Discretizing Delta Functions Supported on Level Sets

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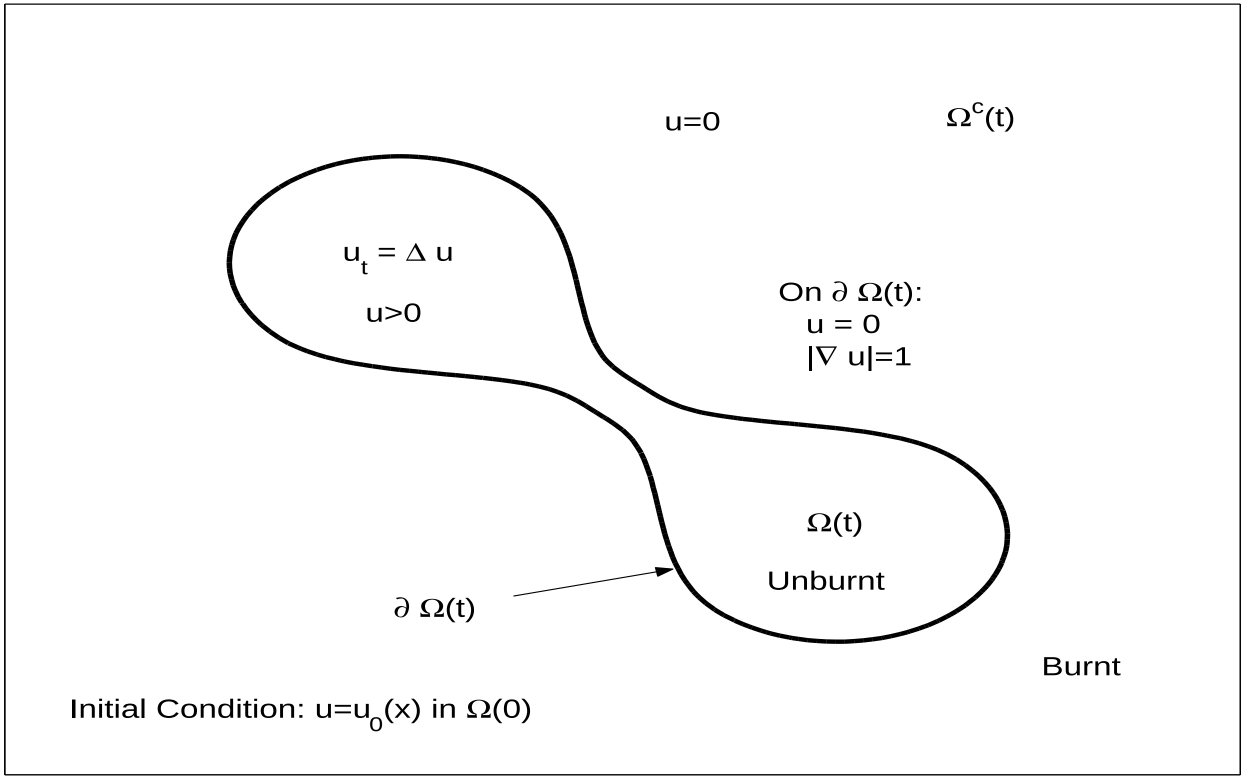
A parabolic free boundary problem



- Related to flame propagation
- Problem has been studied by Caffarelli, Vazquez (1995), others

