Hamiltonian-Preserving Numerical Methods for the Liouville Equation with Discontinuous Hamiltonians

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The Liouville equation

$$f_t + \mathbf{v} \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} V \cdot \nabla_{\mathbf{v}} f = 0\,, \quad t > 0, \quad \mathbf{x}, \mathbf{v} \in R^d$$

where f(t, x, **v**) is the density distribution of a classical particle at

position x, time t, and traveling with velocity v. V(x) is the potential.

It describes the density distribution of a particle whose motion is governed by Newton's Second Law:

$$\frac{d\mathbf{x}}{dt} = \mathbf{v}\,, \quad \frac{d\mathbf{v}}{dt} = -\nabla_{\mathbf{x}} V\,,$$

This is a Hamiltonian system with the Hamiltonian:

$$H = \frac{1}{2}|\mathbf{v}|^2 + V(\mathbf{x})$$

General Liouville equation

$$f_t + \nabla_{\mathbf{p}} H \cdot \nabla_{\mathbf{x}} f - \nabla_x H \cdot \nabla_p f = 0$$

with H=H(x, p) is the Hamiltonian

The bicharacterisitcs:

$$d\mathbf{x}/dt = \nabla_{\mathbf{p}} H$$

$$d\mathbf{p}/dt = -\nabla_{\mathbf{x}} H$$

Semiclassical limit of Schrodinger: $H=1/2\ |\mathbf{p}|^2+V(\mathbf{x})$

Geometrical optics: $H = c(\mathbf{x})\ |\mathbf{p}|$

We will study both problems

Applications

- The Liouville (or Vlasov) equation arises in many physical applications in the microscopic mesoscopic or kinetic scale:

  E.g. Semiconductor, plasma, geometrical optics, wave propagation, etc.

- When coupled with an external field:

  E.g. Vlasov-Poission, Vlasov-Maxwell, etc.

Another application

The Liouville equation also arises from the level set simulation of "**multivalued solutions**" in high frequency waves

- Geometrical optics
- Semiclassical limit of linear Schrodinger equation
- High frequency limit of general symmetric hyperbolic systems: waves, acoustic waves, elastic waves, electro-magnetic waves
- The zero level sets of any quasilinear, multi-D, first order scalar PDEs (hyperbolic equations, Hamilton-Jacobi, etc) solves linear Liouville equations

- References: *Jin-Osher, Cheng-H.L. Liu-Osher, Jin-H.L.Liu-Osher-Tsai*

Discontinuous potential

- The potential V(x) may be a given function, or from an external field

  electric field: Vlasov-Poisson equations

  electromagnetic field: Vlasov-Maxwell equations

- We are interested in the numerical solution of the Liouville equation when the potential V(x) is **discontinuous,** corresponding to a potential barrier
- Potential barriers arise in many physical applications: quantum tunnel effect, semiconductor devise modeling, plasmas, geometric optics, interfaces between different materials, etc.

Discontinuous local wave speed

- We are also interested in the case

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

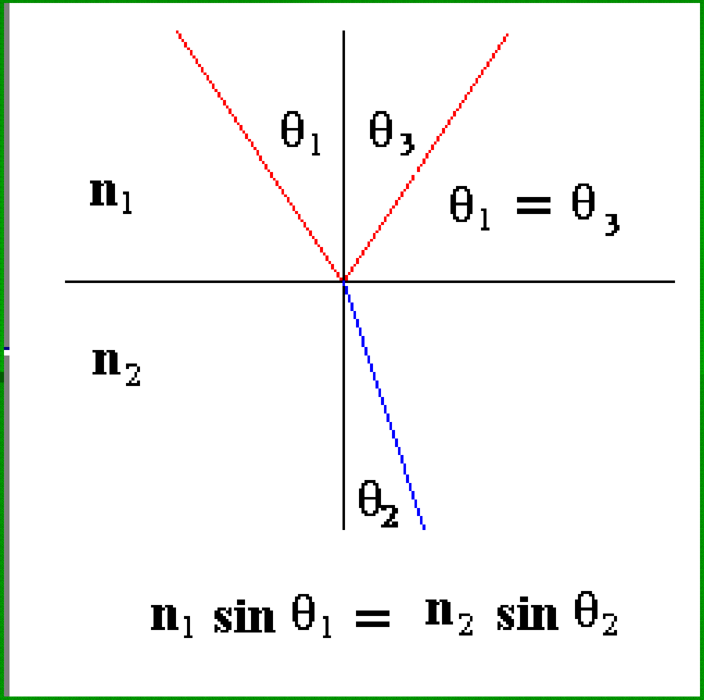
  when c(x) is discontinous, corresponding to waves propagating through different materials
- high frequency or geometrical optics limit of

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

Snell's Law of refraction

- When a plane wave hits the interface,

the angles of incident and transmitted waves satisfy (n=1/c)



Analytic issues

- This is a linear hyperbolic PDE with singular (discontinous + measure valued) coefficients.

  weak solution? Uniqueness?

- Study of geometrical optics limit with interface/boundary: Miller, Bal, Keller, Papanicolaou, Ryzhik

Numerical stability problem

When numerically solving the Liouville equation, which is a linear hyperbolic equation, by an explicit time discretization, the stability condition requires:

$$\Delta t \left[\frac{\max_j |\xi_j|}{\Delta x} + \frac{\max_i |DV_i|}{\Delta \xi} \right] \leq 1.$$

since V'(x)= ∞ at a discontinuity of V, one can smooth out V (Osher, etc.) then Dv_i=O(1/Δx), thus

$\Delta t = O(\Delta x \, \Delta \xi)$

+ poor numerical resolution

Other numerical issues

Another issue is that the Hamiltonian H is a constant across the particle trajectory,

which be **preserved numerically**

It is never a good idea to take derivatives numerically across the interface (incorrect solution!)

Which weak solution does the scheme converges to ?

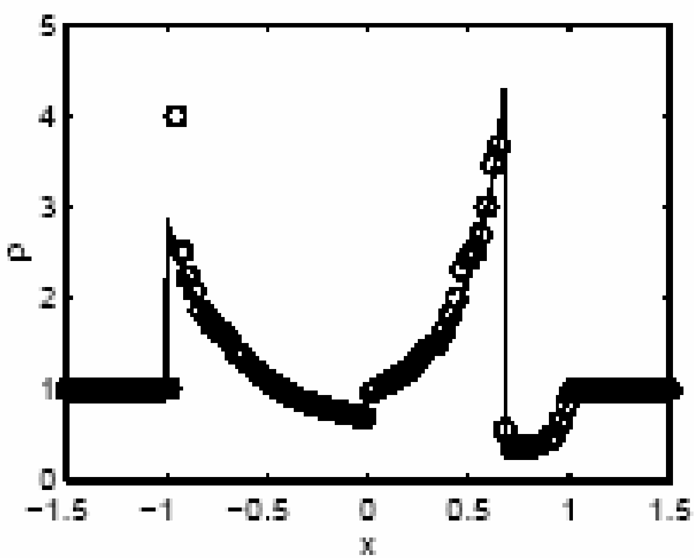
Hamiltonian-preserving schemes

We call a numerical scheme **Hamiltonian-preserving** if it

- Preserves constant Hamiltonian (exactly or with a desired numerical accuracy) along the particle trajectory across the potential barrier

  This provides a section criterion —which is physically relavant— for the unique solution of the underling hyperbolic PDEs

- Allows hyperbolic time step $\Delta t = O(\Delta x, \Delta v)$ for explicit schemes new method



