Computational Methods of Physical Problems with Mixed Scales

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Scales and Physical Laws

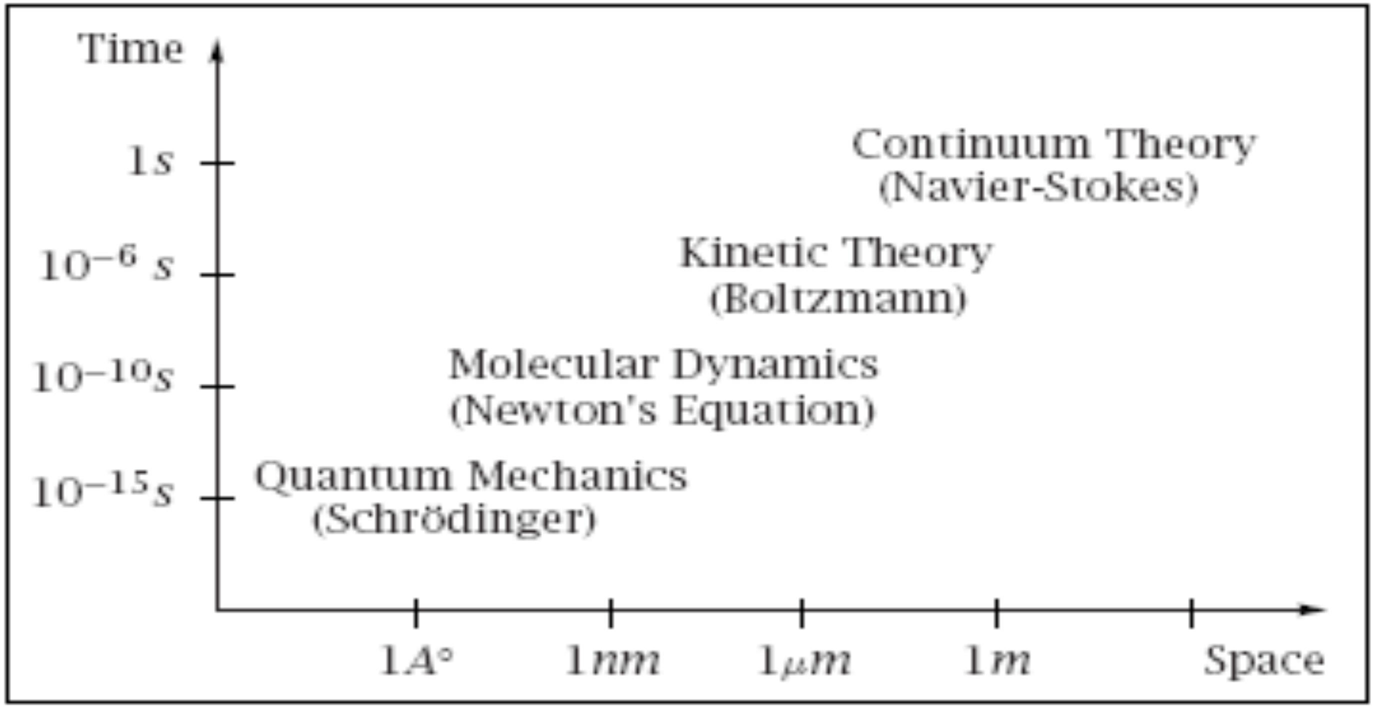


Figure 1. Different laws of physics are required to describe properties and processes of fluids at different scales.

- Figure from E & Engquist, AMS Notice

Connections between these physical laws

- Quantum mechanics → classical mechanics
  Wigner transform and semi-classical limit
  Planck constant →0

- Classical mechanics → Boltzmann Kinetic equations
  BBGKY hierarchy, Grad-Boltzmann limit
  $N \to \infty$, $\sigma \to 0$, $N\sigma^2$ = constant

- Kinetic equations to hydrodynamics equations
  Hilbert and Chapman-Enskog expansions
  Knuden number (mean free path) → 0

Problems of multiple scales

- Physical laws at smaller scales contain laws at larger scales at some level of approximations; they are more accurate but more computationally expensive--very often prohibitively expensive
- Many physical problems contain scales of different orders of magnitude. A multiscale computational method is more efficient than a full small-scale simulation
- Understandings of the mathematical transitions from one scale to another are crucial for and guide the design of multiscale methods

Outline of this tutorial

- The tutorial surveys some (recent) computational methods for

☆ Multi-scale quantum-classical coupling

☆ Multi-scale kinetic-hydrodynamic coupling

I. Battling scales in Quantum mechanics

- Difficulties in a quantum simulation

1) N-body quantum system:

 solve the Schrodinger equation in 3N-dimension: Born-Oppenheimer approximations, Hartree approximation, Hartree-Fock apprimixation, density function theory, etc.

2) Small scale: valid from Angstroms (10^{-10} m) to hundreds of nanometers

We will mainly focus on point 2)

Electromagnetic spectrum

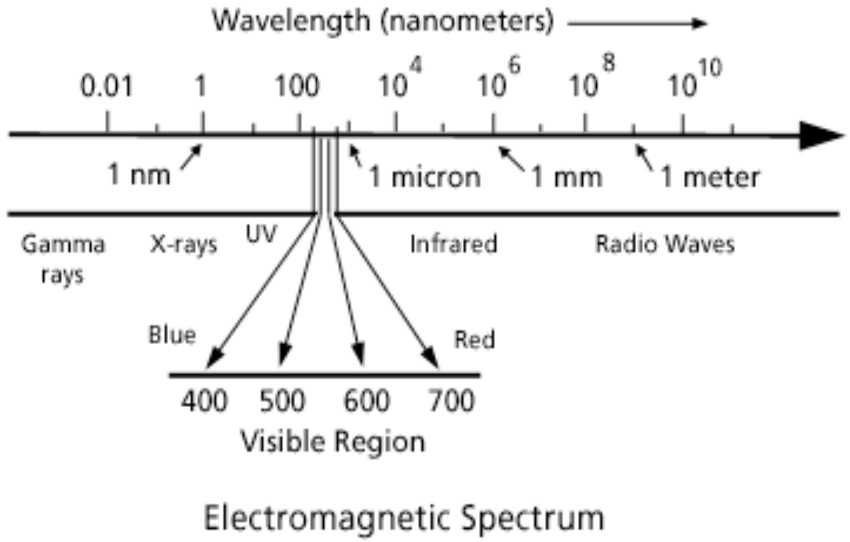


Fig. 1. The electromagnetic spectrum, which encompasses the visible region of light, extends from gamma rays with wave lengths of one hundredth of a nanometer to radio waves with wave lengths of one meter or greater.

- High frequency waves: wave length/domain of computation <<1

Difficulty of high frequency wave computation

- Consider the example of visible lights in this lecture room:

wave length: » 10^{-6} m

computation domain » m

1d computation: 10^{6} » 10^{7}

2d computation: 10^{12} » 10^{14}

3d computation: 10^{18} » 10^{21}

do not forget time! Time steps: 10^{6} » 10^{7}

Linear Schrodinger Equation

$$i\epsilon \psi_t + \frac{\epsilon^2}{2}\Delta\psi - V\psi = 0 \qquad \mathbf{x} \in R^d, \quad t > 0$$
$$\psi(\mathbf{x},0) = A_0(\mathbf{x})e^{i\frac{S_0(\mathbf{x})}{\epsilon}}$$

In this equation, $\psi(\mathbf{x}, t)$ is the complex-valued *wave function*, ϵ is or is playing the role of *Planck's constant*. It is assumed to be small here. The solution ψ and the related physical observables become *oscillatory* in space and time in the order of $O(\epsilon)$, causing all the mathematical and numerical challenges.

