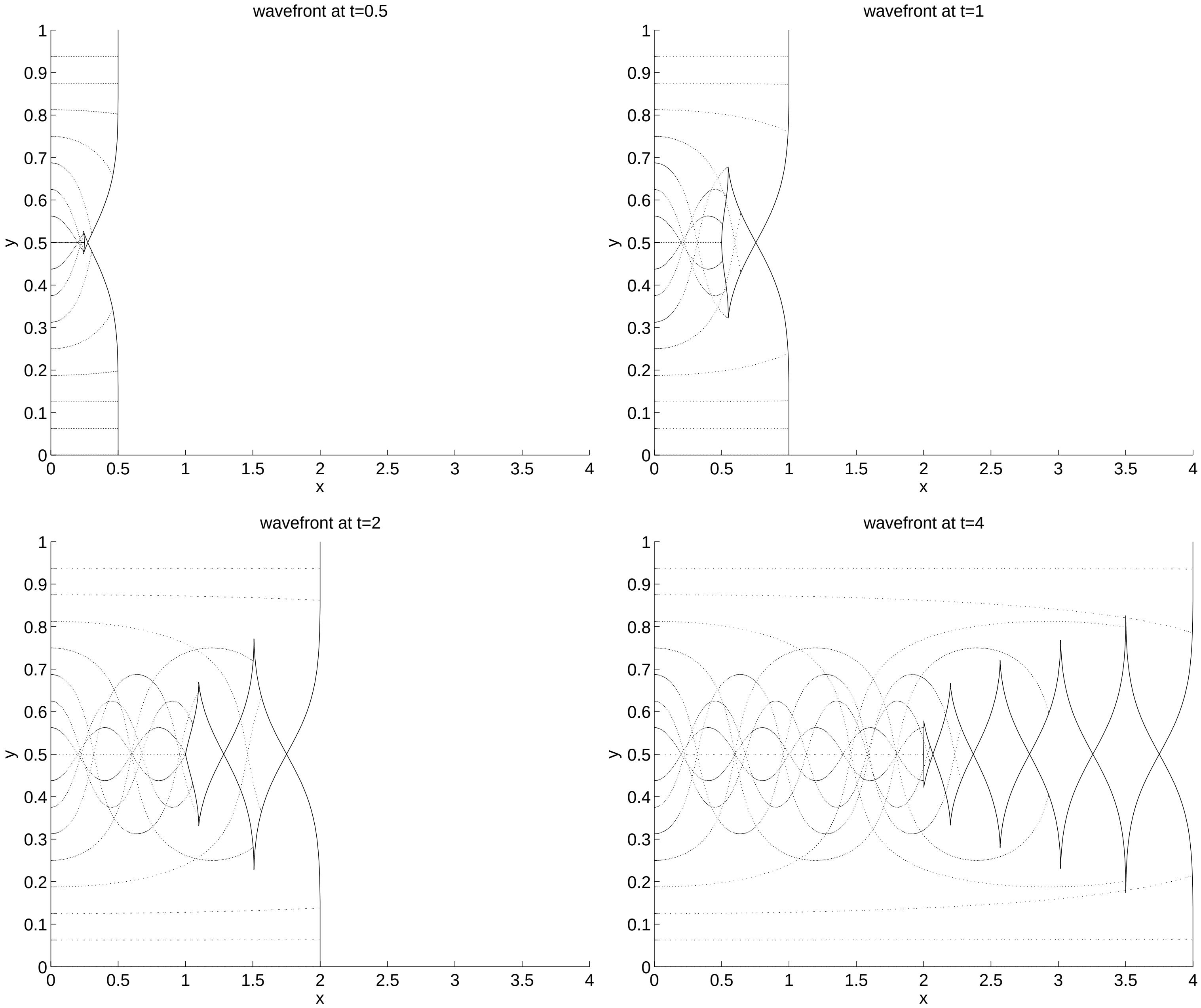
- Velocity field (2D waveguide)

$$c(x, y) = \frac{1}{1 + e^{-64\cdot(y-1/2)^2}}.$$

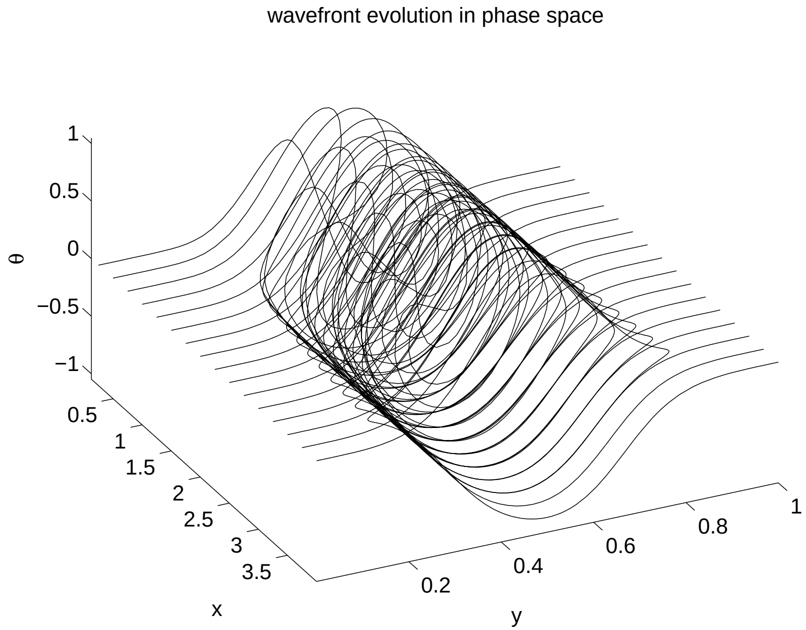


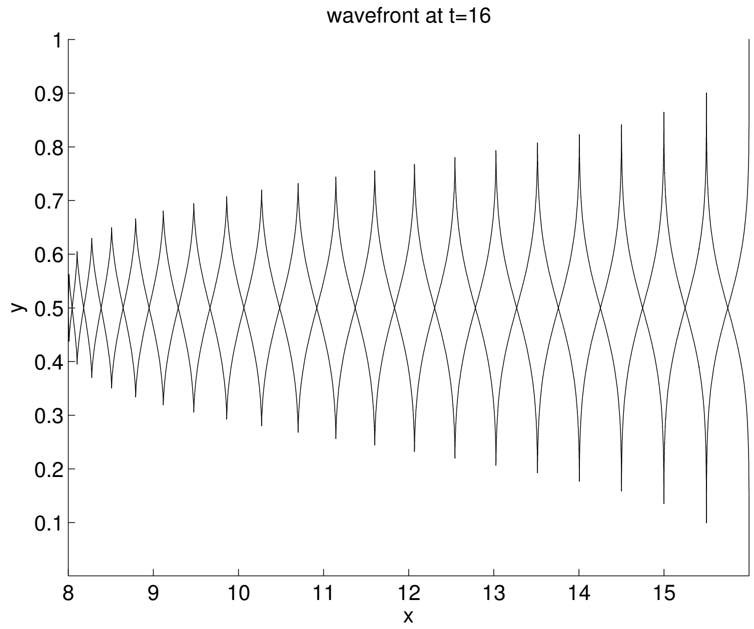
- The initial wave front is a planar wave at $x = 0$.

Example 1: wave front construction



Example 1: wave front construction





MATLAB implementation on a desktop computer with a 2.6GHz CPU and 1GB of memory.

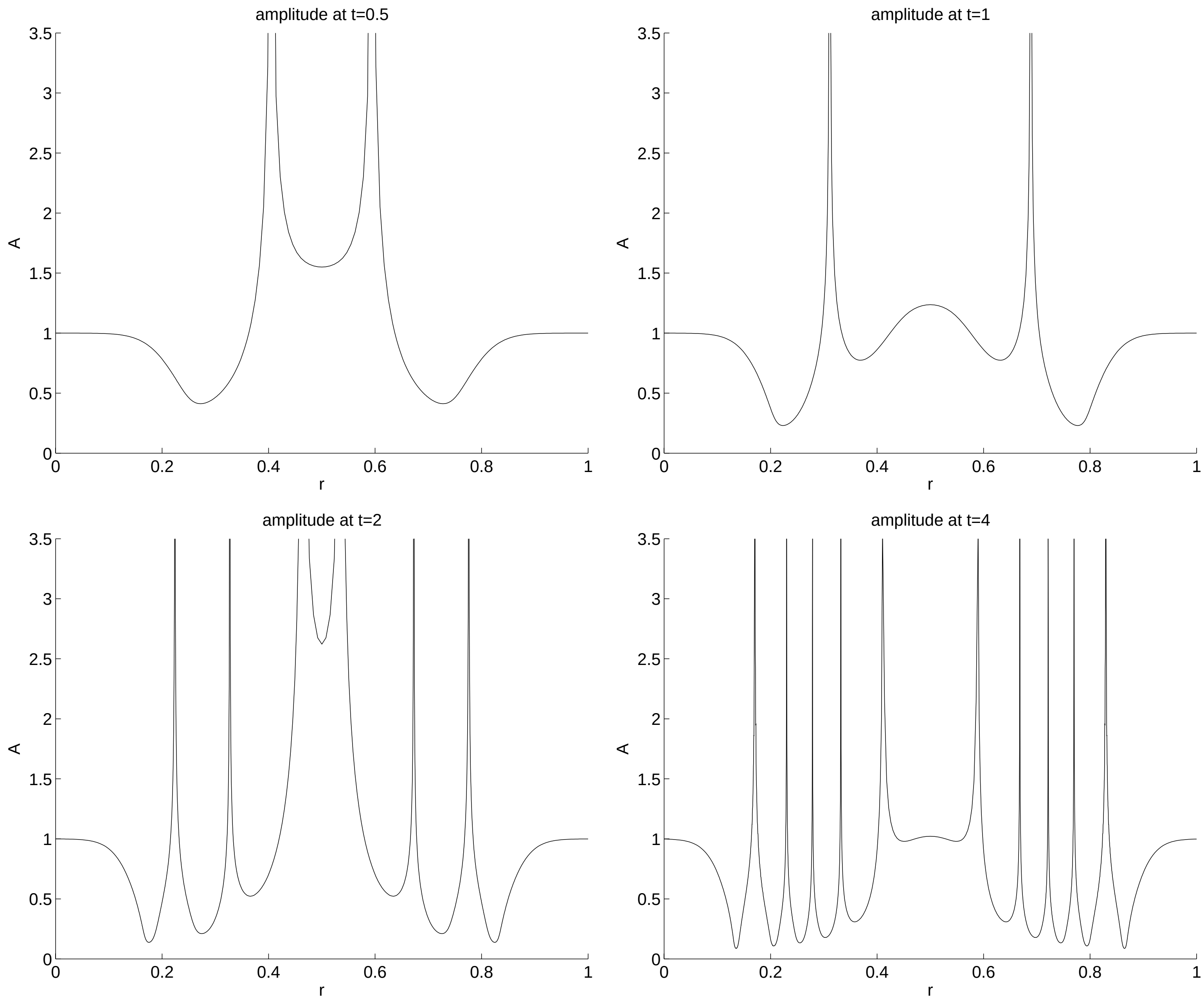
- Uniform grid with 64 points in y and 128 points in θ.
- The construction of $\tilde{g}_{T_0}$ takes about 2 seconds.
- Accuracy of computed phase map is about 10^{-5}.
- Adaptive wave front propagation up to $T = 4$
  - Final wave front has about 600 samples
  - Takes about 0.064 second
  - MATLAB's ODE solver takes about 0.08 second to trace a single ray
  - Speedup factor is about 750