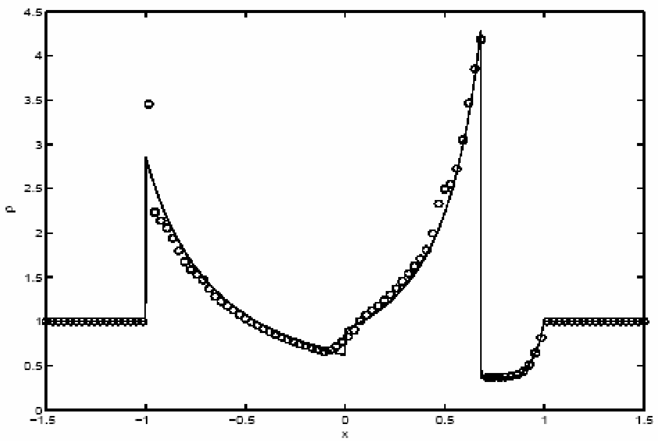
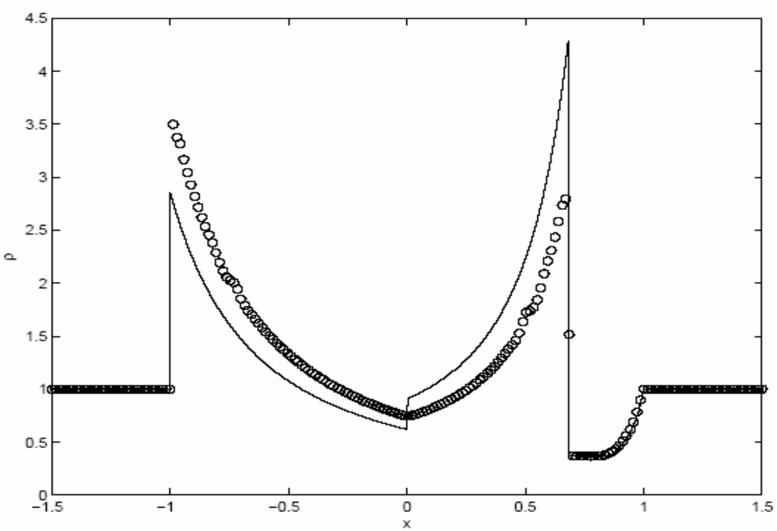


Figure 1 density $\rho(x,t)$ at $t=1$. Solid line: the exact solution; 'o': the numerical solution by standard method on 100×80 mesh with $\Delta t=\frac{1}{4}\Delta\xi$.

smoothing the potential
ignoring the discontinuity



Shallow water equations with bottom topography

A nonlienar hyperbolic systems with source term

$h_t + (hu)_x = 0$
$(hu)_t + (hu^2 + \frac{1}{2} gh^2)_x = -B'(x)gh$

The steady state solution satisfies

$$\frac{1}{2} u^2 + g(h+B) = C$$

so the energy is a constant, even if B is dicontinuous

Well-balanced schemes

How to preserve the steady state numerically?

- A standard shock capturinging scheme does not preserve the constant energy, due to the use of numerical viscosity, when B(x) is discontinuous
- Well-balanced scheme (balance the flux and source term): Roe, Greenberg- LeRoux, Gosse, Perthame-Semioni, LeVeque, Jin, etc.
- Our work is motivated by the well-balanced kinetic scheme of Perthame-Simeoni for the shallow water equations with bottom topography
- The Hamiltonian-preserving schemes are well-balanced schemes at the kinetic level

Particle behavior at potential barrier in classical mechanics

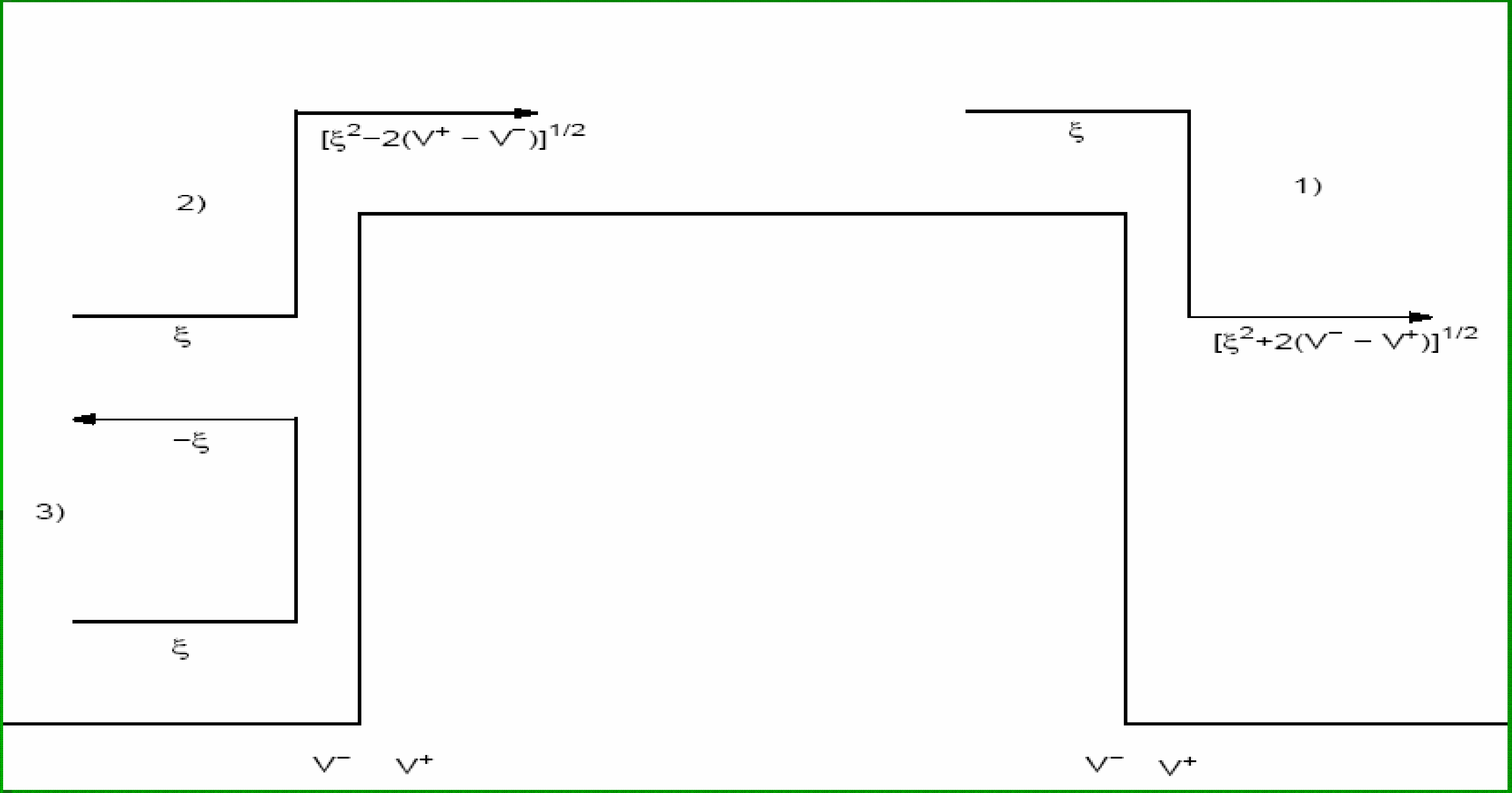
- At a potential barrier, the Hamiltonian H remains a constant along particle trajectory

$$\tfrac{1}{2}(\xi^{+})^2 + V^{+} = \tfrac{1}{2}(\xi^{-})^2 + V^{-}$$

- the density distribution f can be constructed along particle trajectory (upwind)

$$f(x^{-}, \xi^{-}) = f(x^{+}, \xi^{+})$$

Change of momentum at potential barrier



Key idea in Hamiltonian-preserving schemes

- we build in the particle behavior at the potential barrier into the numerical flux

consider a standard finite difference approximation

$$\partial_t f_{ij} + \xi_j \frac{f^-_{i+\frac{1}{2},j} - f^+_{i-\frac{1}{2},j}}{\Delta x} - \frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} \frac{f_{i,j+\frac{1}{2}} - f_{i,j-\frac{1}{2}}}{\Delta \xi} = 0,$$