Free Schrodinger equation (V=0)

If $\psi(x,0)=\exp\,(ik¢\; x/\varepsilon)$, $x\in R^d$

Then $\psi(x, t)=\exp\,[i(\,k\, ¢\; x/\varepsilon-\,|k|^2t/(2\varepsilon)]$

solution is oscillatory in both space and time: wave length $O(\varepsilon)$

No explicit solution for $V \neq 0$

Semiclassical limit of the linear schrodinger equation

If one can find the asymptotic (semiclassical) limit as $\varepsilon \lozenge 0$ then one can just solve the *limiting* equation numerically (no more ε !)

The WKB Method

We assume that solution has the form (*Madelung Transform*)

$$\psi(\mathbf{x}, t) = A(\mathbf{x}, t)e^{i\frac{S(\mathbf{x},t)}{\epsilon}}$$

and apply this ansatz into the Schrodinger equation with initial data.

Separating the real part from the imaginary part, and keeping only the leading order term, one

can get

$$S_t + \frac{1}{2}|\nabla S|^2 + V = 0 \qquad \text{eiconal equation}$$

$$(|A|^2)_t + \nabla \cdot (|A|^2 \nabla S) = 0 \quad \text{transport equation}$$

Pressureless gas equations

Let

$$\rho(t, \mathrm{x}) = |A(t, \mathrm{x})|^2$$
$$\rho(t, \mathrm{x})\mathbf{u}(t, \mathrm{x}) = \rho(t, \mathrm{x})\nabla S(t, \mathrm{x})$$

Then these "fluid variables" satisfy the *pressureless* gas dynamics equations

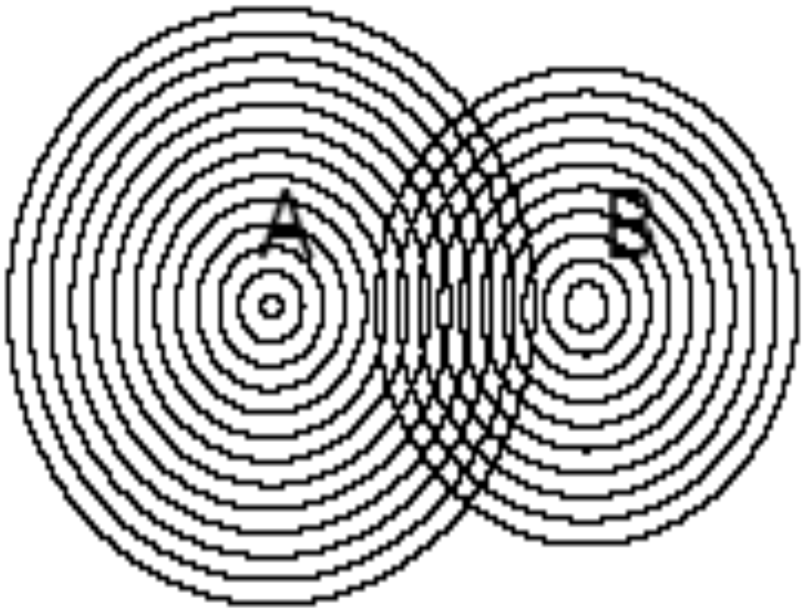
$$\rho_t + \nabla \cdot (\rho\mathbf{u}) = 0,$$
$$(\rho\mathbf{u})_t + \nabla \cdot (\rho\mathbf{u}\mathbf{u}) + \rho\nabla V = 0,$$

Linear superposition vs viscosity solution

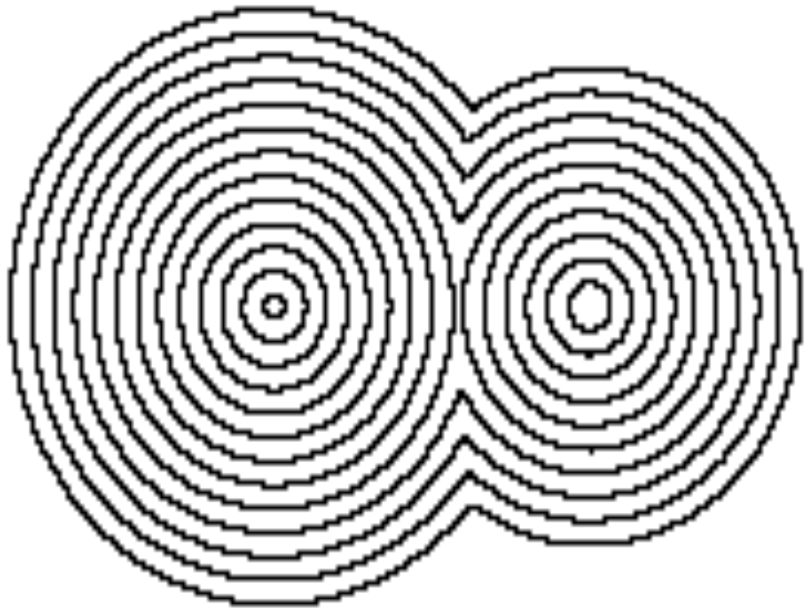
This limit can be justified for smooth solutions (**Grenier** 98). Beyond the singularity (*caustics*) of the eiconal equation this system is no longer the correct *weak solution* of the Semi-classical limit of the Schrodinger equations, even for linear problem.

For example, in the linear case, the Schrodinger equation satisfies the **superposition principle**, while the *viscosity* solution, in the sense of **Crandall and Lions**, for the eiconal equation beyond the caustics, is **not** linearly superimposable.