Example 1: accuracy

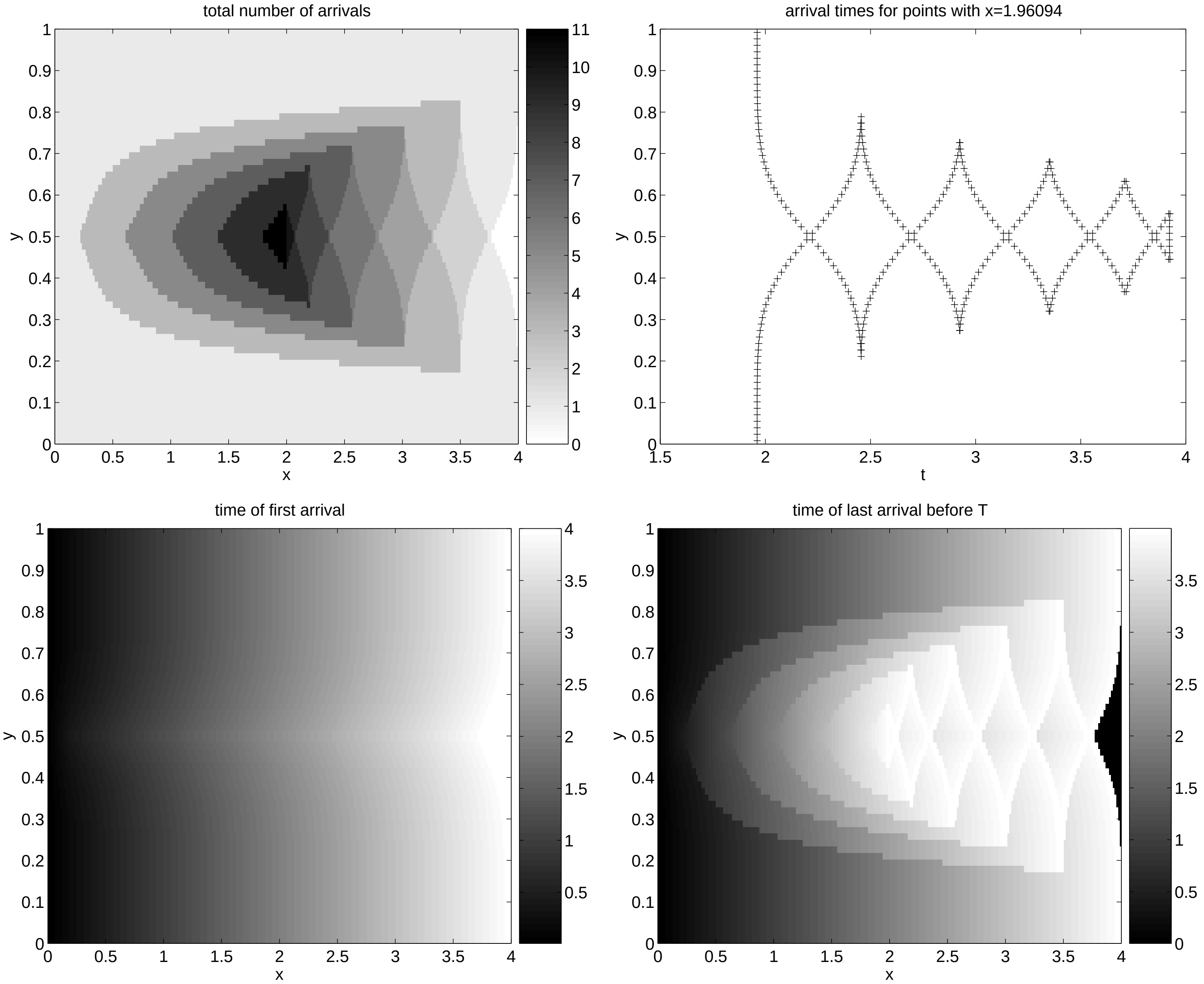
Discretization vs. T_0	0.0625	0.125	0.25	0.5
(16,32)	4.991e-04	1.034e-03	2.316e-03	5.252e-03
(32,64)	2.301e-05	4.563e-05	8.344e-05	3.787e-04
(64,128)	1.274e-06	2.759e-06	5.195e-06	7.343e-06
(128,256)	1.133e-07	1.755e-07	3.901e-07	6.016e-07

High accuracy with small sample size.

Example 1: amplitude computation



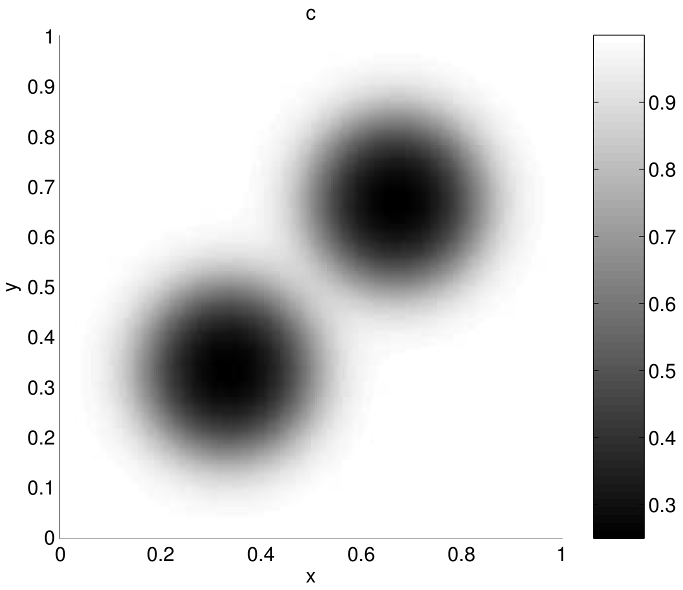
Example 1: multiple arrivals



Example 2

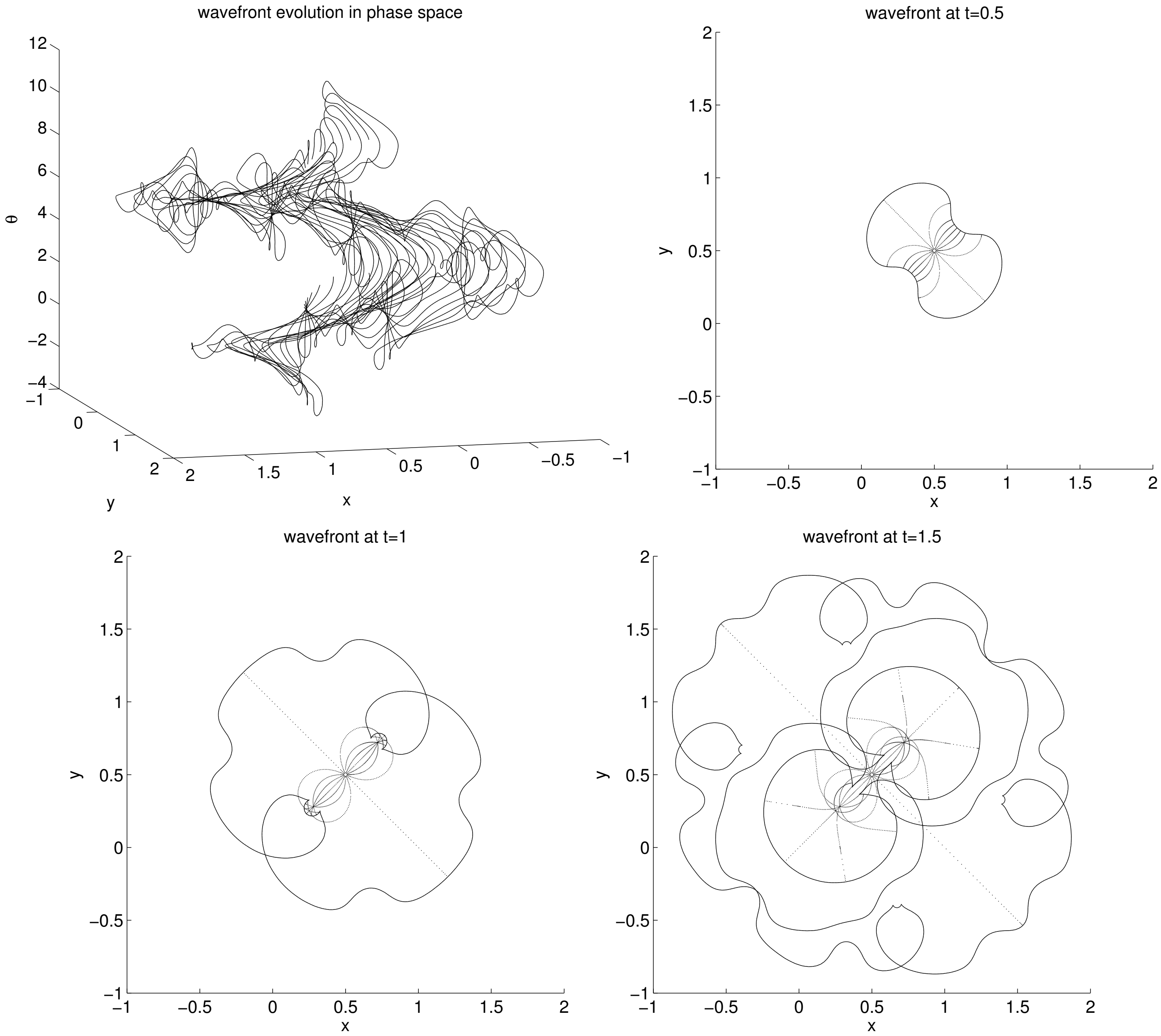
- Velocity field: $a = (1/4, 1/4)$, $b = (3/4, 3/4)$