$f_{I,j+1/2}$, $f^-_{i+1/2,j}$ ---- upwind discretization

$f^+_{i+1/2,\, j}$ ---- incorporating the particle behavior

How to compute numerical flux in x-direcion:
Scheme I (finite difference formulation)

- If at $x_{i+1/2}$ V is continuous, then $f^{+}_{i+1/2,j} = f^{-}_{i+1/2,j;}$
- Otherwise,

  For $\xi_j > 0$,

  If $V^{+}_{i+1/2} > V^{-}_{i+1/2}$, $f^{+}_{i+1/2,j}$ will be obtained from $f^{-}_{i+1/2}(\xi')$, where ξ' is the velocity obtained by

  1) Hamiltonian conservation (if the particle crosses over)

$$\star \ \text{if } \xi_j > \sqrt{2\left(V^{-}_{i+\frac{1}{2}} - V^{+}_{i+\frac{1}{2}}\right)},$$

$$\xi' = \sqrt{\xi_j^2 + 2\left(V^{+}_{i+\frac{1}{2}} - V^{-}_{i+\frac{1}{2}}\right)}$$

$$\text{if } \xi_k \le \xi' < \xi_{k+1} \text{ for some } k$$

$$\text{then } f^{+}_{i+\frac{1}{2},j} = \frac{\xi_{k+1}-\xi'}{\Delta\xi} f_{ik} + \frac{\xi'-\xi_k}{\Delta\xi} f_{i,k+1}$$

The reflection case

2). if the particle was reflected:

$$f^{+}_{i+\frac{1}{2},j} = f_{i+1,k} \text{ where } \xi_k = -\xi_j$$

The other case can be dealt with similarly.

One can also construct higher order scheme by using higher order upwind shock capturing schemes , combined with higher order interpolation to obtain flux at ξ’

The New CFL condition

$$\Delta t \left[\frac{\max_j |\xi_j|}{\Delta x} + \frac{\max_i \left| \frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} \right|}{\Delta \xi} \right] \leq 1.$$

- Note the discrete derivative of V is defined only on **continuous** points of V, thus

$\Delta t = O(\Delta x, \Delta \xi)$

Positivity and l^∞-contraction

- for first order scheme (forward Euler in time + upwind in space), under the “good” CFL condition

$$\text{if } f^n > 0, \text{ then } f^{n+1} > 0;$$

$$\| f^{n+1} \|_{l^\infty (x,\, \xi)} \leq \| f^n \|_{l^\infty (x,\, \xi)}$$

The l^1 stability (V step function)

- If $\| f^0\|_1$ and $\| f^n \|_\infty$ are both bounded, then under the "good" CFL condition, there exists a constant C >0 such that

$$\| f^n\|_1 \leq C \| f^0\|_1$$

Main difficulty of the proof:

carefully estimate the flux at the neighborhood of the barrier

More about the l^1 stability

For singular initial data, the above l^1 stability holds if

Assumption 1

There exists a positive constant ξ_z *such that*

$$\forall (i,j) \in S_z = \{(i,j) |\ \ x_i < x_{m+\frac{1}{2}},\ \ 0 < \xi_j < \xi_z\},$$

it holds that

$$|f^0_{ij}| \le C_1 |f^0|_1 \,.$$

Violation of this condition leads to instability (for semiclassical limit problem for example)

Scheme II: a finite volume approach

By integrating the Liouville equation (2.1) over the cell $[x_{i-1/2}, x_{i+1/2}] \times [\xi_{j-1/2}, \xi_{j+1/2}]$, one gets the following equation

$$\partial_t f_{ij} + \xi_j \frac{f^-_{i+\frac{1}{2},j} - f^+_{i-\frac{1}{2},j}}{\Delta x} - \frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} \frac{f_{i,j+\frac{1}{2}} - f_{i,j-\frac{1}{2}}}{\Delta \xi} = 0. \tag{4.1}$$

The upwind discretization depends on the sign of ξ_j and $\frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x}$. To illustrate the basic idea, we assume $\xi_j > 0$, $\frac{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}}{\Delta x} < 0$ and $V^-_{i+\frac{1}{2}} < V^+_{i+\frac{1}{2}}$ (this is the case when the particle loses momentum from left to right at the barrier). In this case

$$\begin{aligned} f^-_{i+\frac{1}{2},j} &= \frac{1}{\xi_j \Delta \xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \xi f\left(x^-_{i+\frac{1}{2}}, \xi, t\right) d\xi, \\ f_{i,j+\frac{1}{2}} &= \frac{1}{V^-_{i+\frac{1}{2}} - V^+_{i-\frac{1}{2}}} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} V_x f\left(x, \xi^-_{j+\frac{1}{2}}, t\right) dx \end{aligned}$$

where $x^-_{i+\frac{1}{2}}, \xi^-_{j+\frac{1}{2}}$ are the limit from the negative coordinate in the x-and ξ-direction, taking into account that $f(x, \xi, t)$ may be discontinuous at the grid point $x = x_{i+\frac{1}{2}}$ and $\xi = \xi_{j+\frac{1}{2}}$.

Numerical flux

By using the condition (2.5):

$$f^+_{i+\frac{1}{2},j} = \frac{1}{\xi_j \Delta\xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \xi f\left(x^+_{i+\frac{1}{2}}, \xi, t\right) d\xi, = \frac{1}{\xi_j \Delta\xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \xi \overline{f}\left(x^-_{i+\frac{1}{2}}, \xi, t\right) d\xi, \qquad (4.2)$$

where $\overline{f}$ is defined as

$$\overline{f}\left(x^-_{i+\frac{1}{2}}, \xi, t\right) = f\left(x^-_{i+\frac{1}{2}}, \sqrt{\xi^2 + 2\left(V^+_{i+\frac{1}{2}} - V^-_{i+\frac{1}{2}}\right)}, t\right).$$

Using change of variable on (4.2) leads to

$$\begin{aligned} f^+_{i+\frac{1}{2},j} &= \frac{1}{\xi_j \Delta\xi} \int_{\xi_{j-\frac{1}{2}}}^{\xi_{j+\frac{1}{2}}} \xi f\left(x^-_{i+\frac{1}{2}}, \sqrt{\xi^2 + 2\left(V^+_{i+\frac{1}{2}} - V^-_{i+\frac{1}{2}}\right)}, t\right) d\xi \\ &= \frac{1}{\xi_j \Delta\xi} \int_{\sqrt{\xi^2_{j-\frac{1}{2}} + 2\left(V^+_{i+\frac{1}{2}} - V^-_{i+\frac{1}{2}}\right)}}^{\sqrt{\xi^2_{j+\frac{1}{2}} + 2\left(V^+_{i+\frac{1}{2}} - V^-_{i+\frac{1}{2}}\right)}} \xi f\left(x^-_{i+\frac{1}{2}}, \xi, t\right) d\xi. \qquad (4.3) \end{aligned}$$

Numerical integrations

The integral in (4.3) will be approximated by a quadrature rule. Since the end point $\sqrt{\xi^2_{j+\frac{1}{2}} + 2\left(V^+_{i+\frac{1}{2}} - V^-_{i+\frac{1}{2}}\right)}$ in (4.3) may not be a grid point in the ξ-direction. Special care needs to be taken at the both ends of the interval

$$\left[\sqrt{\xi^2_{j-\frac{1}{2}} + 2\left(V^+_{i+\frac{1}{2}} - V^-_{i+\frac{1}{2}}\right)}, \sqrt{\xi^2_{j+\frac{1}{2}} + 2\left(V^+_{i+\frac{1}{2}} - V^-_{i+\frac{1}{2}}\right)}\right]. \qquad (4.4)$$

Stability of Scheme II

If the forward Euler method is used in time, and first order upwind is used in the flux, then ***under the same CFL condition as Scheme I***, Scheme II is

- positive
- l^1 contracting (***for any bounded l^1 initial data***)
- l^∞ stable