Linear superposition vs viscosity solution

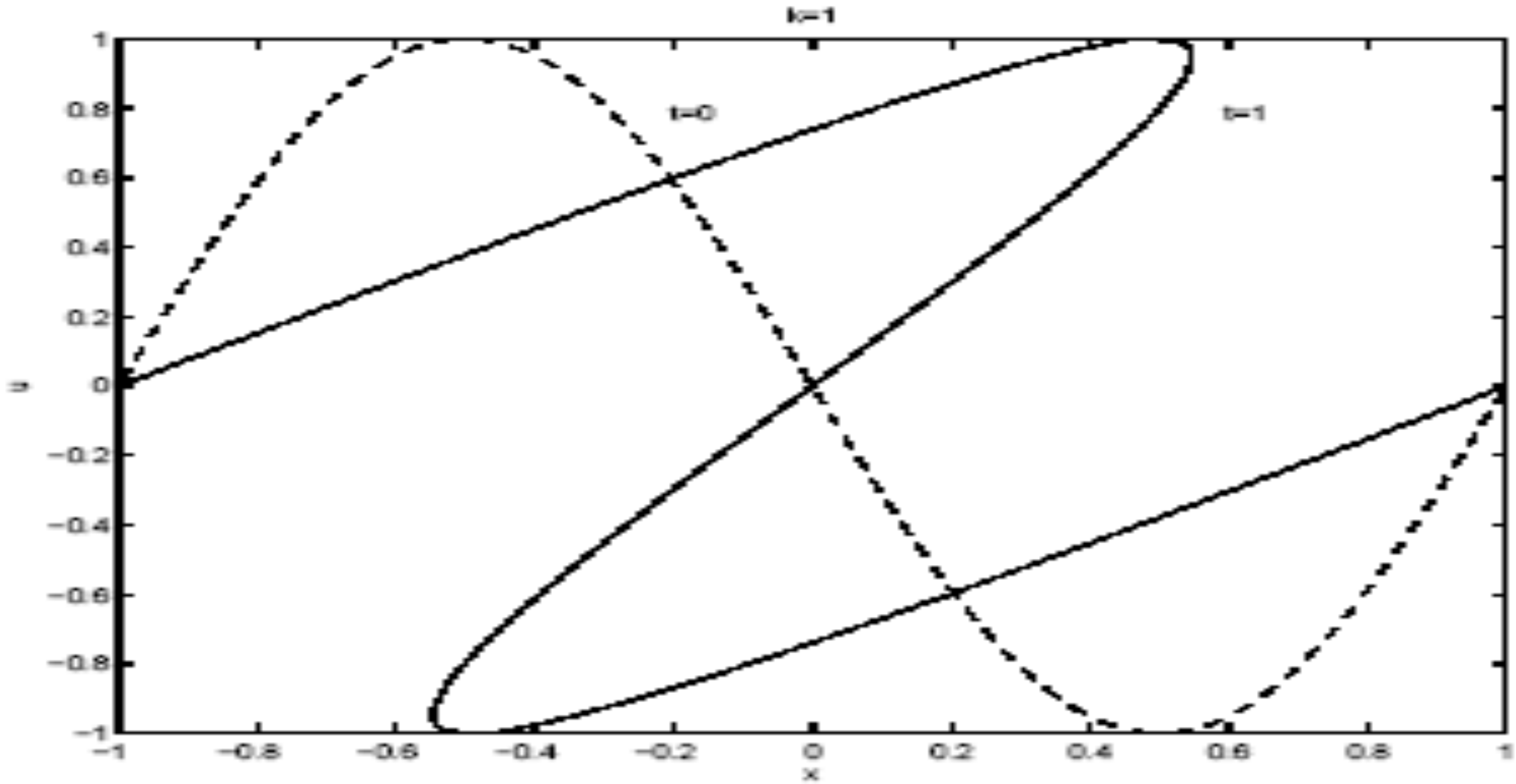


(a) Correct solution



(b) Eikonal equation

Shock vs. multivalued solution



Semi-classical limit in the phase space

Wigner Transform

$$W(x,k)=1/(2\pi)^d \int_{R^d} e^{-i\,k \cdot y}\, \psi(x+\varepsilon y/2)\psi^*(x-\varepsilon y/2)\, dy$$

where ψ^* is the complex conjugate of ψ.

A convenient tool to study the semiclassical limit

Lions-Paul;

Gerard, Markowich, Mauser, Poupaud;

Papanicolaou-Ryzhik-Keller

Moments of the Wigner function

The connection between W^{ε} and ψ is established through the moments

$$\int_{R^d} W^{\epsilon}(\mathrm{x},\mathrm{k})\,d\mathrm{k} = |\psi(\mathrm{x})|^2$$

$$\int_{R^d} \mathrm{k}W^{\epsilon}(\mathrm{x},\mathrm{k})\,d\mathrm{k} = \frac{1}{2i}(\psi\nabla\overline{\psi} - \overline{\psi}\nabla\psi)$$

$$\int_{R^d} |\mathrm{k}|^2 W^{\epsilon}(\mathrm{x},\mathrm{k})d\mathrm{k} = |\nabla\phi(\mathrm{x})|^2$$

The Wigner equation

- W^ε satisfies the Wigner equation

$$W^\varepsilon_t + k \cdot \nabla_x W^\varepsilon - \Theta^\varepsilon[V]\, W^\varepsilon = 0$$

Where

$$\Theta^\varepsilon[V]\, W^\varepsilon = \varepsilon^{-1} /(2\pi)^d \cdot \int_{R^d} e^{ik \cdot y}\, \psi(x-\varepsilon y/2)[V(x+\varepsilon\, y/2)-V(x-\varepsilon\, y/2)]\, dy$$

The semi-classical limit

As $\epsilon \to 0$, the limit Wigner equation is the **Liouville equation** in phase space

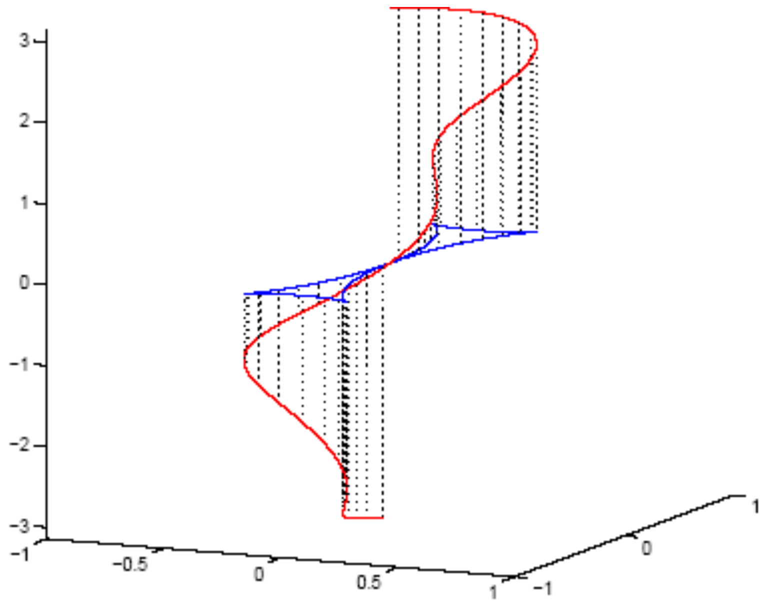
$$W_t + \mathbf{k} \cdot \nabla_{\mathbf{x}} W - \nabla V \cdot \nabla_{\mathbf{k}} W = 0$$

with the initial condition

$$W(0, \mathbf{x}, \mathbf{k}) = |A_0(\mathbf{x})|^2 \delta(\mathbf{k} - \nabla S_0(\mathbf{x}))$$

Semiclassical limit beyond caustics

In the *linear* case, the Liouville equation still holds beyond the caustics; it *unfolds* the caustics in the phase space



Some phase information is missing: Keller-Maslov index

The semiclassical limit for the moments

For smooth solution, the solution

$$\psi(\mathbf{x},t) = A(\mathbf{x},t)e^{i\frac{S(\mathbf{x},t)}{\epsilon}}$$

has a limit

$$W(t,\mathbf{x},\mathbf{k}) = |A(t,\mathbf{x})|^2\delta(\mathbf{k} - \nabla S(t,\mathbf{x}))$$

Applying this ansatz to the Liouville equation one gets the *eiconal* equation for the phase S and *transport* equation for amplitude $|A|^2$, recovering the result by WKB.

Difficulties for computing the semi-classical limit

- In the physical space solution becomes multi-valued
- In phase space, solution in defined in higher dimension, and is singular (measure-valued)

moment methods and level set methods have been developed to deal with these difficulties

Kinetic moment closure

Since the Liouville equation is a *kinetic* equation defined in the *phase* space (**six dimensional** !), it is too expensive to solve numerically. We hope to bring it down to the physical space. This usually requires special density distribution (**Grad, Levermore, extended thermodynamics).**

We are interested in computing the **multivalued** or **multiphased** solutions. If the total number of phases is **finite**, we can find a limiting distribution for W^ε that can be used to close the Liouville equations **exactly**

Multiphase ansatz

Use the **stationary phase method** or the **Fourier integral operators**, one can prove that, if the total number of phases is $N < \infty$, then

$$\psi \approx \sum_{k=1}^{N(\mathbf{x},t)} \psi_k(\mathbf{x},t) = \sum_{k=1}^{N(\mathbf{x},t)} A_k(\mathbf{x},t)\, e^{i\frac{S_k(\mathbf{x},t)}{\epsilon}}.$$

In addition, we have $\mathbf{u}_k(\mathbf{x},t) = \nabla S_k(\mathbf{x},t) \neq \mathbf{u}_j(\mathbf{x},t)$ for $k \neq j$ and A_k's *are bounded away from 0.*

Multiphase ansatz in the semiclassical limit

If one calculates the Wigner function, one can find its limit to be (away from the caustics)

$$w(\mathbf{x}, \mathbf{v}, t) = \sum_{k=1}^{N(\mathbf{x},t)} \rho_k \delta(\mathbf{v} - \mathbf{u}_k)$$

Moreover, each $(\rho_k, \mathbf{u}_k)$ satisfies the pressureless gas equations.