$$c(x,y) = \left(\frac{1}{1 + 3e^{-64|x-a|^2} + 3e^{-64|x-b|^2}} \right)^2$$



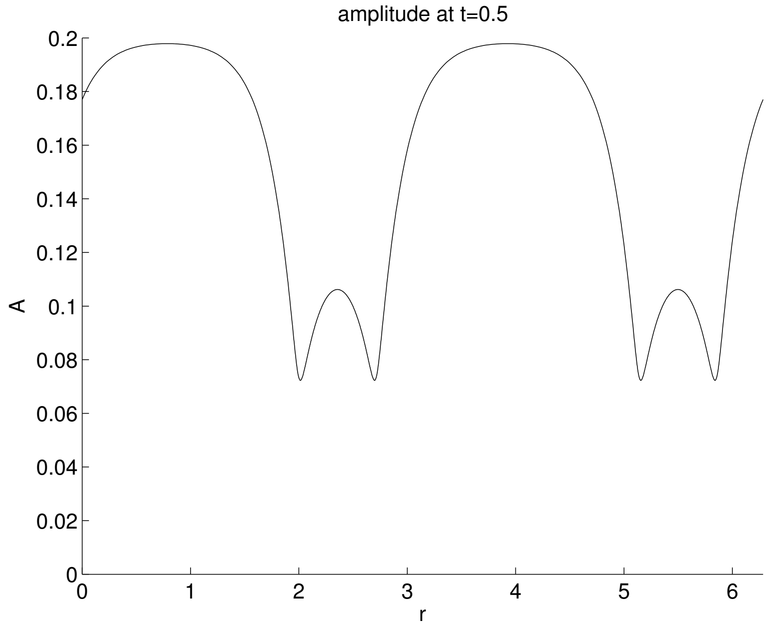
- The initial wave front is a small circle centered at $(1/2, 1/2)$.

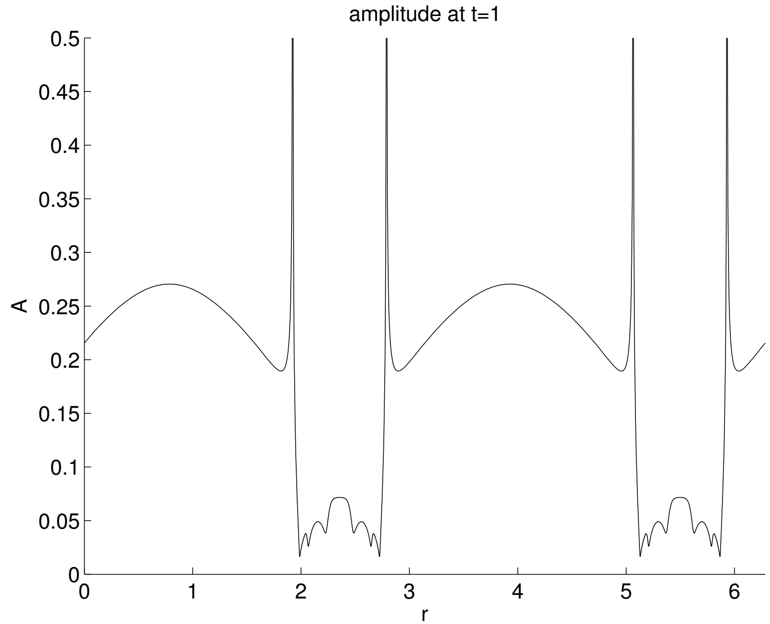
Example 2 (wave front construction)

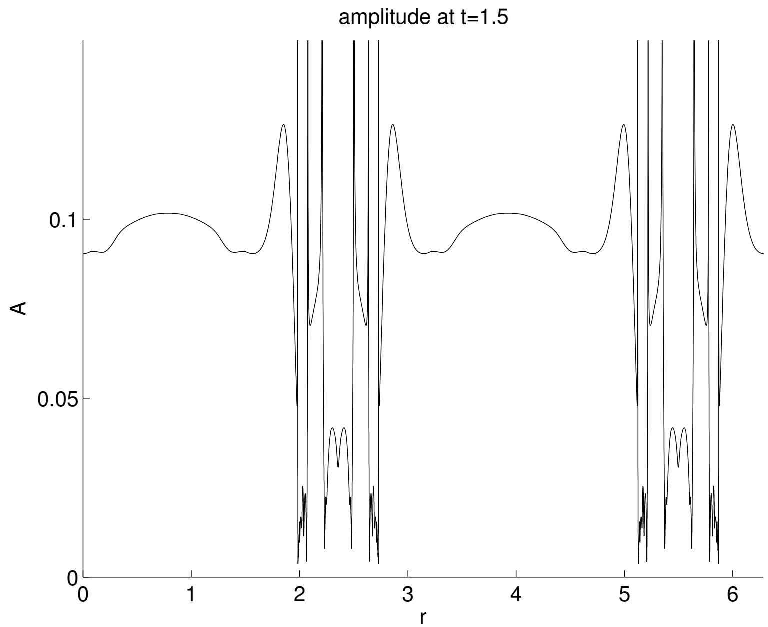


Speed up factor is 200

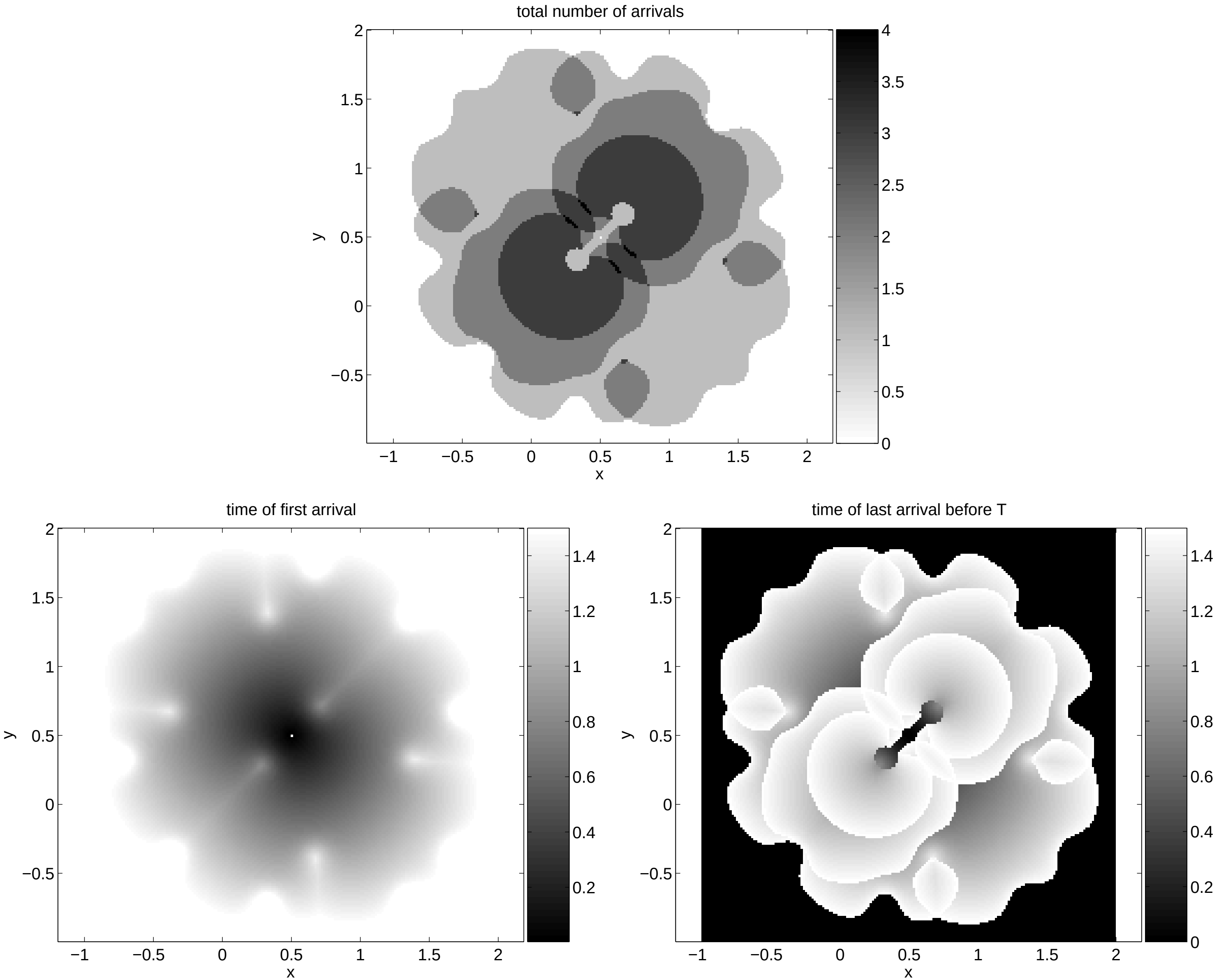
Example 2 (amplitude computation)







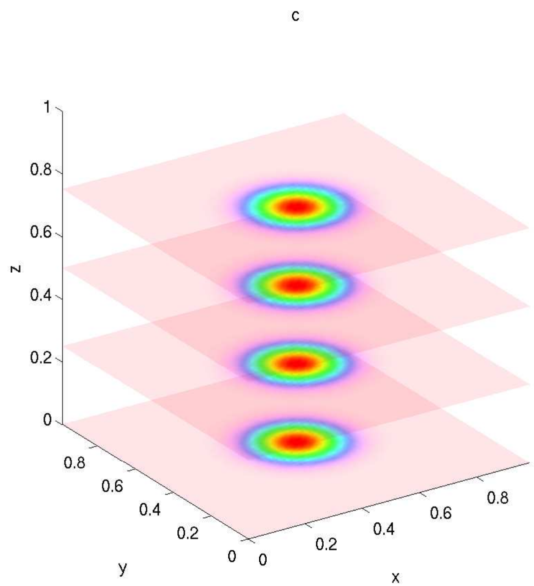
Example 2 (multiple arrivals)