Formulation using delta function

$$u_t = \Delta u - \delta(\tilde{u})$$

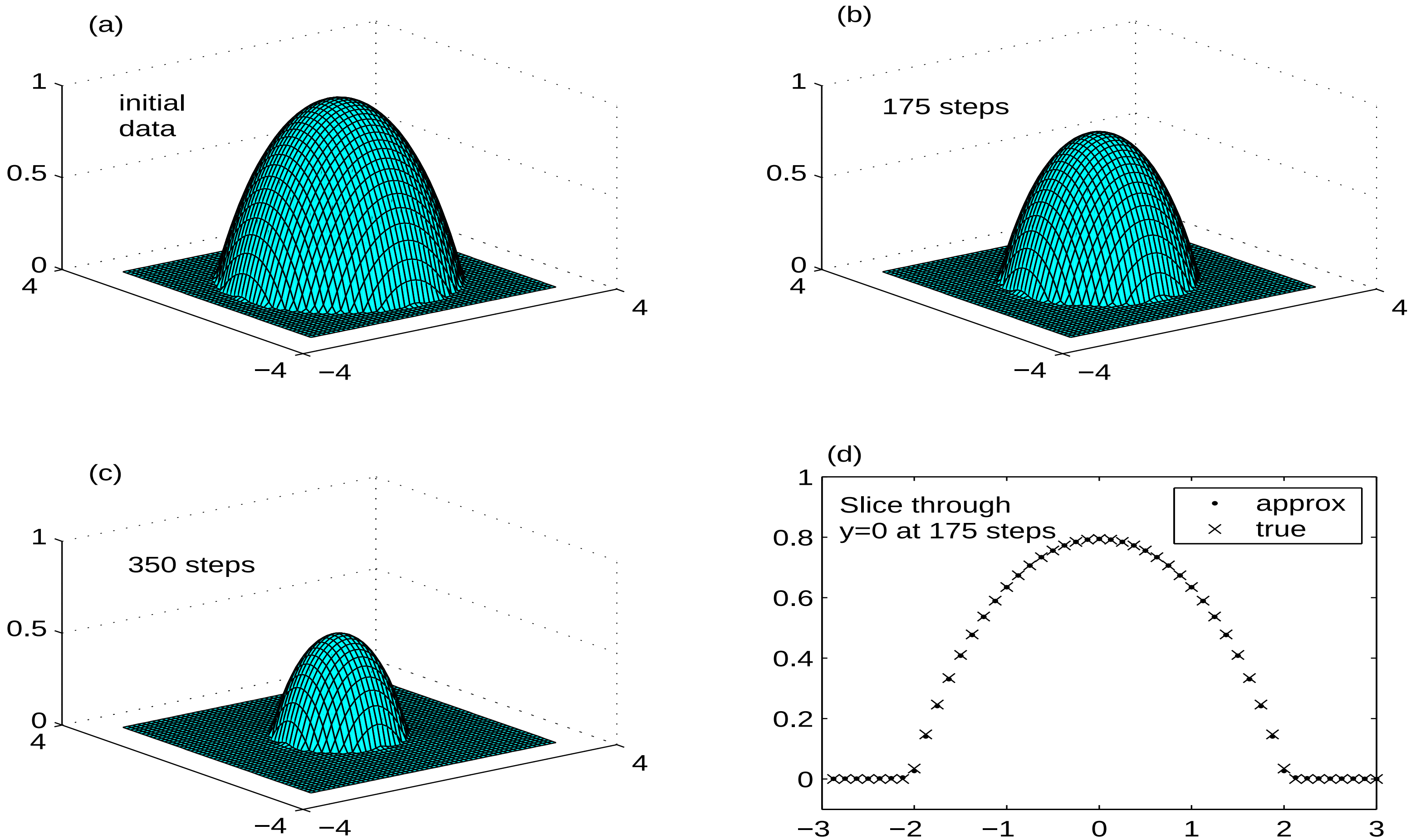
- $\tilde{u}$ is smooth extension of u into burnt region Ω^c
- $\tilde{u} = u > 0$ for $\vec{x}$ in Ω
- $\tilde{u} < 0$ for $\vec{x}$ in Ω^c
- $|\nabla \tilde{u}| = 1$ for $\vec{x}$ on $\partial\Omega$

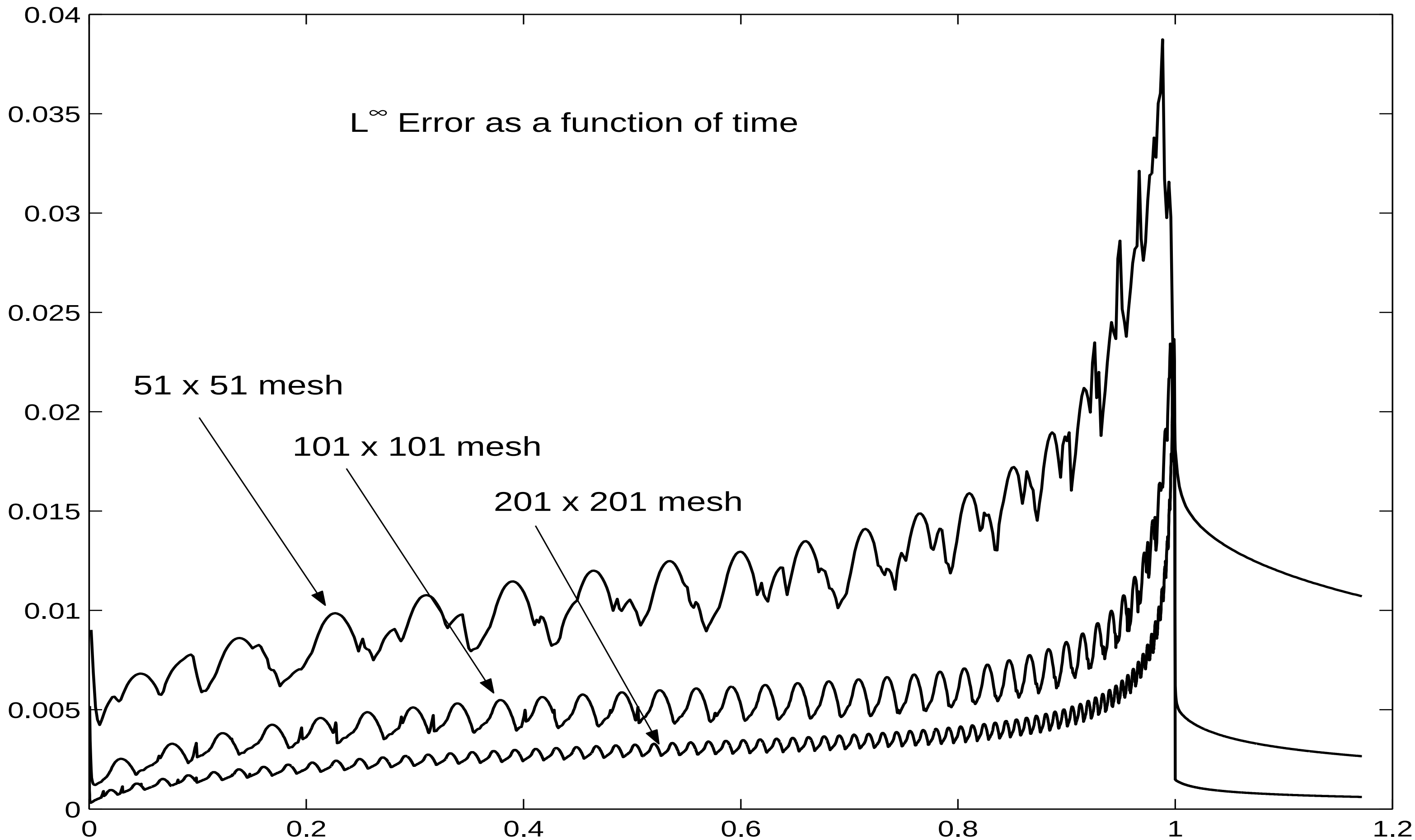
Solve this on $\mathbb{R}^n$. The delta function captures the free boundary.