Sparber, Markowich, Mauser;

Jin-Xiantao Li

Moment equations in 1D (with *X. Li*)

Define the moments

$$m_l = \int_R w(x,v,t)v^l dv, \ \ l = 0, 1, \cdots, 2N.$$

In addition, we define the density and velocity by

$$\rho(x,t) = m_0, \qquad u(x,t) = \frac{m_1}{m_0}.$$

Multiplying the Liouville equation in 1-d by $v^l, l = 0, 1, \cdots, 2N-1$ and integrating over v, one obtains the moment equations in the physical space

$$\begin{aligned}
\partial_t m_0 + \partial_x m_1 &= 0, \\
\partial_t m_1 + \partial_x m_2 &= -m_0 \partial_x V, \\
\cdots\cdots\cdots & \\
\partial_t m_{2N-1} + \partial_x m_{2N} &= -(2N-1) m_{2N-2} \partial_x V.
\end{aligned}$$

Moment closure in 1D

With the multiphase ansatz, one has

$$m_l = \sum_{k=1}^{N} \rho_k u_k^l,\ l = 0, 1, \cdots, 2N.$$

With these one can close the moment system by expressing m_{2N} as a function of $m_0, \cdots, m_{2N-1}$,

$$m_{2N} = F_N(m_0, m_1, \cdots, m_{2N-1}),$$

provided the $2N \times 2N$ system

$$m_l = \sum_{k=1}^{N} \rho_k u_k^l,\ l = 0, 1, \cdots, 2N-1$$

is invertible, allowing us to express $(\rho_k, u_k, k = 1, \cdots, N)$ in terms of $m_0, m_1, \cdots, m_{2N-1}$. If this

A weakly hyperbolic system

- F_N can be defined and consequently the multiphase equations are equivalent to the N pressureless gas equations satisfied by each (ρ_k, u_k)
- The moment systems are

  ---*weakly hyperbolic*—

  the Jacobian is similar to Jordan blocks.

Two phase equations in 1D

If $N = 2$, then one obtains four moment equations

$$\begin{aligned}
\partial_t m_0 + \partial_x m_1 &= 0, \\
\partial_t m_1 + \partial_x m_2 &= -m_0 \partial_x V, \\
\partial_t m_2 + \partial_x m_3 &= -2 m_1 \partial_x V, \\
\partial_t m_3 + \partial_x m_4 &= -3 m_2 \partial_x V,
\end{aligned}$$

with

$$m_4 = \frac{m_3^2 m_0 - 2 m_1 m_2 m_3 + m_2^3}{m_0 m_2 - m_1^2}.$$

Modified flux

Clearly, m_4 is not well-defined if $\frac{m_0 m_2 - m_1^2}{\rho_1 \rho_2} = (u_2 - u_1)^2 = 0$ (when there is just *one* phase). We modify m_4 as follows:

$$m_4 = \begin{cases} \frac{m_3^2 m_0 - 2m_1 m_2 m_3 + m_2^3}{m_0 m_2 - m_1^2}, & \text{if} \quad m_0 m_2 - m_1 \neq 0; \\ \frac{m_2^2}{m_0}, & \text{Otherwise.} \end{cases}$$

Then the moment system is good for both single and double phases, whichever emerges.

Phase boundaries are **undercompressive shocks**

Higher moment equations

Similar moment equations can be obtained for larger N (algebraically the flux becomes increasingly more complicated with larger N and one needs to use numerical procedure to generate the flux F_N for N>5.

F_N is always a rational function of m_0, ⋯, M_{2N-1}, and the zero denominator condition can be used to determine the correct number of phases as was done for N=2. Similar modified flux may also be introduced.

We have also found moment equations for 2-D.

One can estimate the total number of phases in 1-D (*number of intitial inflection points*).

For multi-D physical intuition is needed for such an estimate.

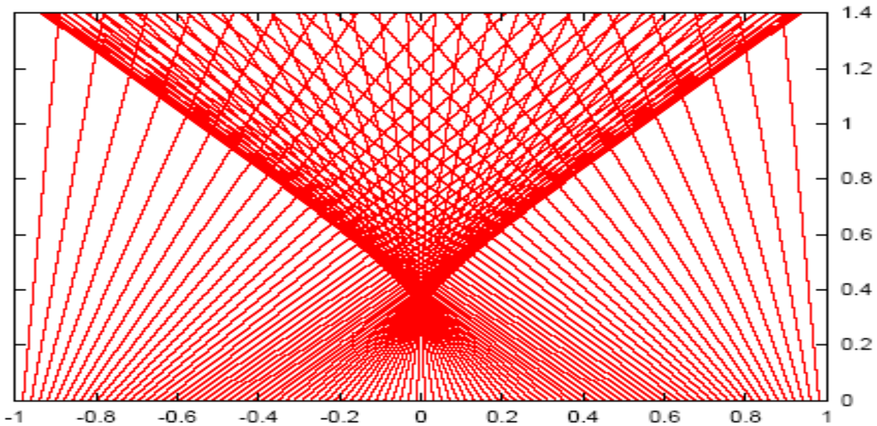
For wave equations moment methods were used by Brenier-Corias, ('84, 98), Engquist-Runborg '96, Gosse '03

Kinetic schemes for moment equations

Since the moment system is only *weakly hyperbolic*, and the flux function cannot be expressed analytically when N is large, the *Godunov* type scheme is out of the question.

On the other hand, since the moment system arises as a moment closure of the kinetic Liouville equation, thus a **kinetic scheme** is the most natural choice for the moment systems.

Burgers' equation



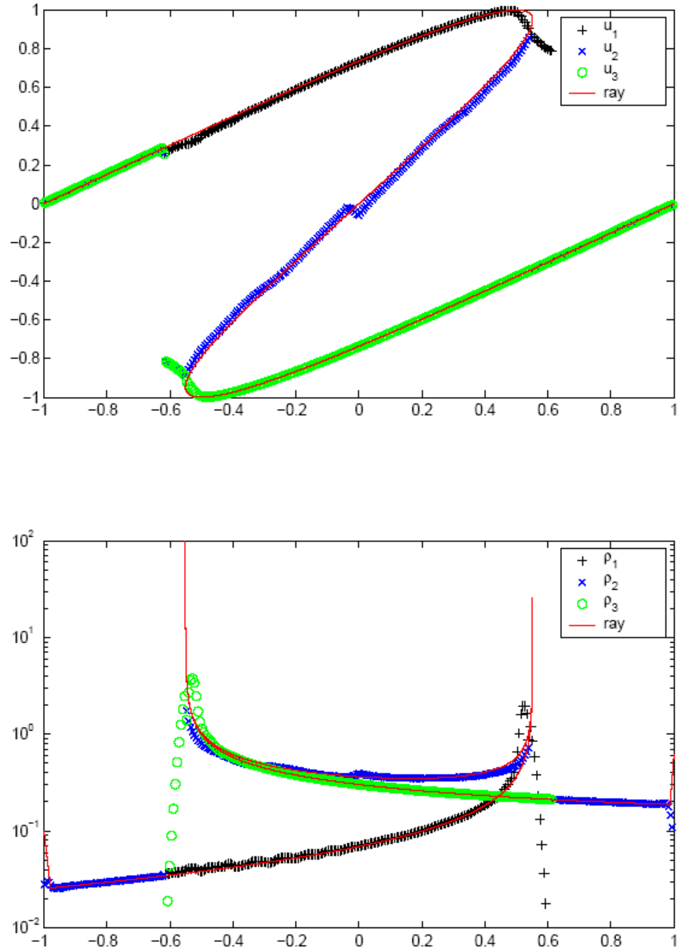


FIGURE 4. Numerical results for $u_{1,2,3}$ (top) and $\rho_{1,2,3}$ (bottom) at time $T = 1$ with (20), $N = 3$ (second order) and $p = 1$.