Example 3

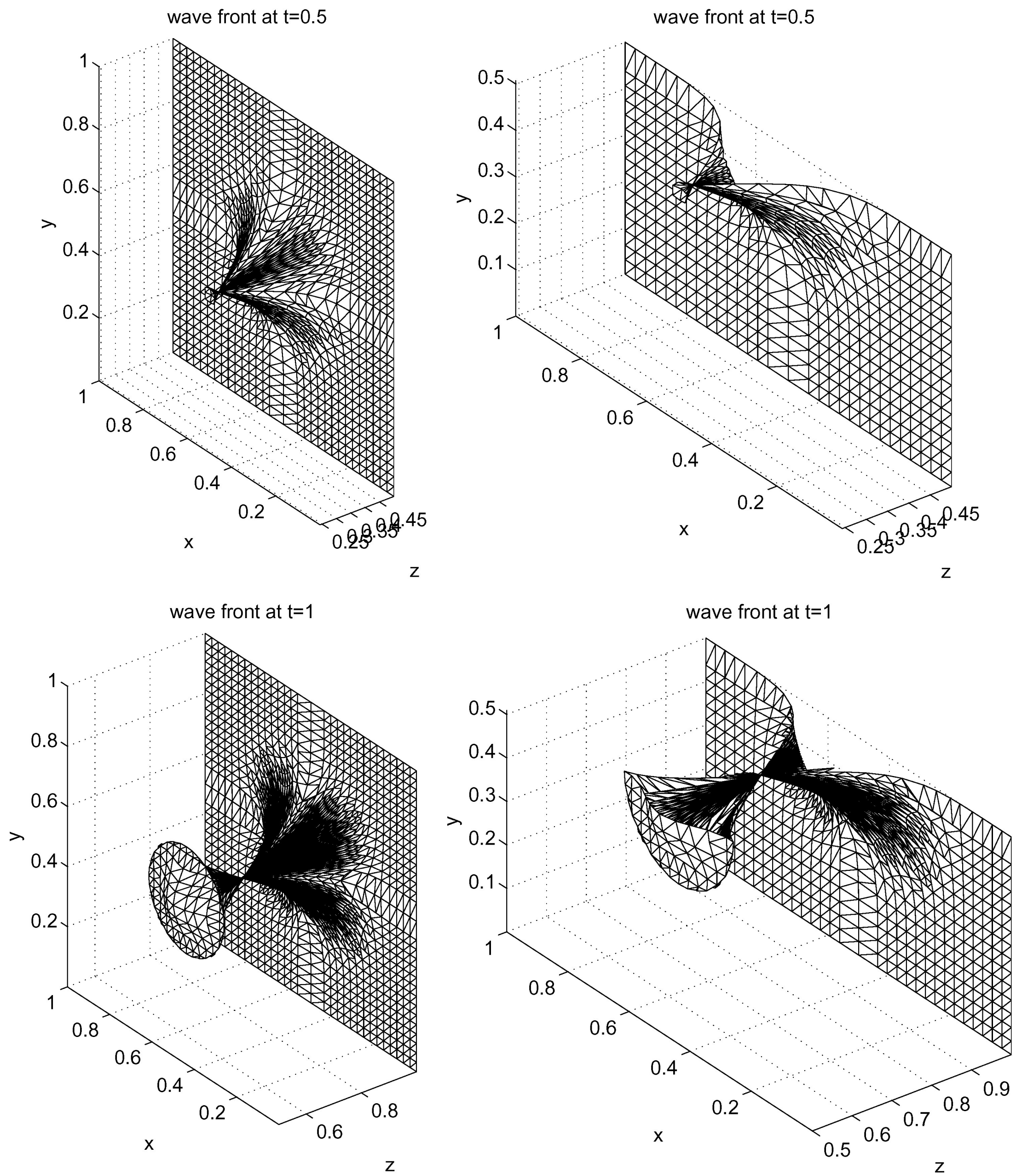
- Velocity field (3D waveguide)

$$c(x,y,z) = \frac{1}{1 + e^{-64\cdot(x-1/2)^2 - 64\cdot(y-1/2)^2}}$$

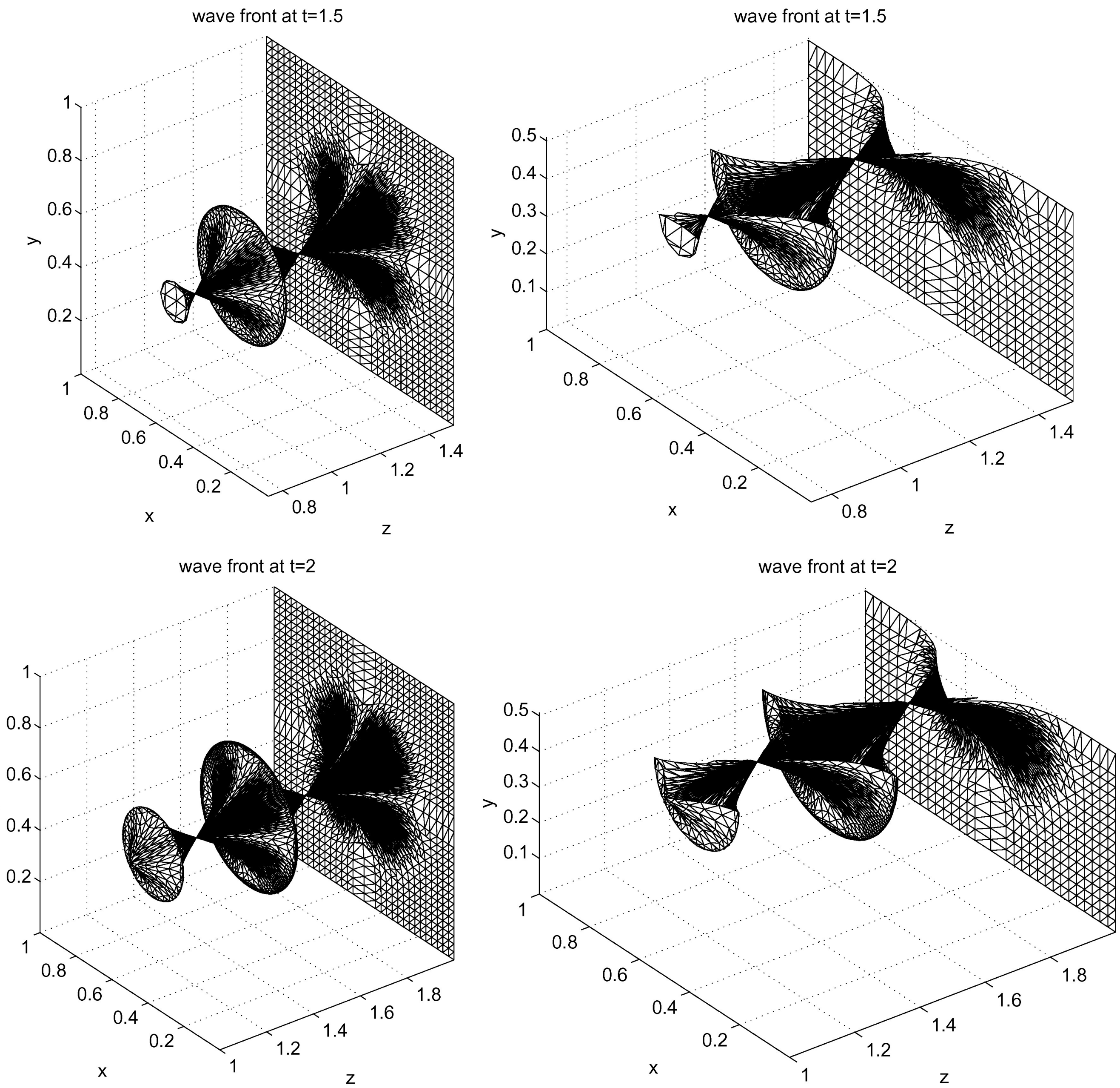


- The initial wave front is a plane wave at $z = 0$.