Difference scheme for $u_t = \Delta u - \delta(\tilde{u})$

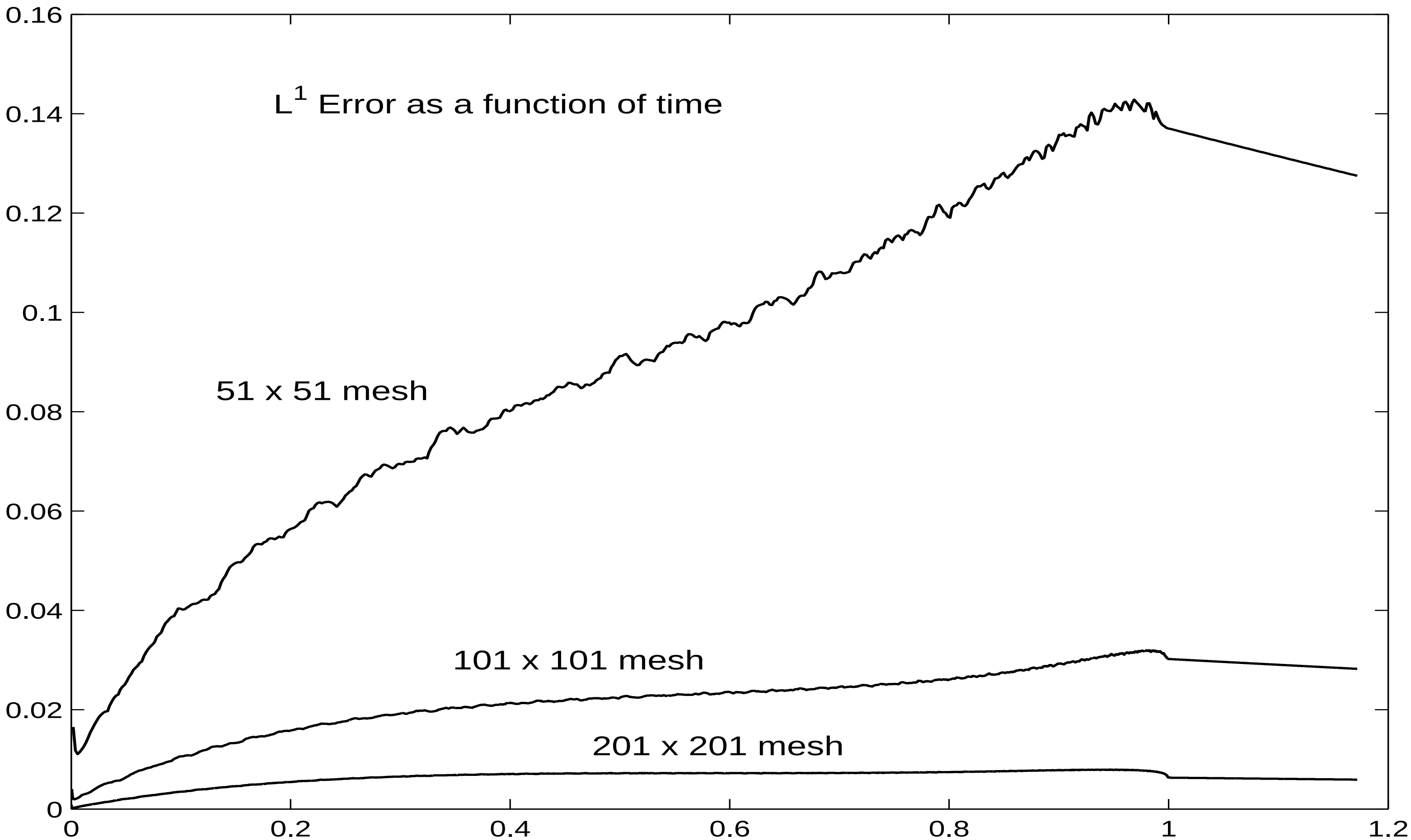
- Regular mesh
- Euler time differencing
- Usual five-point formula for Laplacian
- Use re-distancing method (Peng, Merriman, Osher, Zhao, Kang, 1999) to extend u into burnt region at each step
  - Second order ENO version
- Use FDM2 to approximate delta function

Self similar solution on 51×51 mesh





Sharp drop in error at $t = 1$ due to the fact that the region Ω becomes empty at $t = 1$.