A level set method

- joint work with **S. Osher** (*Comm Math Sci ’03)*
- also see *Cheng-Liu-Osher* (*Comm Math Sci* ’03)
- Liouville-based level set for multivalued fronts: *Engquist-Runborg-Tornberg, Fomel-Sethian, Osher-Cheng-Kang-Shim-Tsai*

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

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}:

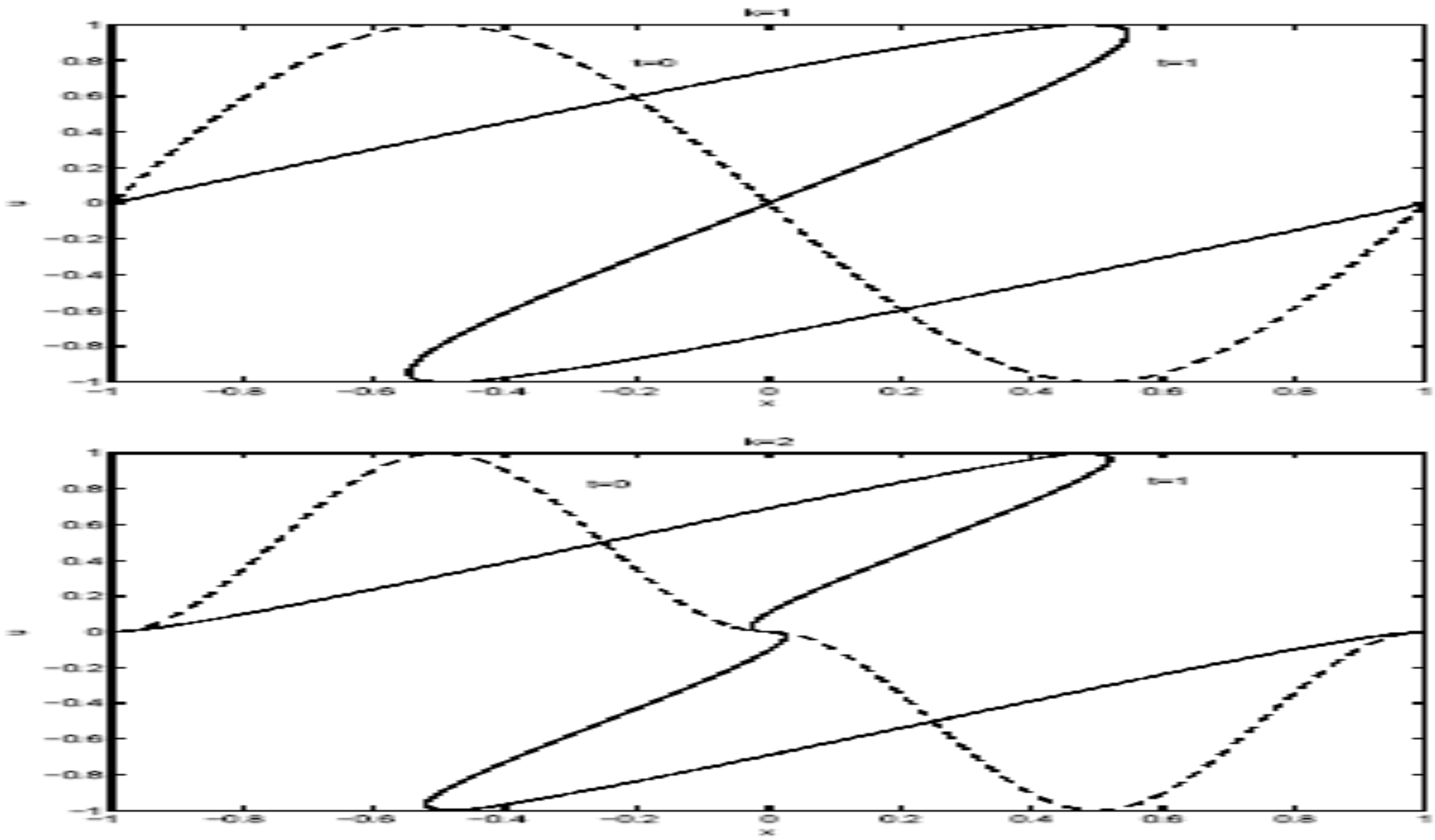
$$\partial_t \phi + \mathbf{F}(p) \cdot \nabla_{\mathbf{x}} \phi - q(\mathbf{x})\, \partial_p \phi = 0\,. \tag{4}$$

The initial condition for ϕ can be chosen simply as

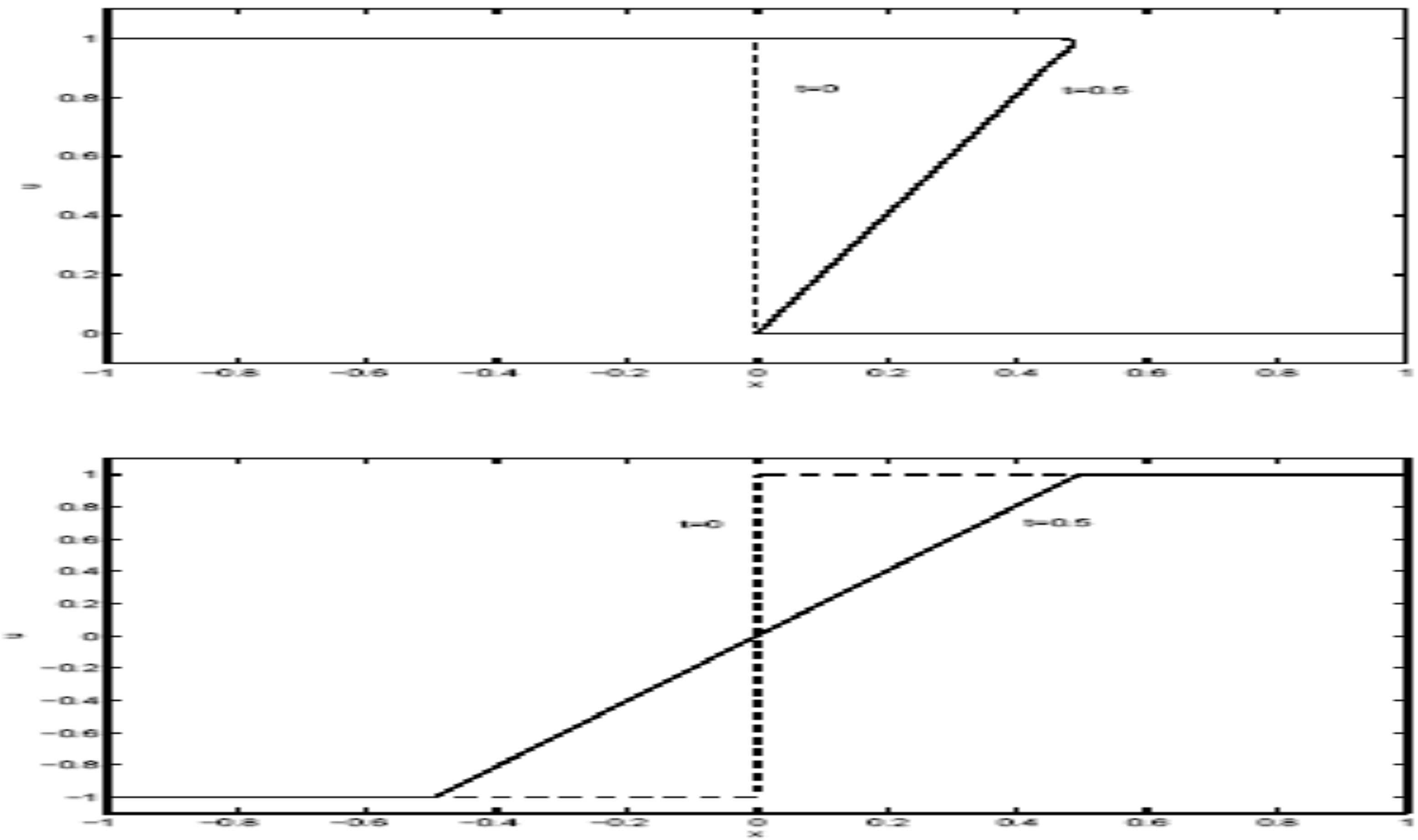
$$\phi(0, \mathbf{x}, p) = p - u_0(\mathbf{x})\,. \tag{5}$$

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).