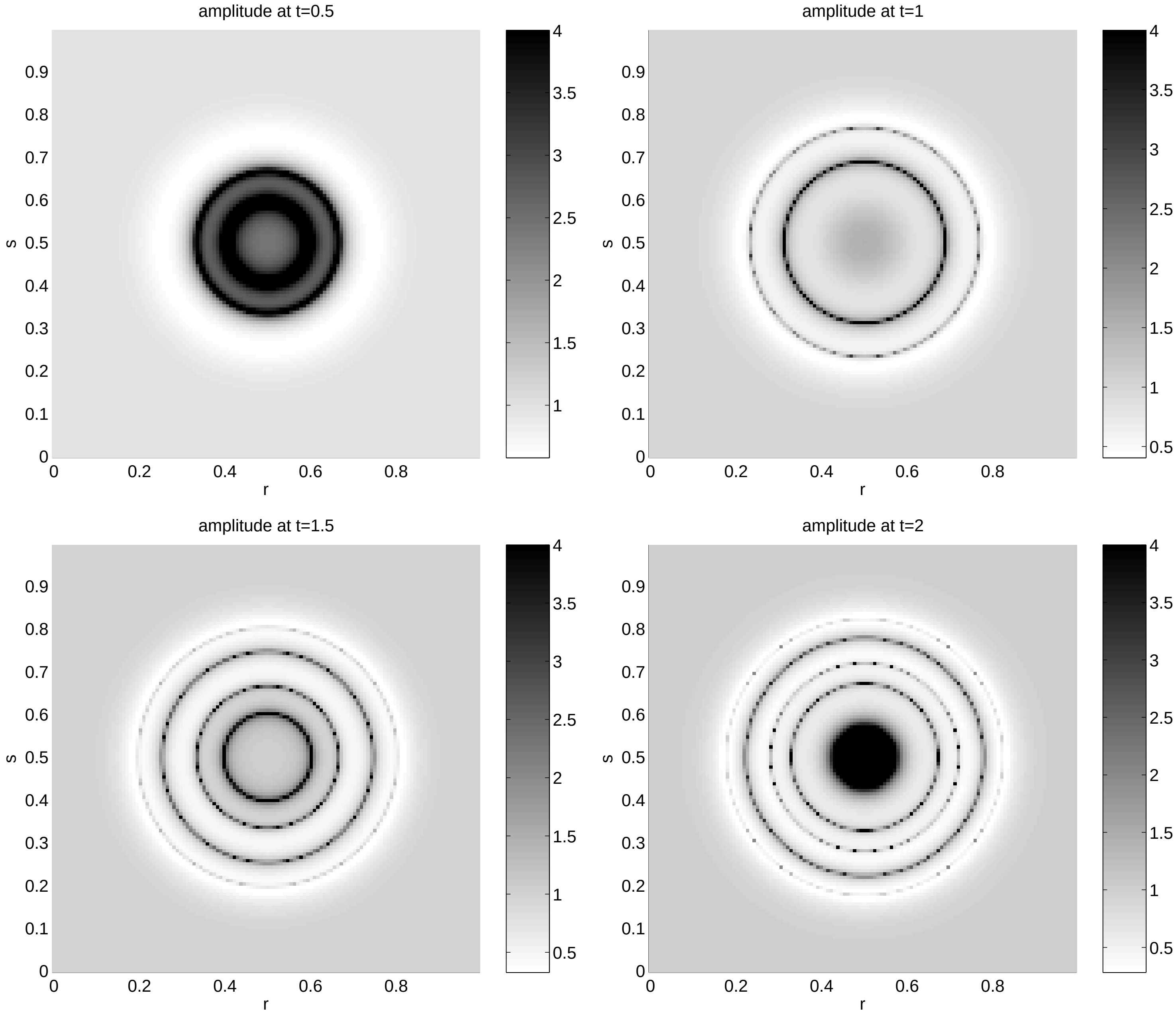
Example 3 (wave front construction)

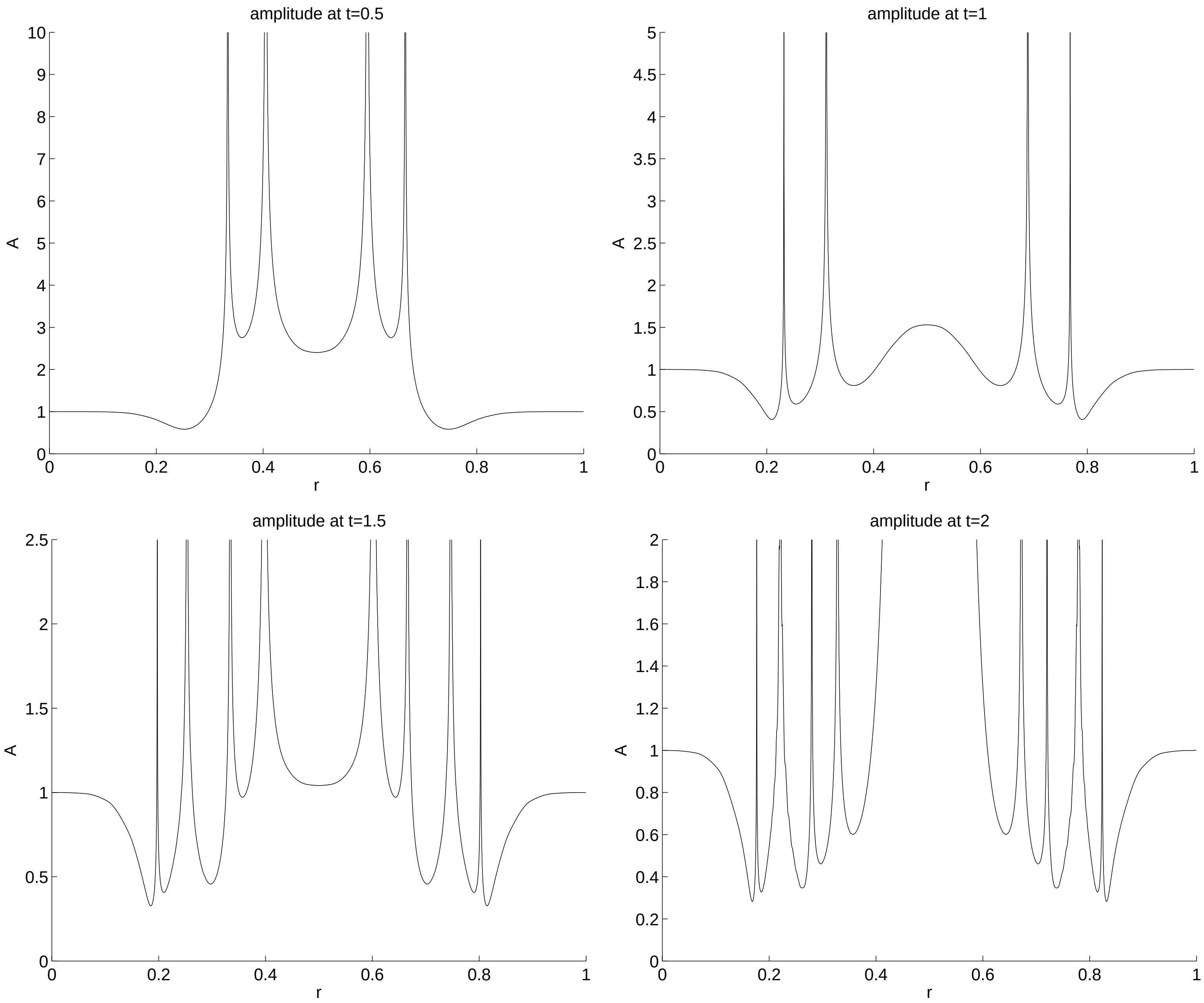


Example 3 (wave front construction)



Example 3 (amplitude computation)




amplitude at t=0.5
amplitude at t=1
amplitude at t=1.5
amplitude at t=2
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r
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0.6
0.8
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10
9
8
7
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0.5
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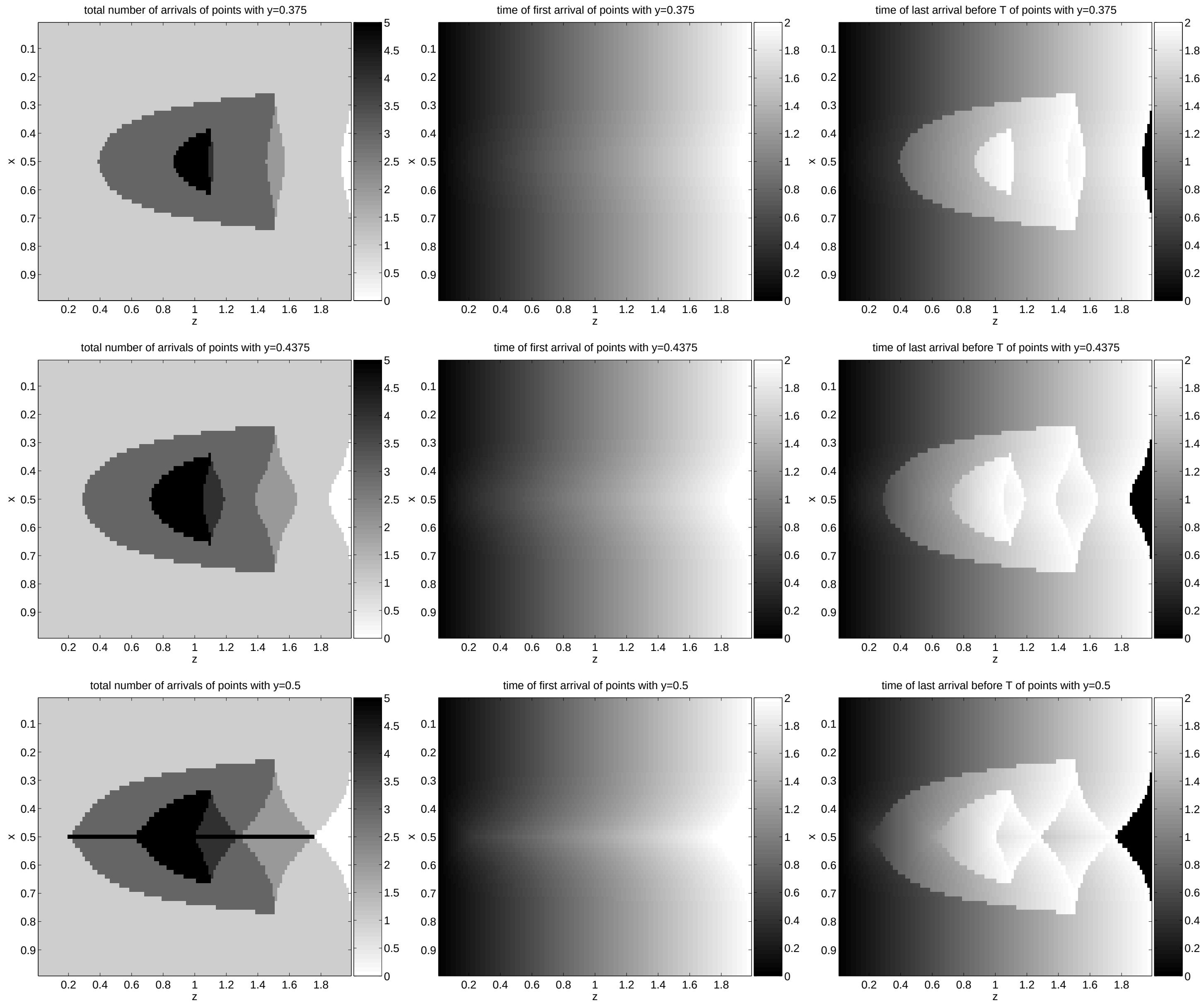
1.4
1.2