L1 Error as a function of time
51 x 51 mesh
101 x 101 mesh
201 x 201 mesh
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
0
0.2
0.4
0.6
0.8
1
1.2

Discretizing delta functions - the setup

- Level set function

$$\vec{u} = (u^1, \ldots, u^m)$$

- $\vec{u} : \mathbb{R}^n \mapsto \mathbb{R}^m, \qquad 1 \leq m \leq n \leq 3$
- $\vec{x} \in \mathbb{R}^n$
- Γ = zero level set = $\{\vec{x} : \vec{u}(\vec{x}) = \vec{0}\}$
- Trying to approximate

$$\Pi_{i=1}^{m} \delta(u^i(\vec{x}))$$

- Everything defined at mesh points of regular mesh, mesh size = h

- Using delta functions to approximate 2 kinds of integrals
  - **Type 1:**

$$\mathcal{I}_1 = \int_{\mathbb{R}^n} f(\vec{x})\, \Pi_{i=1}^{m} \delta(u^i(\vec{x}))\ \|\wedge_m \nabla \vec{u}(\vec{x})\|\ d\vec{x},$$

$$\wedge_m \nabla \vec{u}(\vec{x}) := \nabla u^1(\vec{x}) \wedge \nabla u^2(\vec{x}) \wedge \cdots \wedge \nabla u^m(\vec{x})$$

  - Applications of $\mathcal{I}_1$: volume, arclength, average mean curvature, amplitudes of spherical harmonics
  - **Type 2:**

$$\mathcal{I}_2 := \int_{\mathbb{R}^n} f(\vec{x}) \Pi_{i=1}^{n} \delta(u^i(\vec{x}))\, d\vec{x}$$

  - Application of $\mathcal{I}_2$ in recent level set methods for computing observables for semiclassical Schrödinger equation

$\mathcal{I}_1$ integrals include:

- $m = 1$

$$\mathcal{I}_1 = \int_{\mathbb{R}^n} f(\vec{x})\, \delta(u(\vec{x}))\ \|\nabla u(\vec{x})\|\ d\vec{x}.$$

- $n = 3$, $m = 2$ (Curve in $\mathbb{R}^3$)

$$\mathcal{I}_1 = \int_{\mathbb{R}^3} f(\vec{x})\, \delta(u^1(\vec{x}))\delta(u^2(\vec{x}))\ \left\|\nabla u^1(\vec{x}) \times \nabla u^2(\vec{x})\right\|\ d\vec{x}.$$

- $m = n$

$$\mathcal{I}_1 = \int_{\mathbb{R}^n} f(\vec{x})\, \Pi_{i=1}^{m} \delta(u^i(\vec{x}))\ |\det \nabla \vec{u}(\vec{x})|\ d\vec{x}.$$

FDM algorithms - FDM1 and FDM2

- Both FDM algorithms use discrete version of wedge product formula

$$\delta(u^1)\cdots\delta(u^m) = \frac{\nabla H(u^1)\wedge\cdots\wedge\nabla H(u^m)\;\cdot\;\nabla u^1\wedge\cdots\wedge\nabla u^m}{\left\|\nabla u^1\wedge\cdots\wedge\nabla u^m\right\|^2}.$$

- **FDM1 -** Use discretized wedge product formula with smoothed Heaviside function:

$$H^{C,\epsilon}(z) = \begin{cases} 0, & z < \epsilon \\ \frac{1}{2} + \frac{z}{2\epsilon} + \frac{1}{2\pi}\sin\left(\frac{\pi z}{\epsilon}\right), & -\epsilon \le z \le \epsilon \\ 1, & \epsilon < z \end{cases}$$

Usually use $\epsilon = 1.5h$

FDM2 - Two steps.

- **Step 1:** Compute discrete version of

$$H(u^i) = \frac{\nabla I(u^i) \cdot \nabla u^i}{\|\nabla u^i\|^2}, \quad i = 1, \ldots, m.$$

- The function I is the primitive of H:

$$I(z) := \int_0^z H(\zeta)\, d\zeta = \max(0, z)$$

- **Step 2:** Plug these discrete Heaviside functions into discrete version of

$$\delta(u^1) \cdots \delta(u^m) = \frac{\nabla H(u^1) \wedge \cdots \wedge \nabla H(u^m) \ \cdot \ \nabla u^1 \wedge \cdots \wedge \nabla u^m}{\|\nabla u^1 \wedge \cdots \wedge \nabla u^m\|^2}.$$

- No smoothing involved - no parameters.

The wedge product delta function formulas - without wedges

- Codimension 1:

$$\delta(u) = \frac{\nabla H(u) \ \cdot \ \nabla u}{\|\nabla u\|^2}$$

- $n = 3$, $m = 2$

$$\delta(u^1)\,\delta(u^2) = \frac{\nabla H(u^1) \times \nabla H(u^2) \ \cdot \ \nabla u^1 \times \nabla u^2}{\|\nabla u^1 \times u^2\|^2}$$

- Full codimension ($m = n$)

$$\delta(u^1)\cdots\delta(u^n) = \frac{\det \nabla \vec{H}}{\det \nabla \vec{u}}, \quad \vec{H} := \big(H(u^1), \ldots, H(u^n)\big)$$

Codimension one ($m = 1$)

- Codimension one problem (using different techniques different from FDM1, FDM2) studied earlier by
  - Engquist, Tornberg, Tsai
  - Smereka
- Both FDM1 and FDM2 known to be consistent (theorem)
- Numerical experience - For codimension one, FDM1 is first order or better, FDM2 is second order

Higher Codimension Problems

- Not as well understood as codimension one problems
- Constructing consistent approximations not trivial
- FDM algorithms
  - Generally very accurate, but may not be be consistent in some situations
  - Consistent when combined with gradient normalization

Other approximate delta functions for comparison

- Product of pointwise delta functions - **PDF**

$$\delta^h_{PDF}(\vec{x}_{\mathbf{k}};\vec{u}) := \Pi_{i=1}^m \delta^{L,\epsilon}(u^i(\vec{x}_{\mathbf{k}}))$$