Multivalued solution to the Burgers equation



Riemann problem for Burgers' equation



Burger’s equation with harmonic osccilator forcing

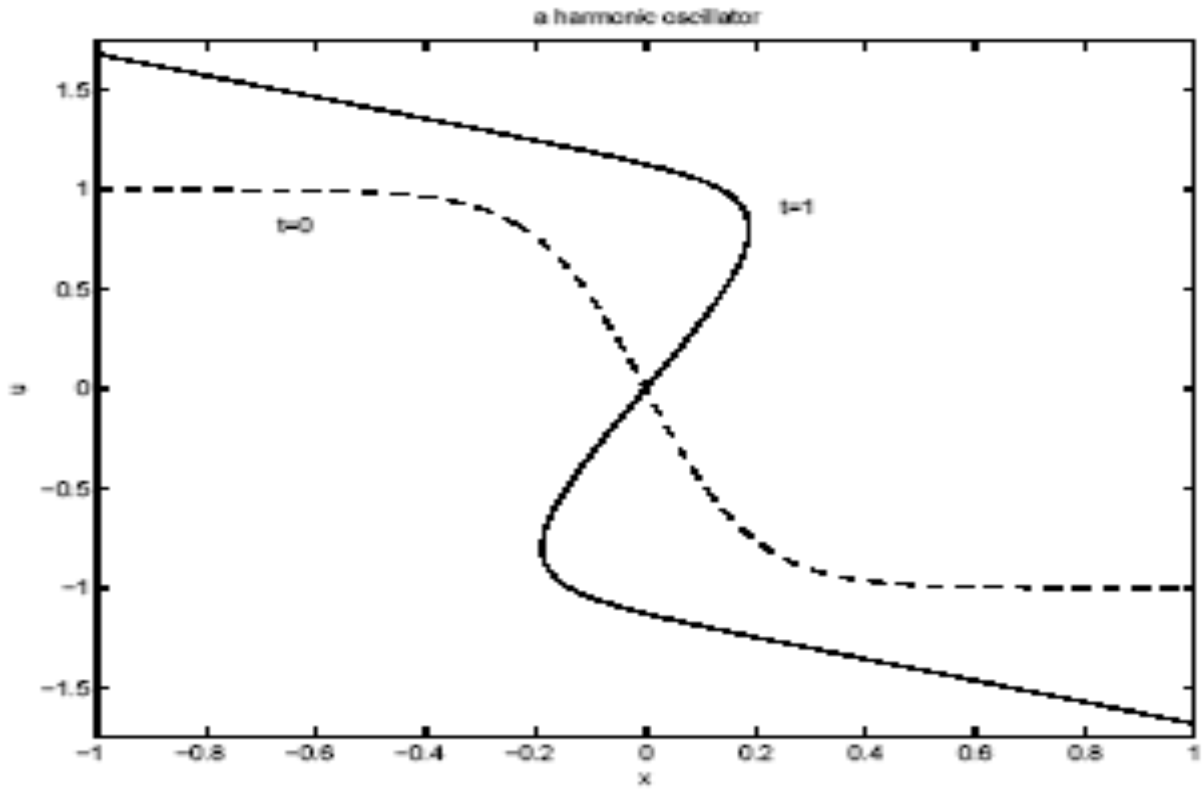
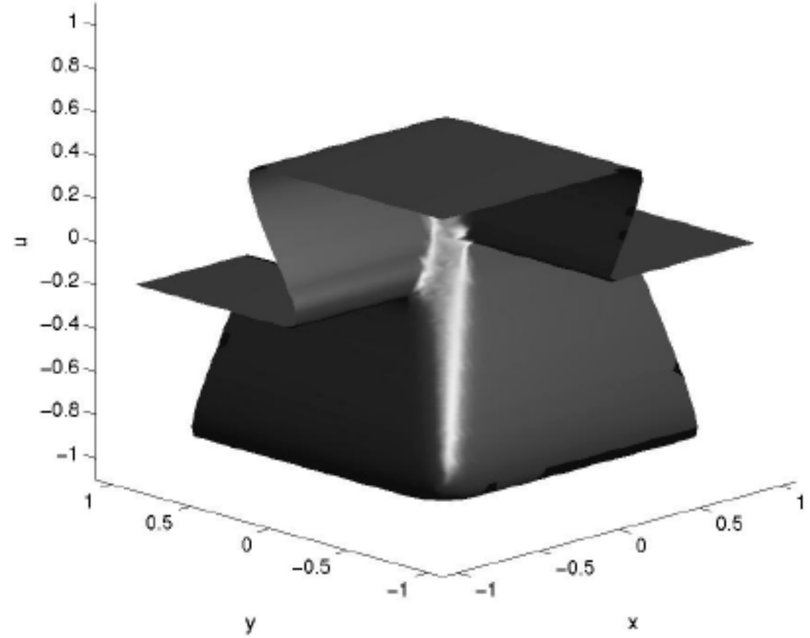


FIG. 4.3. *The numerical solutions of the harmonic oscillator case.*

Riemann problem for 2d Burgers



- $uu_t+uu_x+uu_y=0$

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,

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

(13)

Then one can show that ϕ_i satisfies

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

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

Initial condition

A convenient initial condition for each ϕ_i, $i = 1, \ldots, n$ can be taken as:

$$\phi_i(0, \mathbf{x}, \mathbf{p}) = p_i - u_i(\mathbf{x}) \,. \tag{15}$$

One should use the signed distance function if the initial data are discontinuous.

Local level set method can be used to reduce the cost to $O(N^d \ln N)$

2d Hamilton-Jacobi

Density and other physical observables

If one is interested in also computing the density, or other physical observables (momentum, energy, etc.), the solving directly the continuity equation

$$\rho_t + \nabla \cdot \rho \mathbf{u} = 0$$

will be difficult when $\mathbf{u}$ is multivalued.

One can of course solve the Liouville equation

$$W_t + \mathbf{k} \cdot \nabla_{\mathbf{x}} W - \nabla V \cdot \nabla_{\mathbf{k}} W = 0$$

with the measure-valued initial data

$$W(0, \mathbf{x}, \mathbf{k}) = |A_0(\mathbf{x})|^2 \delta(\mathbf{k} - \nabla S_0(\mathbf{x}))$$

This involves 1) approximating the delta function initially and then 2) numerically evolving a "delta" function in time.

Due to numerical dissipation the accuracy will be low.