Multidimensions

- Multi-d problems can be solved with the same idea using *dimension-by-dimension*
- We are yet to develop methods to treat barriers not aligned with grids, or curved potential barrier

An application

One application of the Liouville equation is to compute the

- geometrical optics
- semiclassical limit of linear Schrodinger equation

$$f_t + \mathbf{v} \cdot \nabla_{\mathbf{x}} f - \nabla_{\mathbf{x}} V \cdot \nabla_{\mathbf{v}} f = 0\,,$$

$$f(\mathbf{x}, \mathbf{v}, 0) = \rho_0(\mathbf{x}) \delta(\mathbf{v} - \mathbf{u}_0(\mathbf{x}))$$

Physical observables include

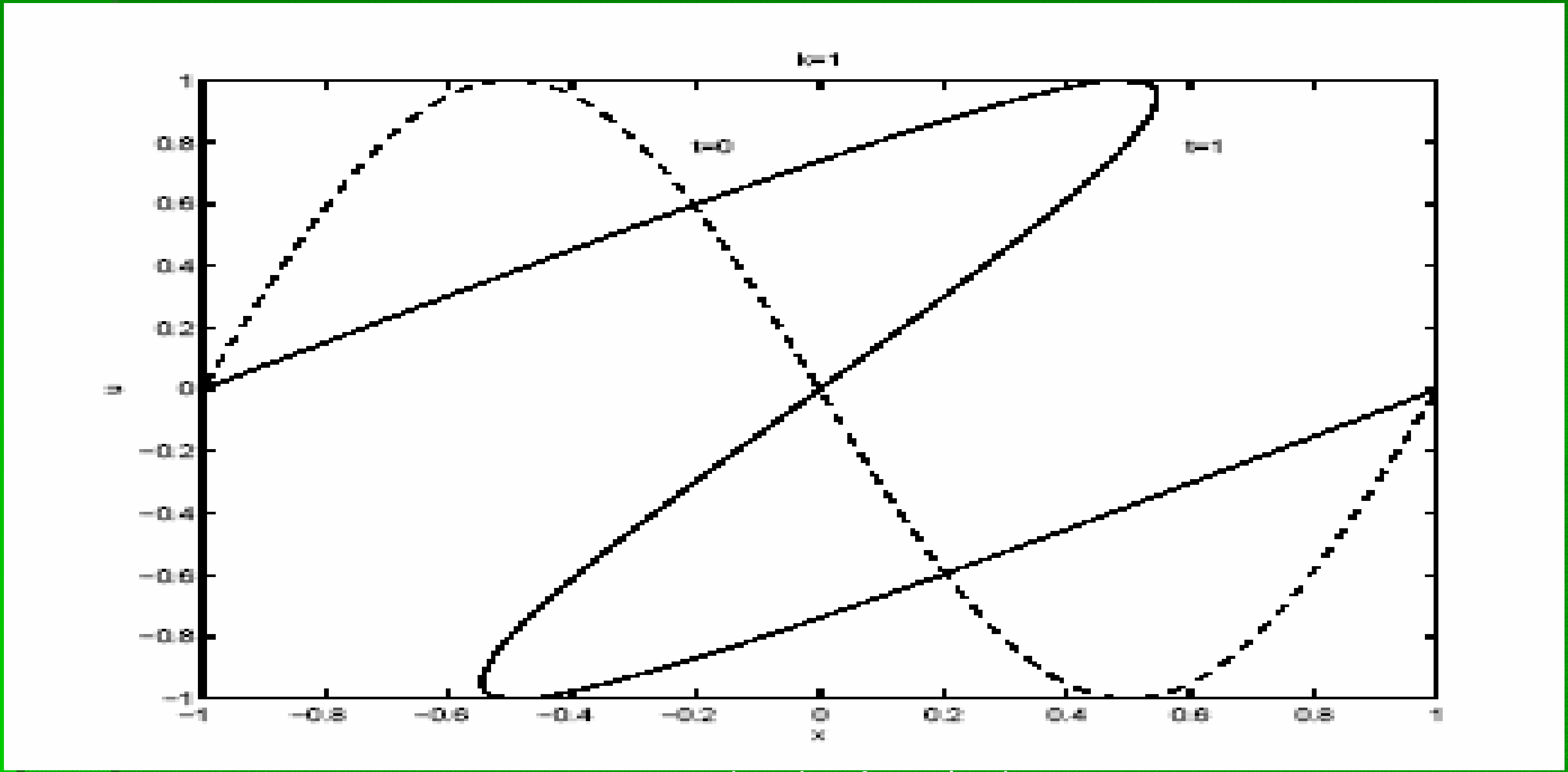
Position density

$$\rho(\mathbf{x}, t) = \int f(\mathbf{x}, \mathbf{v}, t) d\mathbf{v},$$

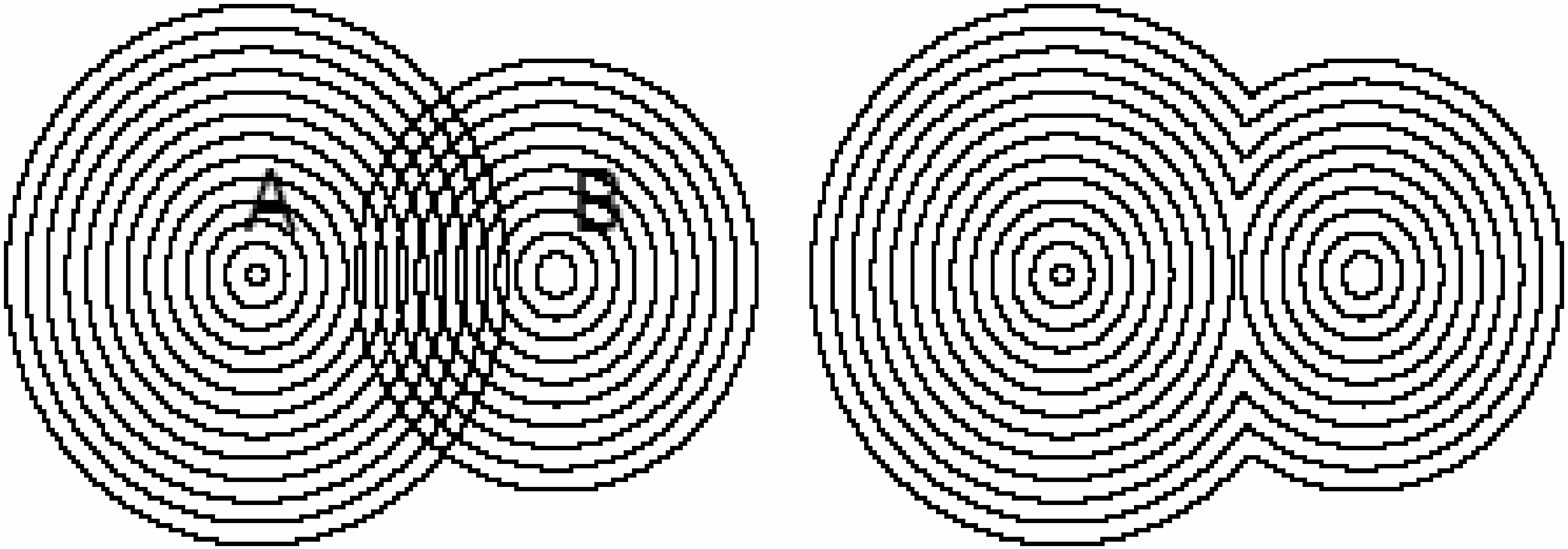
velocity

$$\mathbf{u}(\mathbf{x}, t) = \frac{1}{\rho(\mathbf{x}, t)} \int f(\mathbf{x}, \mathbf{v}, t) \mathbf{v} \, d\mathbf{v}$$

Shock vs. multivalued solution



Linear superposition vs viscosity solution



(a) Correct solution (b) Eikonal equation

Quasilinear hyperbolic equations

Based on a mathematical formulation in *Courant-Hilbert*.