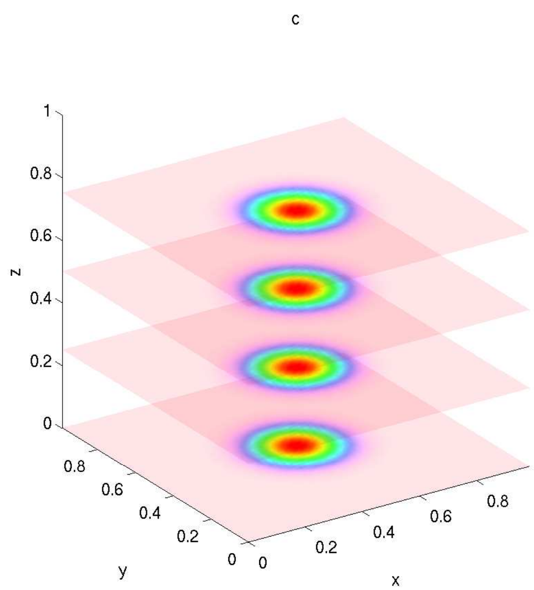
Example 3 (multiple arrivals)



Example 4

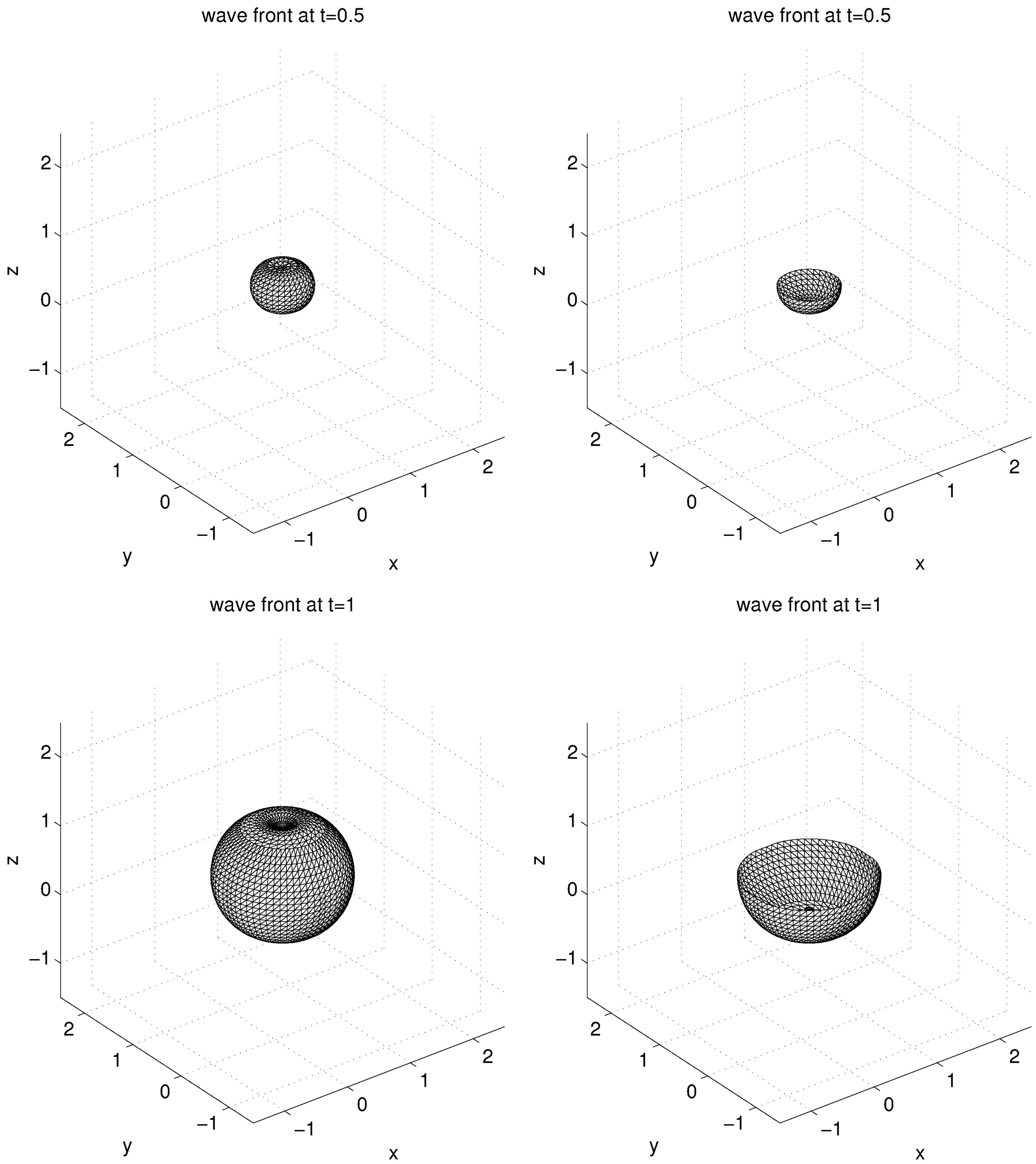
- Velocity field (3D waveguide)

$$c(x, y, z) = \frac{1}{1 + e^{-64(t(x-1/2)^2 + (y-1/2)^2)}}$$



- The initial wave front is a small sphere centered at $(1/2, 1/2, 1/2)$.

Example 4


wave front at t=0.5
wave front at t=0.5
wave front at t=1
wave front at t=1
z
y
x
2
1
0
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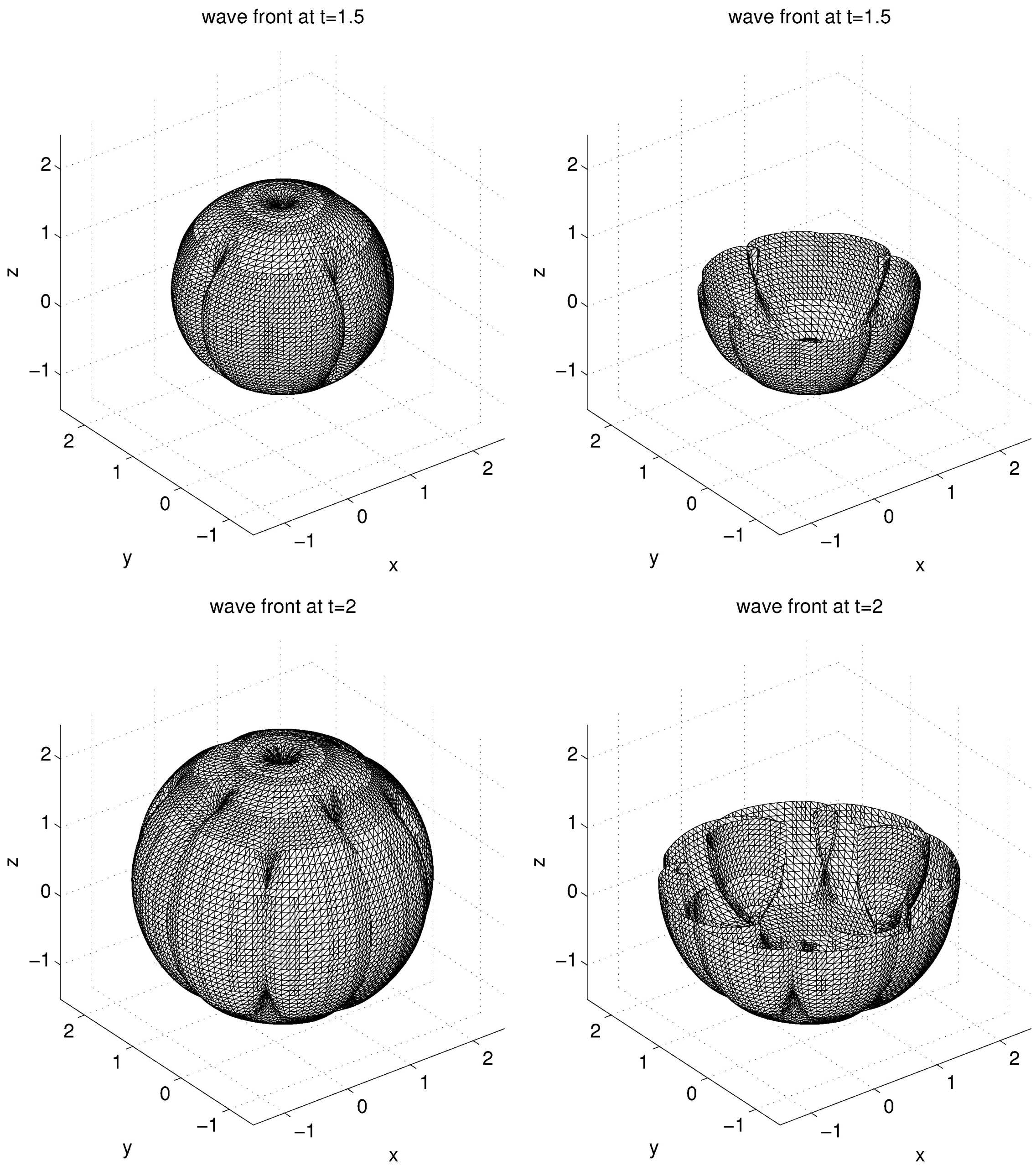
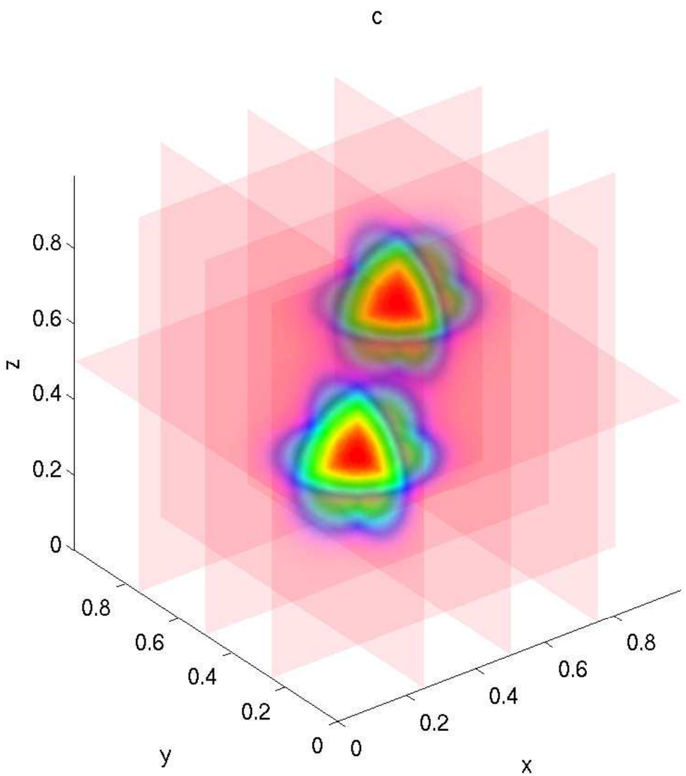
Example 4


wave front at t=1.5
z
y
x
wave front at t=1.5
z
y
x
wave front at t=2
z
y
x
wave front at t=2
z
y
x