Phase space computation of physical observables

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

We now consider the following two problems.

$$\partial_t f + \mathbf{k} \cdot \nabla_{\mathbf{x}} f - \nabla V \cdot \nabla_{\mathbf{k}} f = 0\,,$$
$$f(0, \mathbf{x}, \mathbf{k}) = \rho_0(\mathbf{x})\,;$$

$$\partial_t \phi + \mathbf{k} \cdot \nabla_{\mathbf{x}} \phi - \nabla V \cdot \nabla_{\mathbf{k}} \phi = 0\,,$$
$$\phi(0, \mathbf{x}, \mathbf{k}) = \mathbf{k} - \mathbf{u}_0(\mathbf{x})\,.$$

we can prove that

$$W(t, \mathbf{x}, \mathbf{k}) = f(t, \mathbf{x}, \mathbf{k})\delta(\phi(t, \mathbf{x}, \mathbf{k}))\,. \tag{16}$$

Recovering the physical observables (moments)

The physical observables of the Liouville equation are thus given by

$$\overline{\rho} = \int W \, d\mathbf{k} = \int f(t, \mathbf{x}, \mathbf{k}) \delta(\phi(t, \mathbf{x}, \mathbf{k})) \, d\mathbf{k} \,,$$
$$\overline{\rho \mathbf{u}} = \int \mathbf{k} W \, d\mathbf{k} = \int \mathbf{k} f(t, \mathbf{x}, \mathbf{k}) \delta(\phi(t, \mathbf{x}, \mathbf{k})) \, d\mathbf{k} \,.$$

We only evaluating the delta function numerical at the end (postprocessing)!

Evolving delta function or not

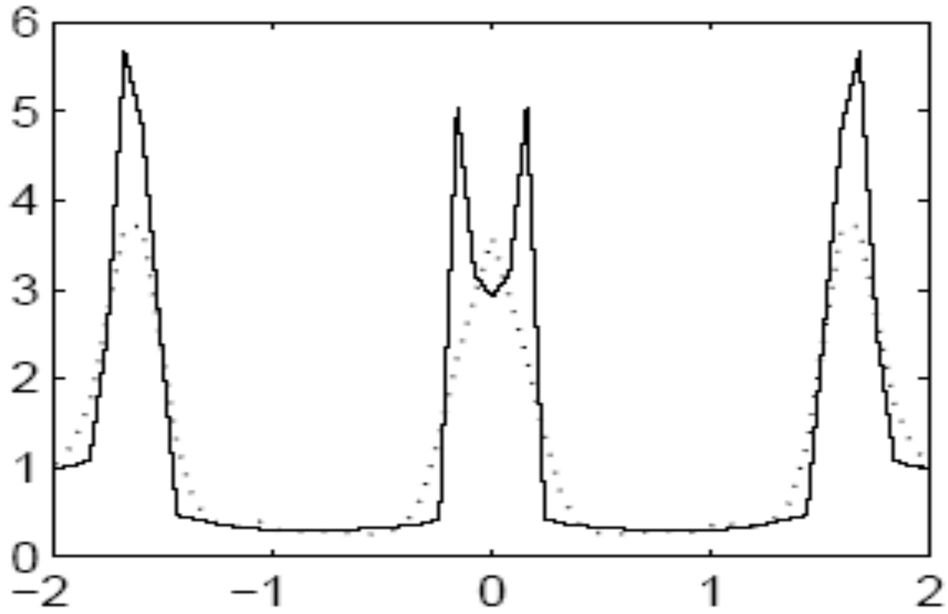
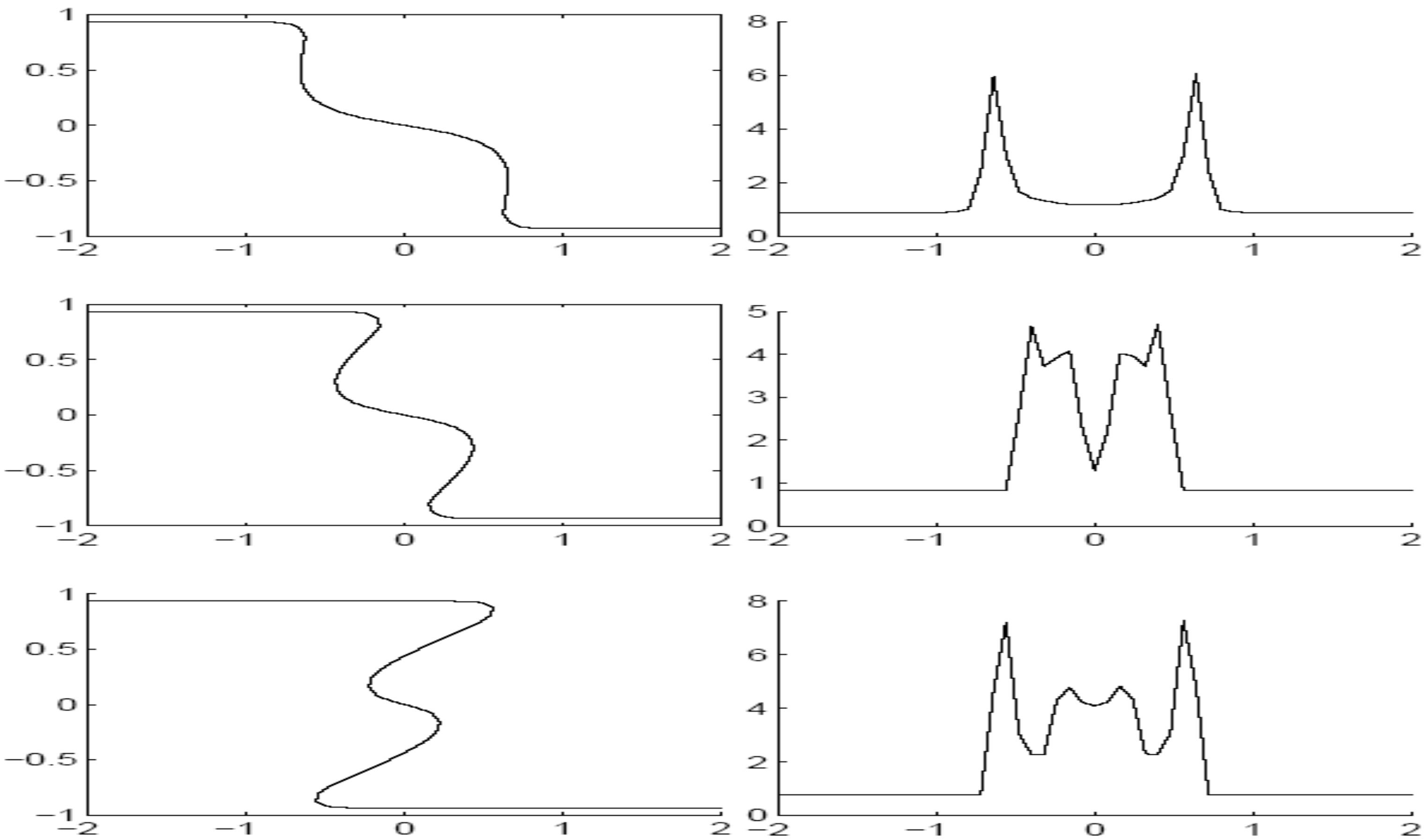


FIGURE 3.1. Comparison of the density computed from evolving the delta function initial data (dotted curve) and the proposed level set approach (solid curve). These are numerical solutions to the problem described in Example 3.2.