We consider Let $u(t, \mathbf{x}) \in \Re$ be a scalar satisfying an initial value problem of an d-dimensional first order hyperbolic PDE with source term:

(1) $$\partial_t u + \mathbf{F}(u) \cdot \nabla_{\mathbf{x}} u + q(\mathbf{x}) = 0 \,,$$

(2) $$u(0, \mathbf{x}) = u_0(\mathbf{x}) \,.$$

Here $\mathbf{F}(u) : \Re^d \longrightarrow \Re^d$ is a vector, and $q : \Re^d \longrightarrow \Re$ is the source term. We introduce a level set function $\phi(t, \mathbf{x}, p)$ in dimension $d + 1$, whose zero level set is the solution u:

(3) $$\phi(t, \mathbf{x}, p) = 0 \qquad \text{at} \qquad p = u(t, \mathbf{x}) \,.$$

Therefore we evolve the entire solution u as the zero level set of ϕ.

The level set equation

One can easily show that the level set function satisfies a simple linear hyperbolic equation in R^{d+1}:

$$\partial_t \phi + \mathbf{F}(p) \cdot \nabla_{\mathbf{x}} \phi - q(\mathbf{x})\, \partial_p \phi = 0\,. \tag{4}$$

The initial condition for ϕ can be chosen simply as

$$\phi(0, \mathbf{x}, p) = p - u_0(\mathbf{x})\,. \tag{5}$$

if $u_0(\mathbf{x})$ is ocntinuous, or as the *signed distance function* if $u_0(\mathbf{x})$ is discontinuous (so ϕ is always continuous).

Multidimensional Hamilton-Jacobi equations

Consider the time dependent, d-dimensional Hamilton-Jacobi equation

(6) $$\partial_t S + H(\mathbf{x}, \nabla_{\mathbf{x}} S) = 0\,,$$

(7) $$S(0, \mathbf{x}) = S_0(\mathbf{x})\,.$$

Introduce $\mathbf{u} = (u_1, \cdots, u_d) = \nabla_{\mathbf{x}} S$. Taking the gradient on the H-J equation, one gets an equivalent (at least for smooth solutions) form of the Hamilton-Jacobi equation

(8) $$\partial_t \mathbf{u} + \nabla_{\mathbf{x}} H(\mathbf{x}, \mathbf{u}) = 0\,,$$

(9) $$\mathbf{u}(0, \mathbf{x}) \equiv \mathbf{u}_0(\mathbf{x}) = \nabla_{\mathbf{x}} S_0(\mathbf{x})\,.$$

Level set equation for H-J

We use d level set functions $\phi_i = \phi_i(t, \mathbf{x}, \mathbf{p})$, $i = 1, \cdots, d$, where $\mathbf{p} = (p_1, \cdots, p_d) \in \Re^d$, such that the intersection of their zero level sets yields $\mathbf{u}$, namely,

$$\phi_i(t, \mathbf{x}, \mathbf{p}) = 0 \qquad \text{at} \quad \mathbf{p} = \mathbf{u}(t, \mathbf{x})\,, \qquad i = 1, \cdots, d \tag{13}$$

Then one can show that ϕ_i satisfies

$$\partial_t \phi + \nabla_{\mathbf{p}} H \cdot \nabla_{\mathbf{x}} \phi - \nabla_{\mathbf{x}} H \cdot \nabla_{\mathbf{p}} \phi = 0\,. \tag{14}$$

It is the Liouville equation, which is linear hyperbolic with variable coefficients since in (**??**) $H = H(\mathbf{x}, \mathbf{p})$.

How to deal with measure-valued solution?

In physical space, the density and velocity may become **multivalued** after the formation of caustics, causing tremendous numerical difficulties.

Directly solving this measure-valued solution (by approximating the initial delta function numerically) leads to poor numerical resolution.

Scheme I is also unstable for such initial data

The level set method

By Jin, H.L. Liu, S. Osher and R. Tsai, *J. Comp. Phys*. 05

Decompose f into ϕ and ψ_i (i=1, ⋯ d)

ϕ and ψ_i both solve the same Liouville equation with initial data

$$\phi(\mathbf{x},\mathbf{v},0) = \rho_0(\mathbf{x})\,, \quad \psi_i(\mathbf{x},\mathbf{v},0) = v_i - u_{i0}(\mathbf{x})$$

then f = $\phi(\mathbf{x},\mathbf{v},t)\Pi_{i=1}^{d}\delta(\psi_i)$

and

$$\rho(\mathbf{x},t) = \int \phi(\mathbf{x},\mathbf{v},t)\Pi_{i=1}^{d}\delta(\psi_i)d\mathbf{v},$$

$$\mathbf{u}(\mathbf{x},t) = \int \phi(\mathbf{x},\mathbf{v},t)\mathbf{v}\Pi_{i=1}^{d}\delta(\psi_i)d\mathbf{v}/\rho(\mathbf{x},t)$$

Level set for multivalued solutions

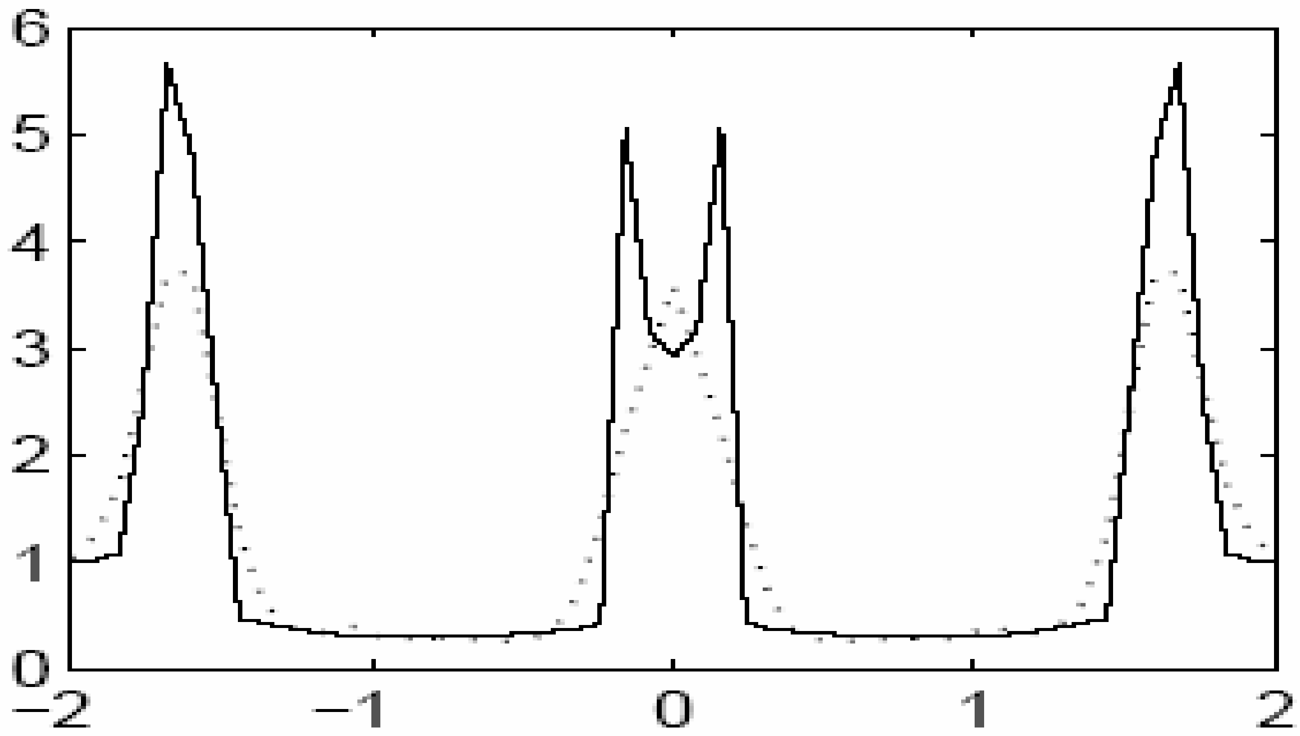
Note that ψ_i is the level set function to compute the multivalued solution of velocity u

Jin and Osher, *Comm. Math. Sci* 2003

Cheng, Liu and Osher, *Comm. Math. Sci* 2003

By using this decomposition we compute the Liouville equation with l^∞ data. The delta function is needed only at the post processing step when we need to evaluate the moments ρ and u !