We use $\epsilon = 2h$ in the linear hat delta function

$$\delta^{L,\epsilon}(z) = \begin{cases} \frac{1}{\epsilon}\left(1 - \left|\frac{z}{\epsilon}\right|\right), & |z| < \epsilon \\ 0, & |z| \geq \epsilon. \end{cases}$$

- Product of pointwise delta functions with local ϵ - **PDFL**

Same as above with

$$\epsilon = 2\max\left(1, |\det \nabla \vec{u}_{\mathbf{k}}|\right) h$$

Used by Jin, Liu, Osher, Tsai for $\mathcal{I}_2$ type integrals

A grid misalignment experiment

- Level set functions are linear, signed distance functions, and gradients are orthogonal:
$$u(x,y) = \cos(\theta)\cdot x - \sin(\theta)\cdot y,$$
$$v(x,y) = \sin(\theta)\cdot x + \cos(\theta)\cdot y,$$
- Integrand is $f(x,y) \equiv 1$
- $\mathcal{I}_1 = \mathcal{I}_2 = 1$.
- Let θ vary between 0 and $\pi/2$.
- Mesh refinement not required for this linear problem.

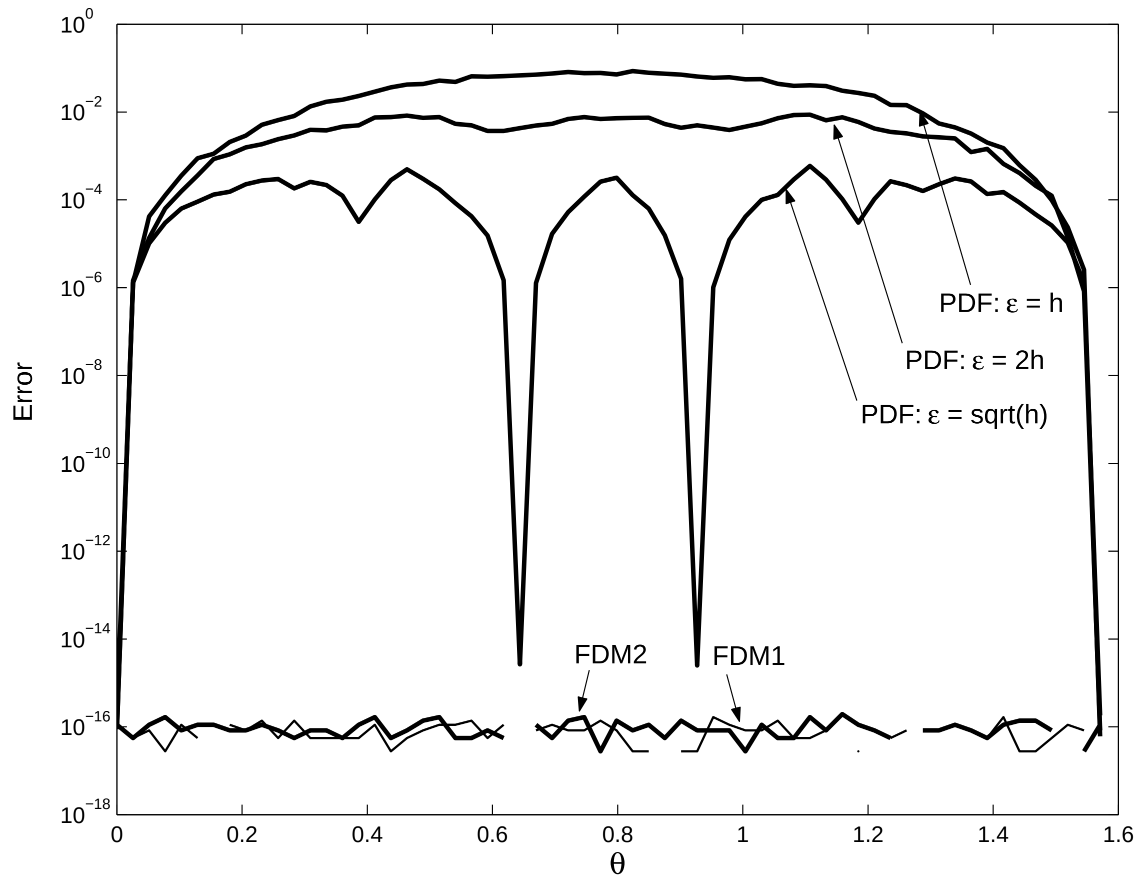


Figure 1: Example 1. Error in approximating $\mathcal{I}_1 = \mathcal{I}_2$ for the case of $n = 2$, $m = 2$ as a function of grid misalignment.

Full Gradient Normalization - FGN

- For full codimension problems ($m = n$)
- Replace $\vec{u}_{\mathbf{k}}$ by $\vec{v}_{\mathbf{k}}$ and $f_{\mathbf{k}}$ by $g_{\mathbf{k}}$ where

$$\vec{v}_{\mathbf{k}} := \left[\nabla^h \vec{u}_{\mathbf{k}}\right]^{-1} \vec{u}_{\mathbf{k}}, \qquad g_{\mathbf{k}} = \begin{cases} f_{\mathbf{k}}, & \text{for } \mathcal{I}_1 \\ f_{\mathbf{k}} / \left|\det \nabla^h \vec{u}_{\mathbf{k}}\right|, & \text{for } \mathcal{I}_2. \end{cases} \tag{1}$$

  and before computing approximate delta function.