Example 5

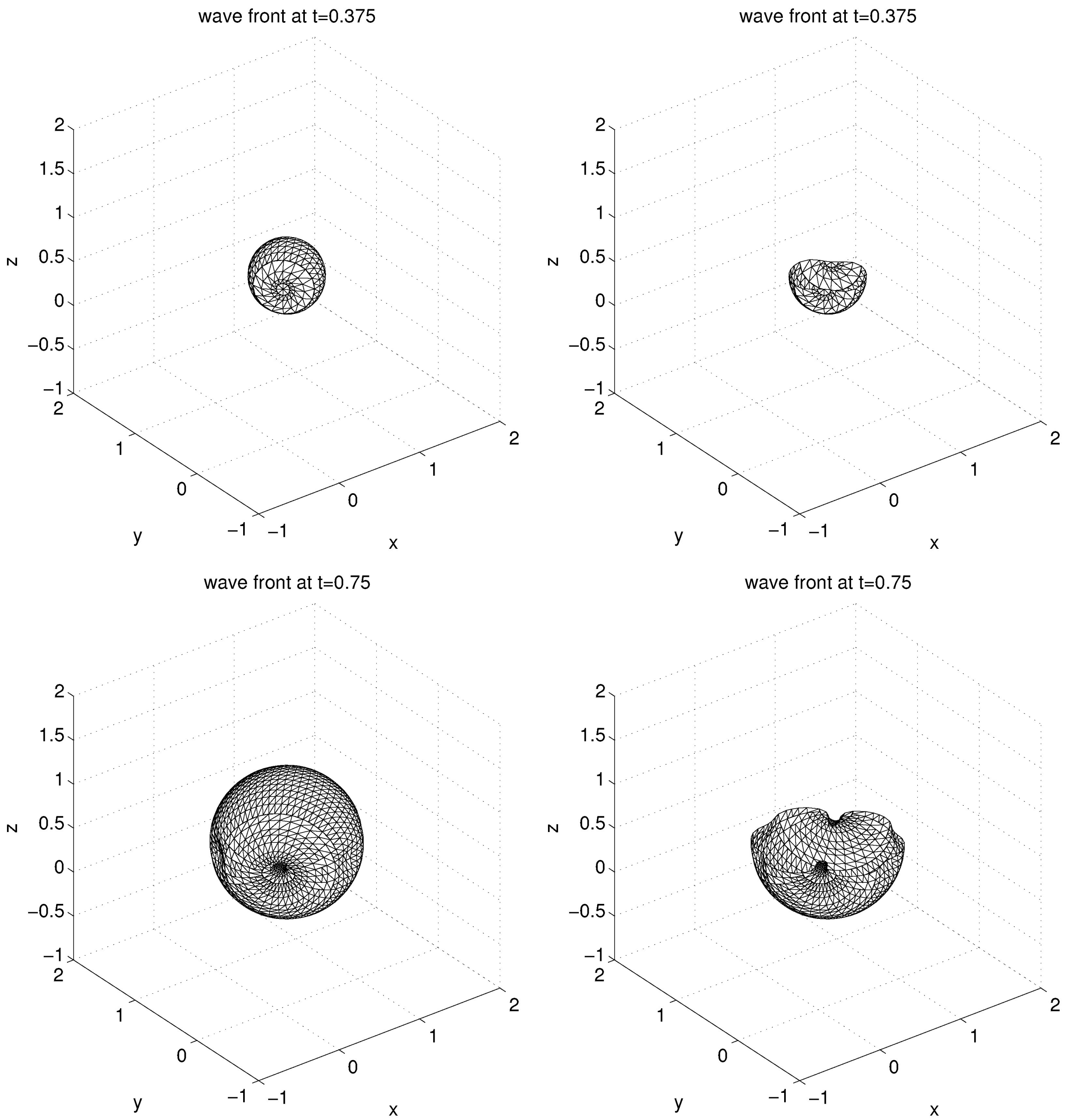
- Velocity field: $\boldsymbol{a} = (1/4, 1/4, 1/2)$, $\boldsymbol{b} = (3/4, 3/4, 1/2)$

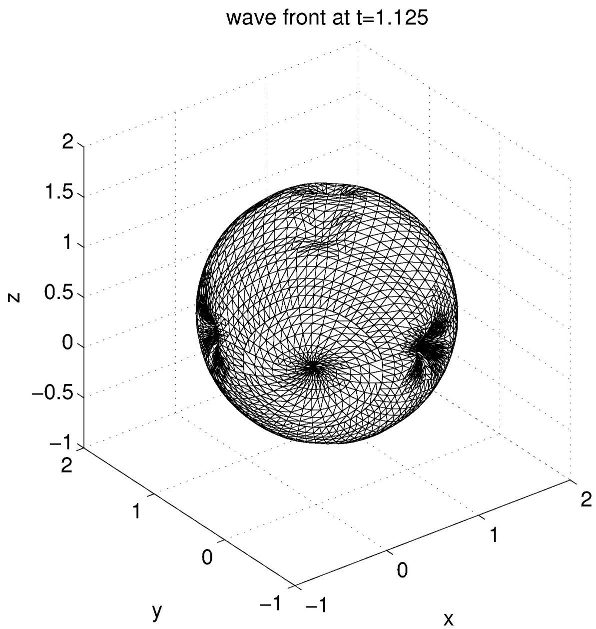
$$c(x, y) = \frac{1}{1 + 3e^{-64|x-a|^2} + 3e^{-64|x-b|^2}}$$

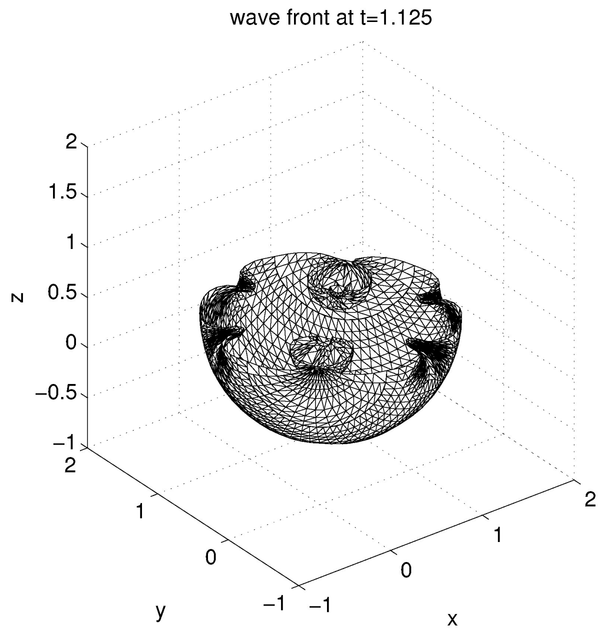


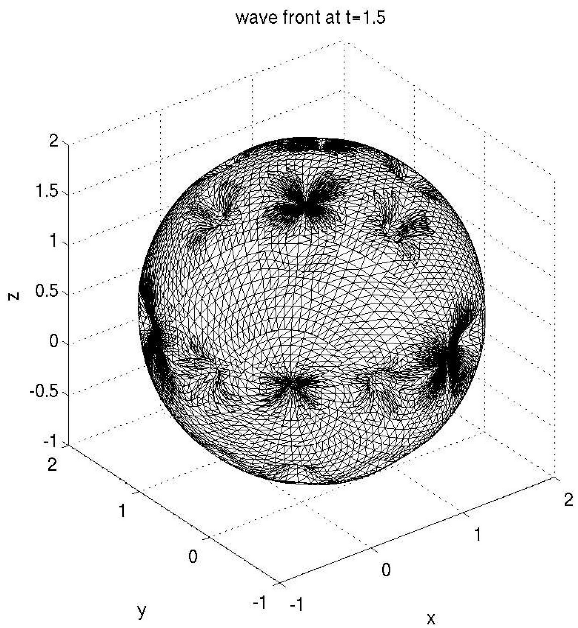
- The initial wave front is a small sphere centered at $(1/2, 1/2, 1/2)$.

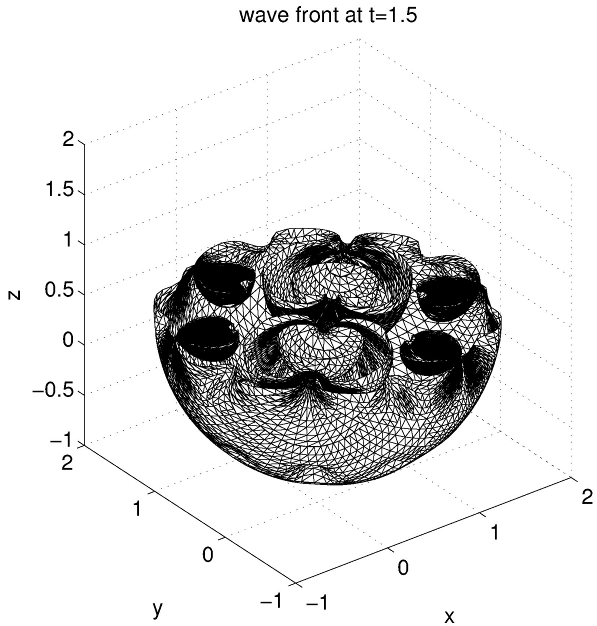
Example 5


wave front at t=0.375
wave front at t=0.375
wave front at t=0.75
wave front at t=0.75
x
y
z
−1
−0.5
0
0.5
1
1.5
2


wave front at t=1.125
z
y
x


wave front at t=1.125
z
y
x


wave front at t=1.5
z
y
x


wave front at t=1.5
z
y
x

- $T_0 = 0.0625$ and $\tau = 2^{-10}$ in the wave front construction algorithm.
- Cartesian grid with 16, 16, 16, 32 and 16 points in x, y, z, θ and ϕ.
- $\tilde{g}_{T_0}$ is constructed within 900 second and has accuracy around 10^{-4}.
- Adaptive wave front propagation up to $T = 1.5$. The final wave front is resolved with $37,000$ samples.