Initial delta or not



Downstream discontinuity

- If V is discontinuous, the solution of ψ, even with a continuous initial data, become discontinuous with the discontinuity in the downstream of the potential barrier

This will affect the numerical accuracy

Numerical accuracy

It is well known that the l^1 convergence of a discontinuous solution to linear hyperbolic equation is **halfth order**

Thus a scheme solving the Liouville equation with a discontinous V has only **halfth-order** l^1 convergence.

Evaluating the moments through a singuler kernel also introduces a halfth order error

Thus the error for both f and the moments are halfth order.

Example 1

$$V(x) = \begin{cases} 0.2 & x < 0 \\ 0 & x > 0 \end{cases}$$

$$f(x, \xi, 0) = \begin{cases} 1 & x \leq 0, \xi > 0, \sqrt{x^2 + \xi^2} < 1, \\ 1 & x \geq 0, \xi < 0, \sqrt{x^2 + \xi^2} < 1, \\ 0 & \text{otherwise}, \end{cases}$$

Initial data (non-zero part)

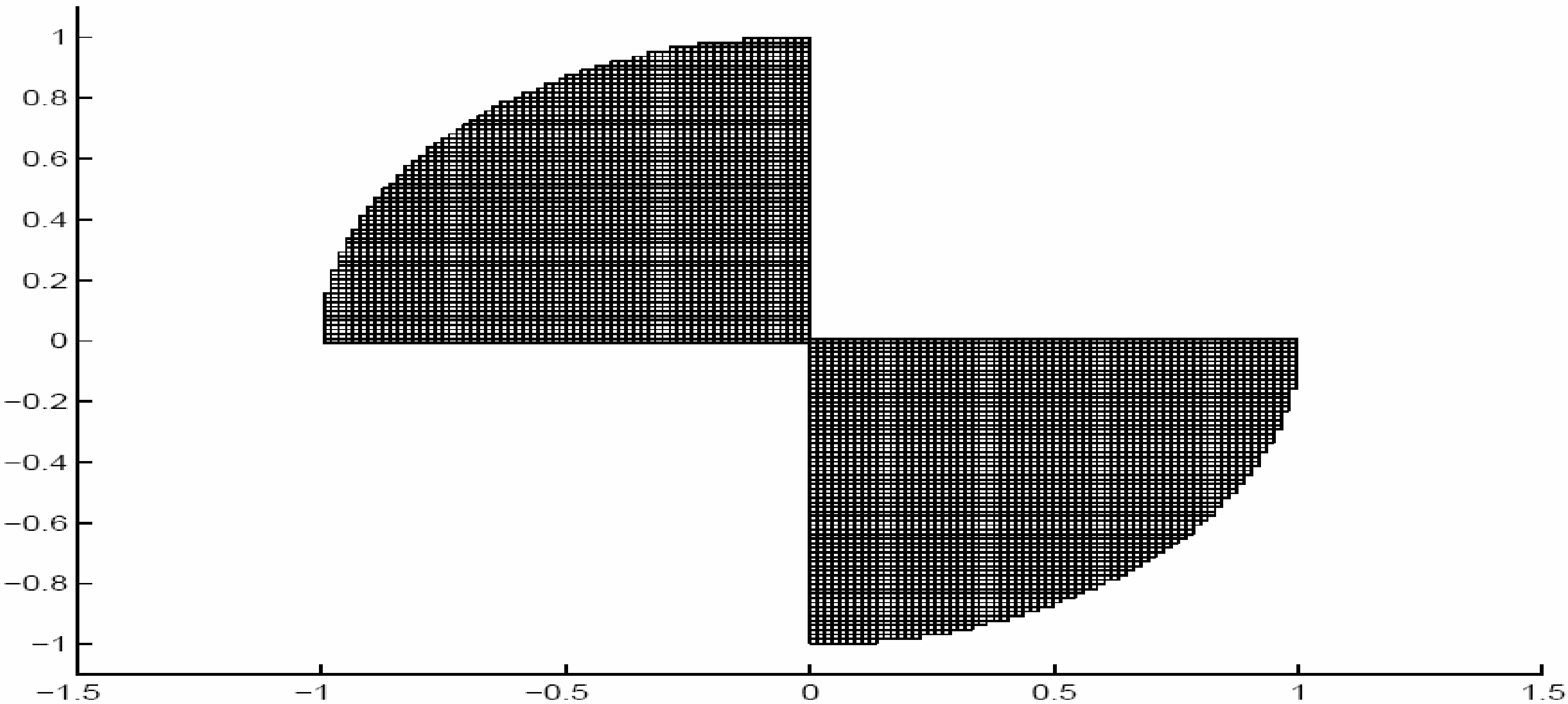
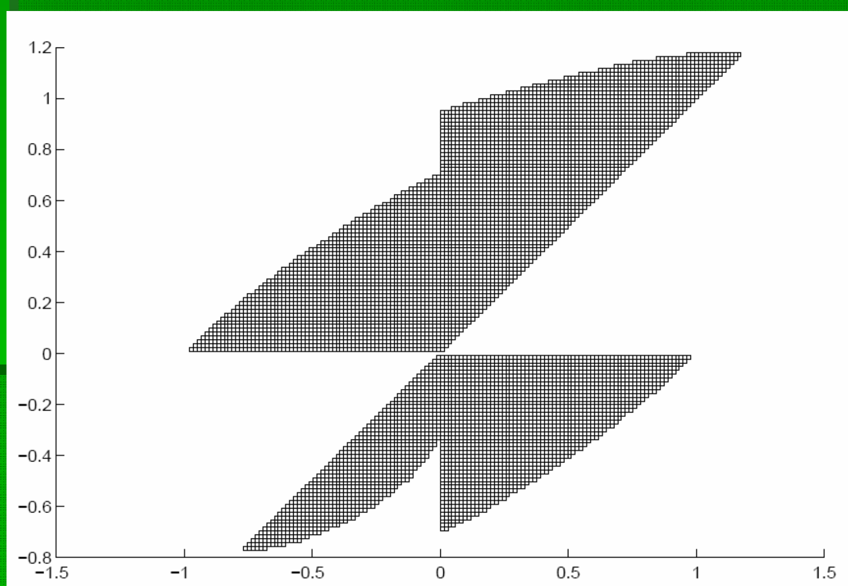


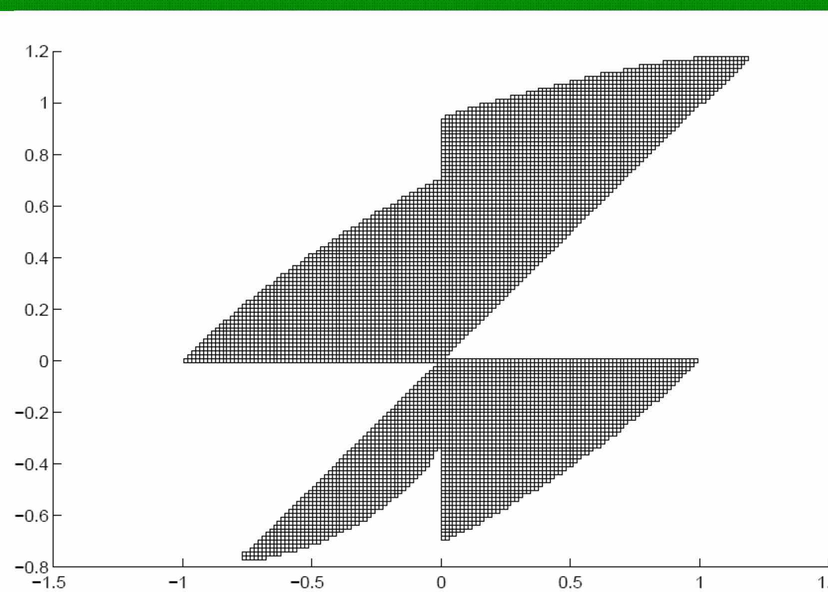
Figure 9.1 Example 9.1, the non-zero part of the initial data $f(x, \xi, 0)$ in (9.2). The horizontal axis is position, the vertical axis is velocity.