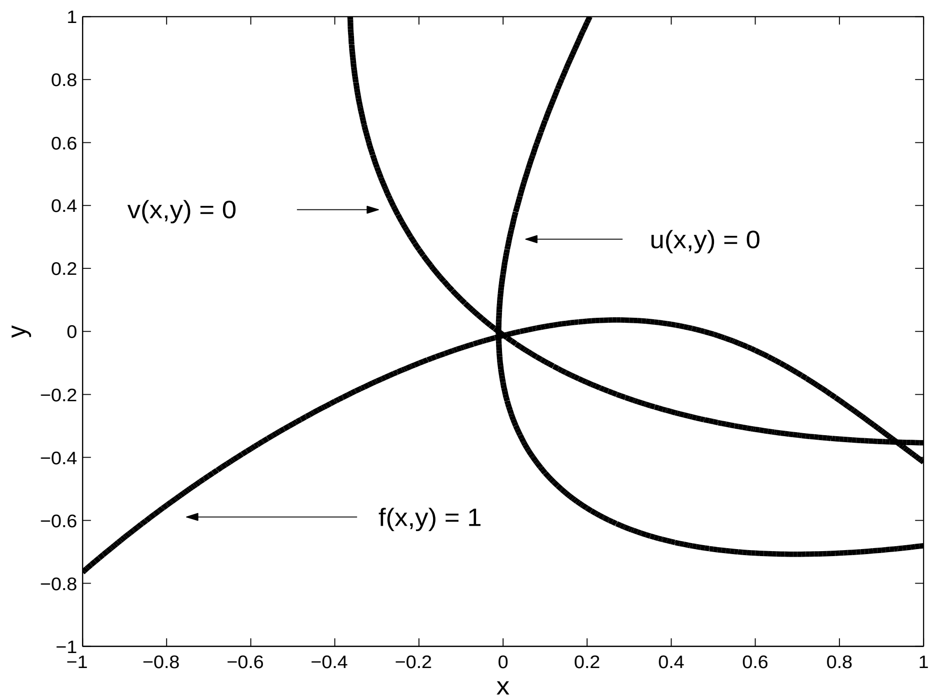
- Resulting level functions are approximately signed distance, gradients are approximately orthogonal, and approximately aligned with mesh.
- Combined algorithms are consistent
  - FDM1-FGN
  - FDM2-FGN
  - PDF-FGN, PDFL-FGN

A full codimension $\mathcal{I}_1$ example. $n = m = 2$

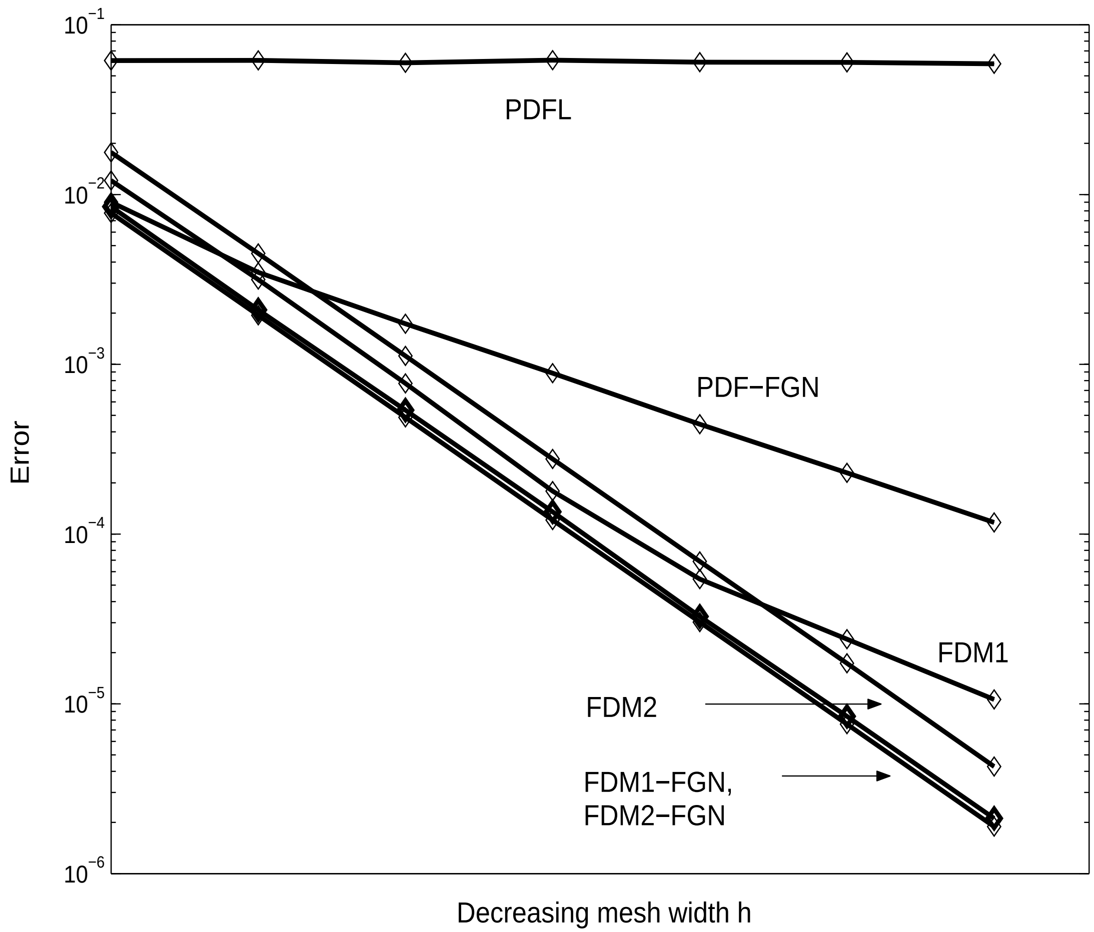
$$u(x,y) = y - x(x-1), \qquad v(x,y) = \frac{1}{2}x^2 - y$$

$$f(x,y) = (x-1)^4 + (y+1)^2 - 1$$

To create misalignment with mesh, everything rotated by 45 degrees



Errors for full codimension $\mathcal{I}_1$ example. (n=m=2)