Summary

The phase flow method: novel approach to integrate ODEs.

- Bootstrapping in time domain using the group property of the phase flow.
- Efficient and accurate
- Inserting rays is effortless
- Many applications: e.g. geodesic flows on surfaces
- Further developments: piecewise smooth velocity fields

Epilogue: Curvelet and Wave Equations

New curvelet multiscale pyramid

- Multiscale
- Multi-orientations
- Parabolic (anisotropy) scaling

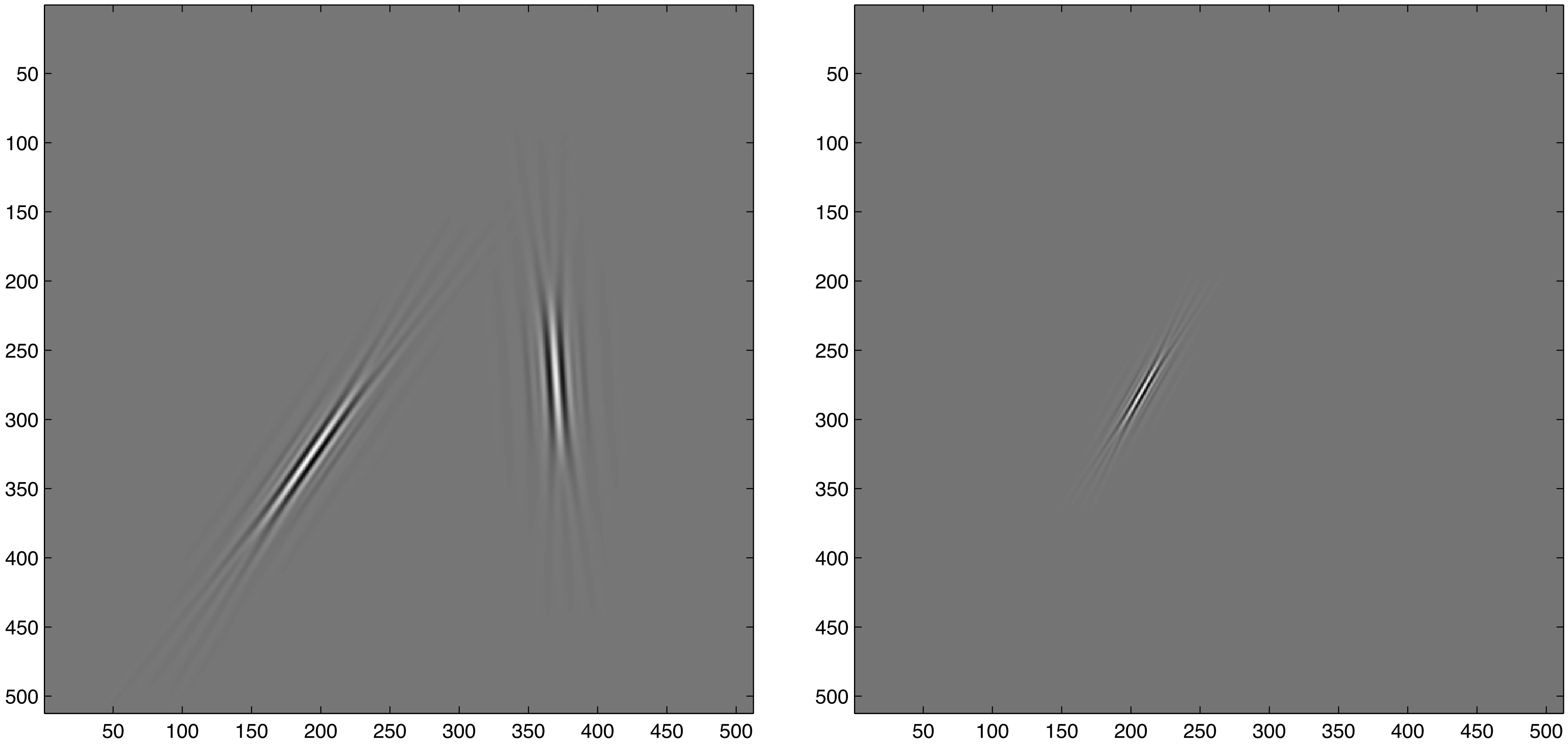
$$width \approx length^2$$

- Indexed by phase space

Curvelet expansion

$$f = \sum_{\mu} \langle f, \varphi_\mu \rangle \varphi_\mu \qquad ||f||_2^2 = \sum_{\mu} \langle f, \varphi_\mu \rangle^2$$

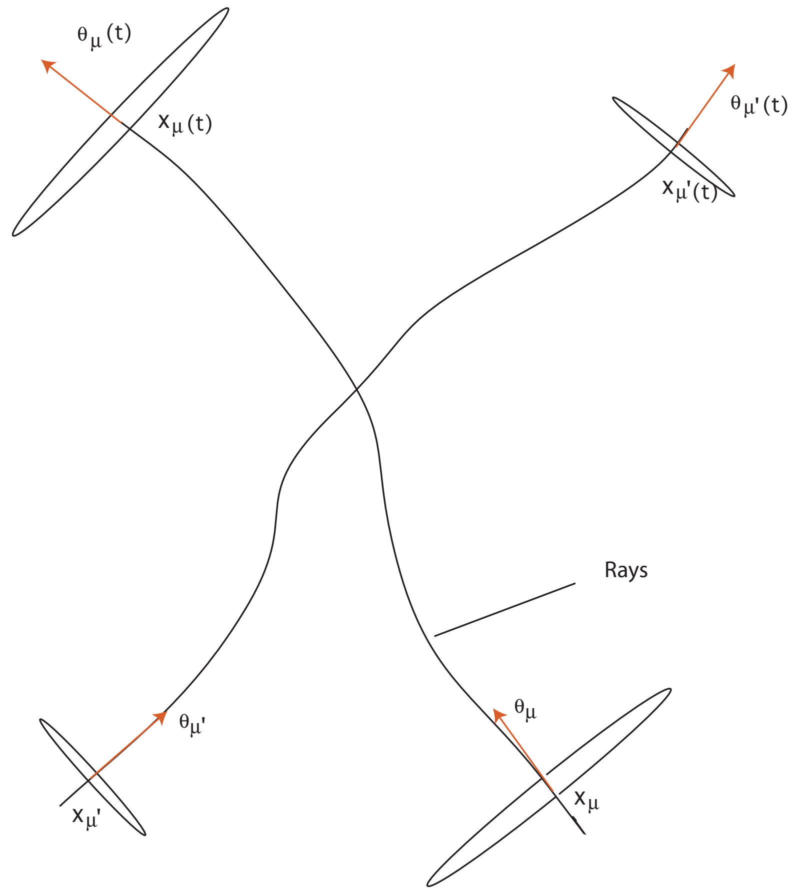
Digital Curvelets



Curvelets and Wave Equations, I

$$u_{tt} - c^2(x)\Delta u = 0$$

The action of the wave propagator on a curvelet is well- approximated by a rigid motion along the Hamiltonian flow.



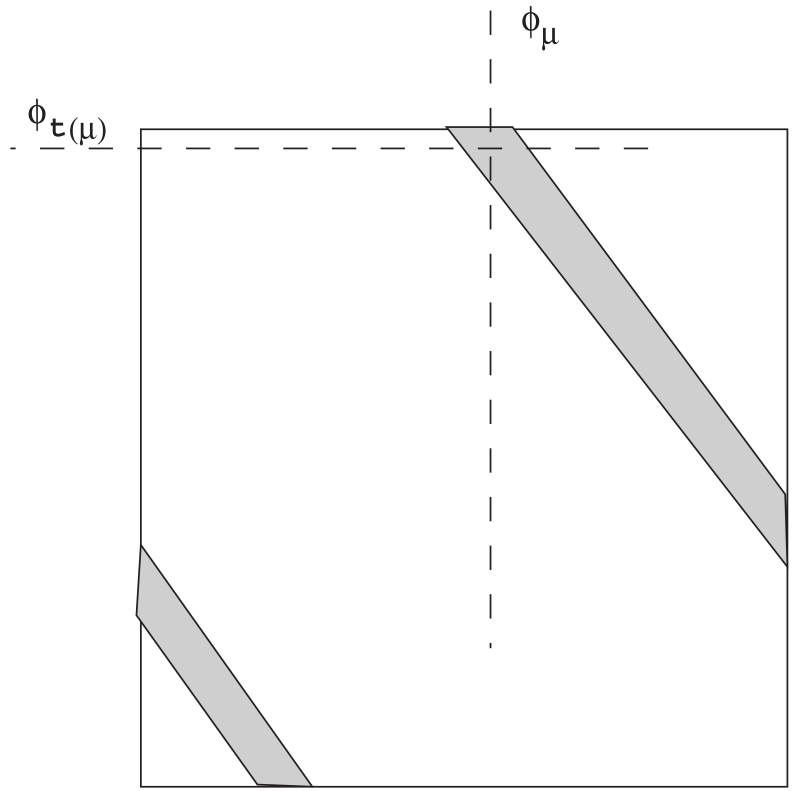
Curvelets and Wave Equations, II

Wave equation

$$u_{tt} - c^2(x)\Delta u = 0,$$

with $u(0, x)$ and $u_t(0, x)$ as initial data.

The curvelet matrix of a wide range of wave propagators is optimally sparse: the coefficients decay nearly exponentially fast away from a shifted diagonal.



Sketch of the curvelet representation of the wave propagator

Fast Wave Propagation?

$$u_t = e^{-Pt} u_0$$

$$\begin{array}{ccc} u_0 & \xrightarrow{e^{-Pt}} & u_t \\ F \downarrow & & \downarrow F \\ \theta_0 & \xrightarrow[A(t)]{} & \theta_t \end{array}$$

For any t, $A(t)$ is sparse

Background: Fast and accurate Digital Curvelet Transform is available (with Demanet, Donoho and Ying).