comparison

Exact solution



solution by Scheme I



L^1 error

Table 1 Example 9.1, l^1 error of numerical solutions on different meshes

mesh	50×51	100×101	200×201
Scheme I	0.245192	0.155871	0.093817
Scheme II	0.246248	0.156963	0.094275

Example 2 (semiclassical limit problem)

$$V(x) = \begin{cases} 0.2 & x < 0 \\ 0 & x > 0 \end{cases}$$

$$f(x, \xi, 0) = \delta(\xi - w(x))$$

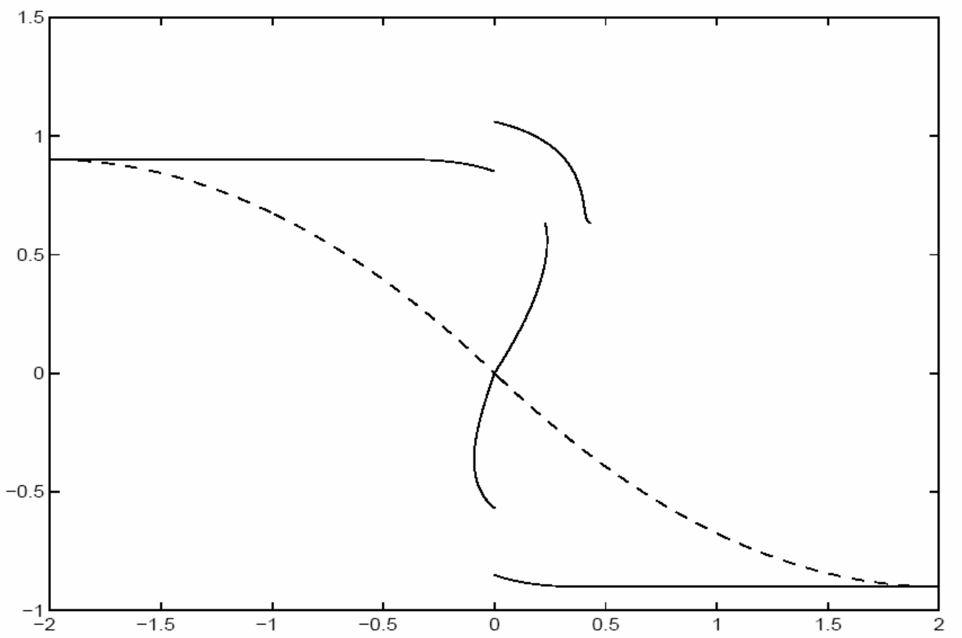
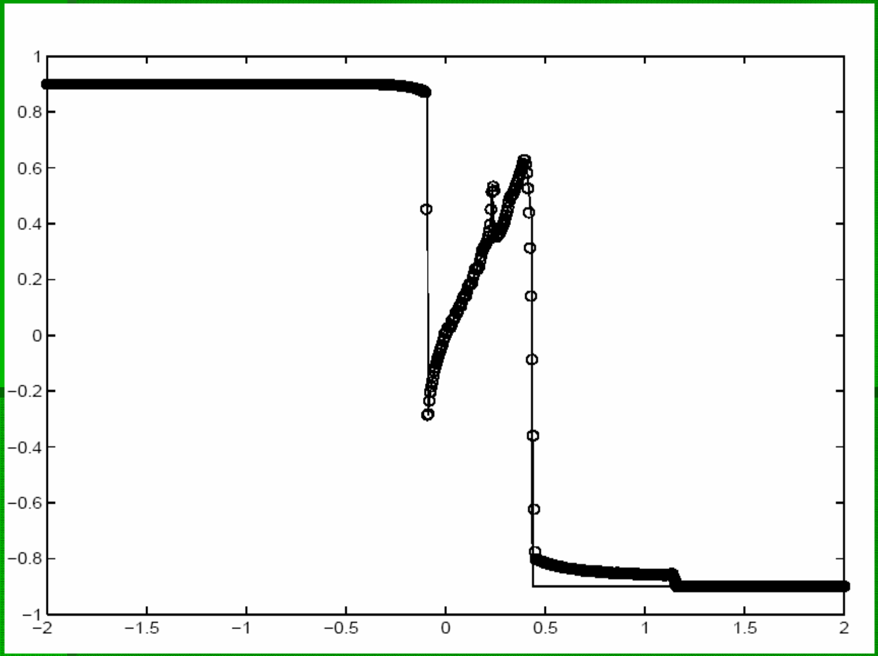


Figure 9.4 Example 9.2, velocity profile $w(x)$. Dashed line: initial velocity profile; Solid line: velocity profile $u(x,t)$ at $t = 1.8$. The horizontal axis is position, the vertical axis is velocity.

Solution by 800 x 640 mesh

Averaged Velocity density



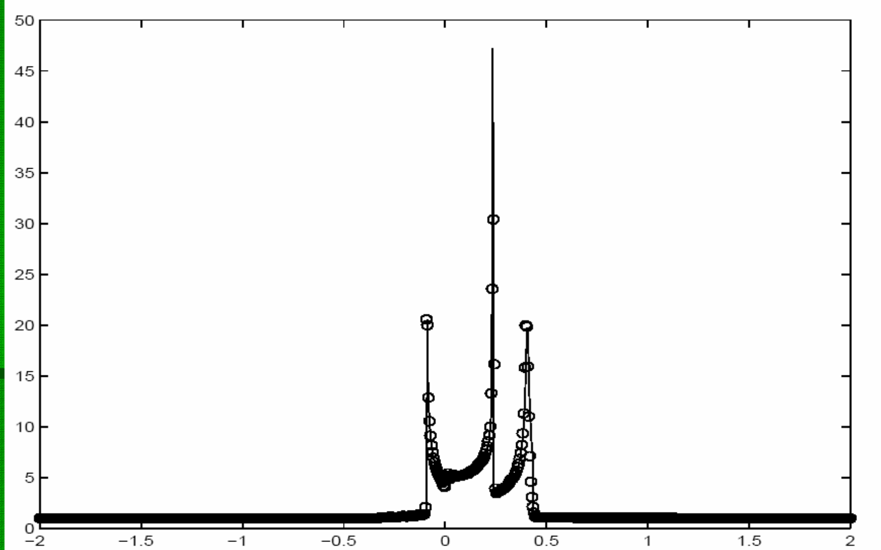


Figure 9.6 Example 9.2, density in physical space at $t = 1.8$. Solid line: exact solution; 'o': numerical solution using a 800×641 cell.