A codimension two $\mathcal{I}_1$ problem in $\mathbb{R}^3$

- Two surfaces that intersect in a pair of **helices**

$$u(x,y,z) = 1 - (x^2 + y^2), \qquad v(x,y,z) = x\sin(z) - y\cos(z),$$

$$f(x,y,z) = \begin{cases} \sin^4(z/2 - \pi/2)\,\cos(v(x,y,z)/2), & -\pi < z < \pi \\ 0, & \text{otherwise} \end{cases}$$

To create misalignment with mesh, rotated everything by

$$A = \begin{bmatrix} 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \\ 0 & -1/\sqrt{2} & 1/\sqrt{2} \\ 2/\sqrt{6} & -1/\sqrt{6} & -1/\sqrt{6} \end{bmatrix}$$

Partial Gradient Normalization (PGN)

- For problems where $n = 3$, $m = 2$
- What PGN accomplishes:
  - Level set functions are approximately signed distance
  - Gradients are approximately orthogonal
- Like Gram-Schmidt

Starting with level functions $u_{\mathbf{k}}$, $v_{\mathbf{k}}$, **orthogonalize:**

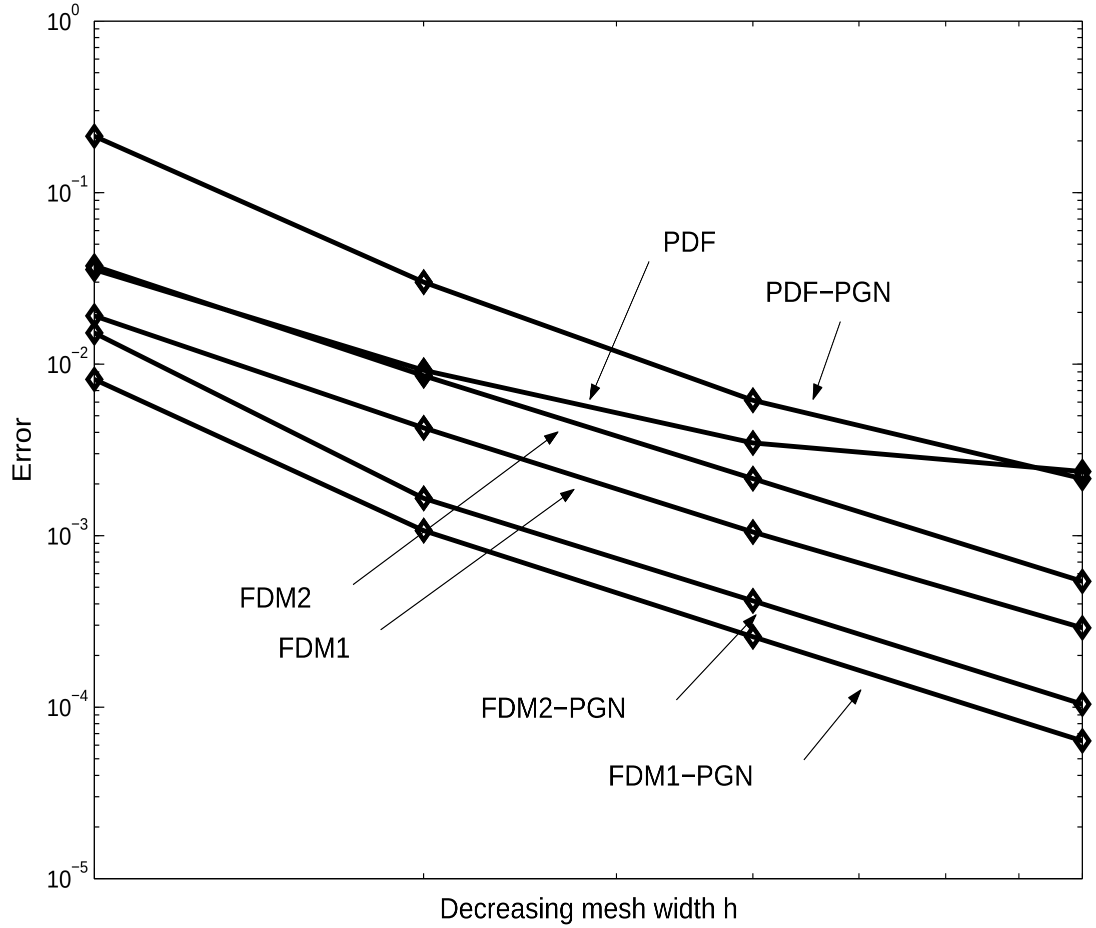
$$\tilde{v}_{\mathbf{k}} = v_{\mathbf{k}} - c u_{\mathbf{k}}, \quad c = \frac{\nabla^h u_{\mathbf{k}} \cdot \nabla^h v_{\mathbf{k}}}{\nabla^h u_{\mathbf{k}} \cdot \nabla^h u_{\mathbf{k}}},$$