Five branch solution (velocity and density)



Another example

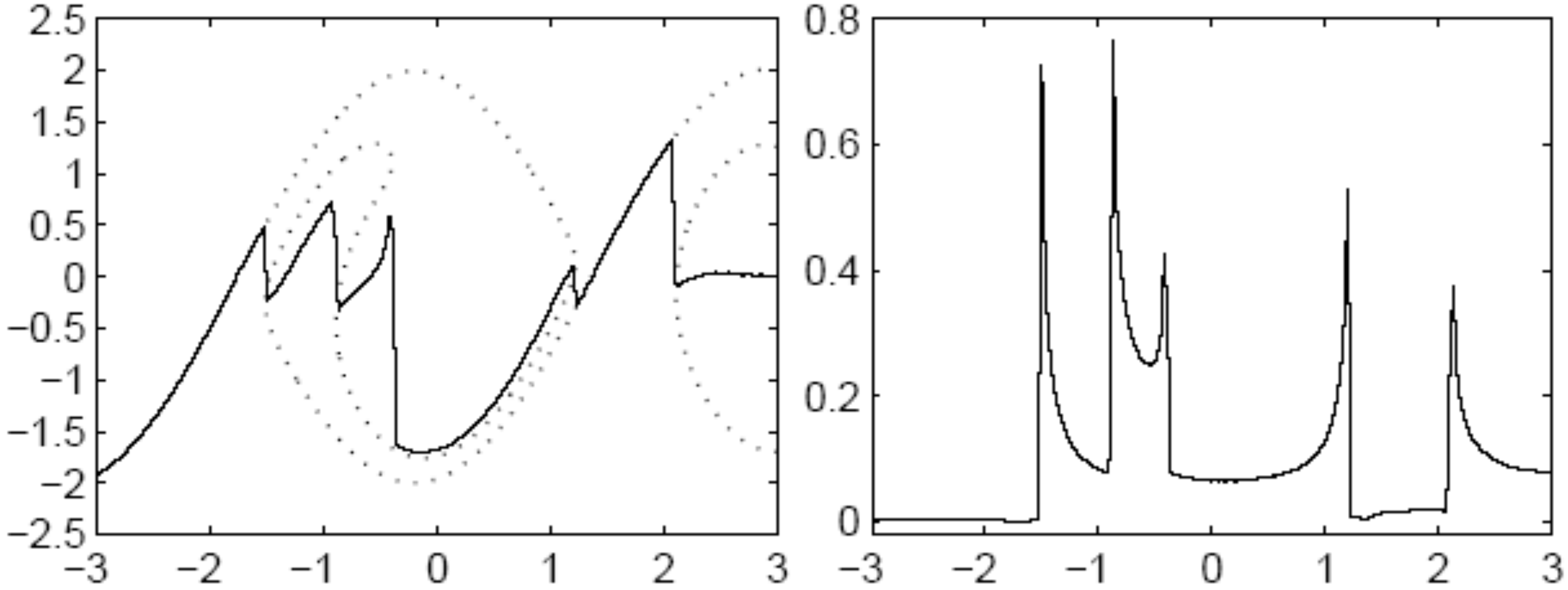


FIGURE 3.10. 200 grid points are used. The dotted line and the solid line in the plot on the left correspond respectively to the multivalued phase gradient and its average ($\bar{u}$). The plot on the right is the corresponding density $\bar{\rho}$ at $T = 18.0$.

2d computation (density)

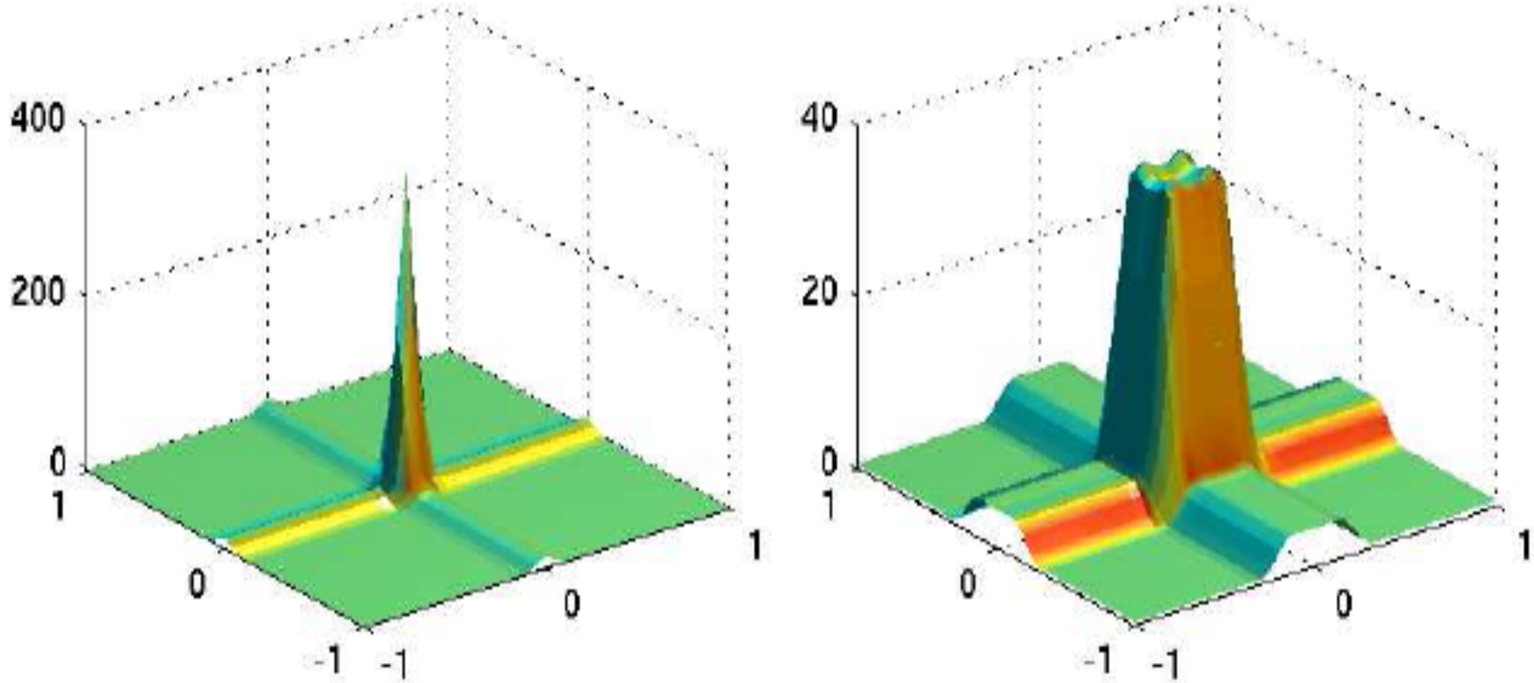


FIGURE 3.11. $T = 1.0$ and 1.25. 40 grid points.

Phase shift

- We are also able to include the Keller-Maslov index into the level set formulation in order to take into account the phase shift at caustics

Jin and X. Yang (JSC 08)

Other topics/issues

Diffractions

—can combine with Geometric Theory of diffractions (*J. Keller*)

Runborg-Matemed; Jin-Yin

Other topics/issues

Gaussian beam methods —accurate even at caustics

$$\varphi_{la}^{\varepsilon}(t, \boldsymbol{x}, \boldsymbol{y}_0) = A(t, \boldsymbol{y}) e^{iT(t, \boldsymbol{x}, \boldsymbol{y})/\varepsilon}$$

$$T(t, \boldsymbol{x}, \boldsymbol{y}) = S(t, \boldsymbol{y}) + \boldsymbol{p}(t, \boldsymbol{y}) \cdot (\boldsymbol{x} - \boldsymbol{y}) + \frac{1}{2}(\boldsymbol{x} - \boldsymbol{y})^{\top} M(t, \boldsymbol{y})(\boldsymbol{x} - \boldsymbol{y}) + O(|\boldsymbol{x} - \boldsymbol{y}|^3),$$

Where A and M are complex (Haller,Popov, Ralston, …)

Level set/complex Liouville equations can also be used

(*Leung-Raslton-Qian-Burridge, Jin-Wu-Yang*)