L^1 error for density

Table 3 l^1 error of the numerical averaged velocity ρ on different meshes

mesh	200×161	400×321	800×641
Scheme I	0.170247	0.116522	0.073458
Scheme II	0.170900	0.128646	0.081642

Example 2: a 2D semiclassical limit problem

$$f_t + \xi f_x + \eta f_y - V_x f_\xi - V_y f_\eta = 0$$

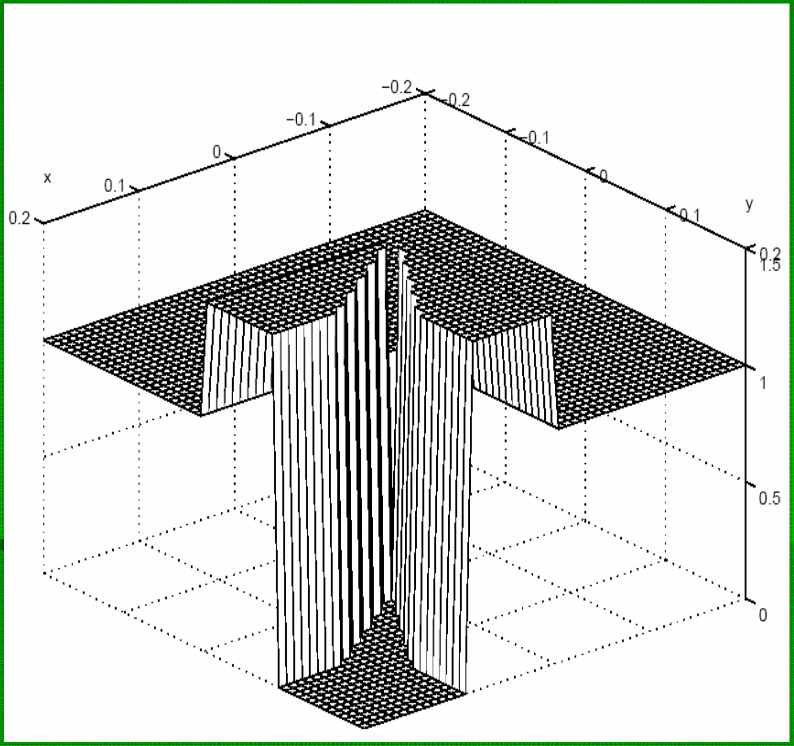
$$V(x,y) = \begin{cases} 0.1, & x > 0, y > 0, \\ 0, & \text{else} \end{cases}$$

$$f(x,y,\xi,\eta,0) = \rho(x,y,0)\delta(\xi - p(x,y))\delta(\eta - q(x,y)),$$

$$\rho(x,y,0) = \begin{cases} 0 & x > -0.1, y > -0.1 \\ 1 & \text{else} \end{cases},$$

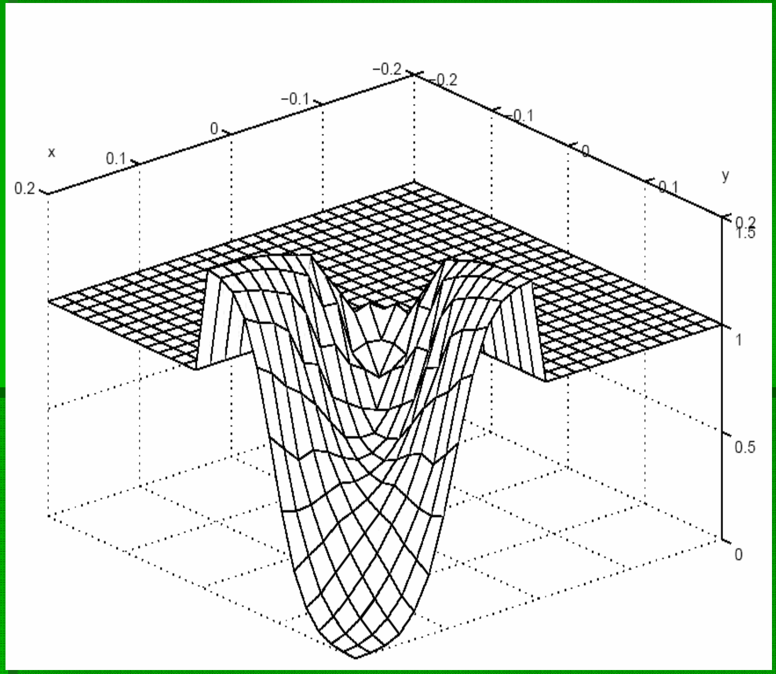
$$p(x,y) = q(x,y) = \begin{cases} 0.4 & x > 0, y > 0 \\ 0.6 & \text{else} \end{cases}.$$

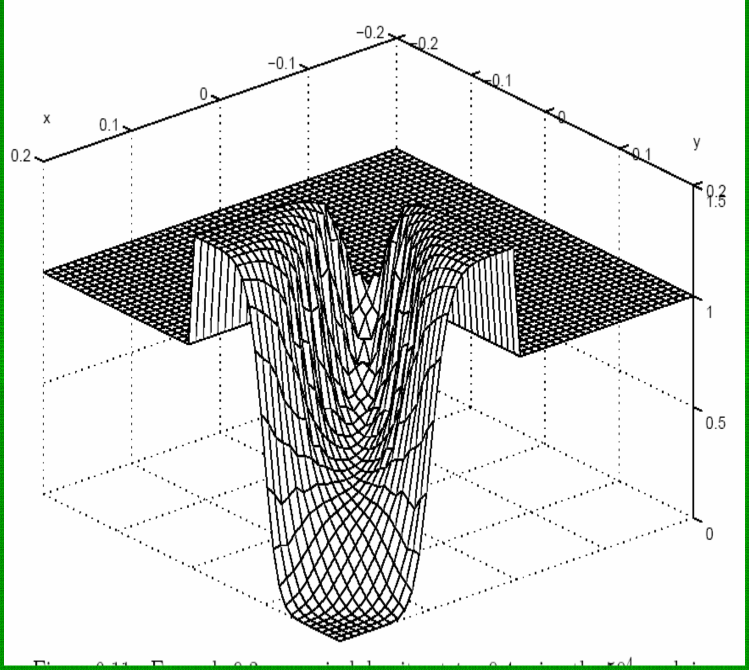
Exact density at t=0.4



Numerical density by Scheme I

- 26^4 mesh 50^4 mesh





l^1 error

Table 4 l^1 error of numerical densities on $[0, 0.2] \times [0, 0.2]$ using different meshes

mesh	14^4	26^4	50^4
Scheme I	0.01851	0.01417	0.01029
Scheme II	0.01864	0.01527	0.01257

High frequency waves with discontinuous wave speed

The high frequency (geometrical optics) limit of wave equations

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

is the Liouville equation with $H=c(\mathbf{x})|\mathbf{p}|$

$$f_t + c(x)\, p/|p| \cdot \nabla_x f + |p|\, \nabla c(x) \cdot \nabla_p f = 0$$

We have also constructed similar Hamiltoian-Preserving schemes for $c(\mathbf{x})$ discontinuous

Hamiltonian-preserving=Snell's Law

- We can show that the Hamiltonian preservation is equivalent to Snell's law for a plane wave hits a flat interface.

Transmission and reflection

We can extend our algorithm to the case when both transmission and reflection coexist

$f(x,\xi) = \alpha_T f(x^-, \xi^-) + \alpha_R f(x^+, \xi^+)$

α_R: reflection rate

α_T: transmission rate

$$\alpha_R + \alpha_T = 1$$

New numerical difficulty

The decomposion idea of Jin-Liu-Osher-Tsai does not apply here, and one has to use the delta initial data numerically

Since the solution to the ODEs (bicharacteristics) bifurcates at interface with given probability to transmit or being reflected

Stability results

- We obtained similar stability results for the scheme for the wave equations, even when both transmission and reflection coexist

Other possible applications

When there is an external field:

acoustic waves, elastic waves,

Vlasov-Poission, Vlasov-Maxwell, etc.

The principle of Hamiltonian-preserving can certainly be used in these systems

Other ongoing projects

- A Monte-Carlo particle method for Hamiltonian systems with discontinuous Hamiltonians (with F. Bai and L. Wu)
- Quantum Liouville equation (with K. Novak):

  we aim at developing "semiclassical Liouville approach to quantum potential barrier"
- Elastic wave (with X. Liao)
- When the interface is not aligned with the grids, or curved interface, etc.
- Diffraction: incorporate GTD into the numerical flux…