Then **normalize:**

$$\hat{u}_{\mathbf{k}} = u_{\mathbf{k}} / \sqrt{\nabla^h u_{\mathbf{k}} \cdot \nabla^h u_{\mathbf{k}}}$$

$$\hat{v}_{\mathbf{k}} = \tilde{v}_{\mathbf{k}} / \sqrt{\nabla^h v_{\mathbf{k}} \cdot \nabla^h v_{\mathbf{k}} - c^2 \nabla^h u_{\mathbf{k}} \cdot \nabla^h u_{\mathbf{k}}},$$

Errors for helix $\mathcal{I}_1$ example. ($n = 3$, $m = 2$)



A full codimension $\mathcal{I}_1$ example in $\mathbb{R}^3$

$$\begin{cases} u(x,y,z) & = \sqrt{(x-2)^2+(y-3)^2+(z-1)^2}-\sqrt{14}, \\ v(x,y,z) & = \sqrt{(x+1)^2+(y-2)^2+(z-3)^2}-\sqrt{14}, \\ w(x,y,z) & = \sqrt{(x+3)^2+(y-1)^2+(z+2)^2}-\sqrt{14}, \end{cases}$$

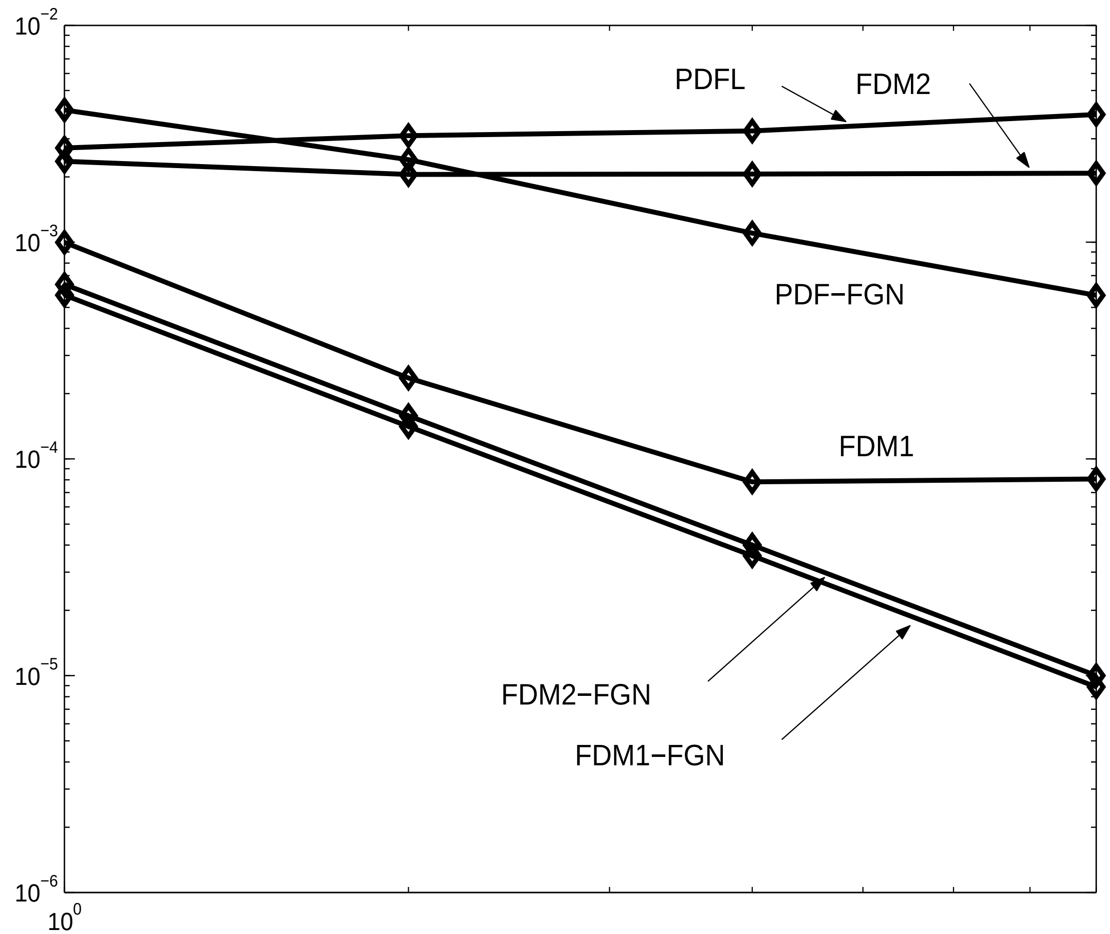
$$f(x,y,z) = e^x \cos(y)\cos(z)$$

Level functions intersect at origin. $\mathcal{I}_1 = 1$

Jacobian $\approx .802$ at intersection point

Level functions are signed distance

Errors for 3D full codimension $\mathcal{I}_1$ example. ($n = 3$, $m = 3$)



Computing observables for semiclassical limit of Schrödinger equation

- Using approach of Jin, Liu, Osher, Tsai (2005), and Liu, Osher, Tsai (2006)
- Solve Liouville equations for $w(\vec{x},\vec{p},t)$, $\vec{x}\in\mathbb{R}^n$, $\vec{p}\in\mathbb{R}^n$

$$w_t + \vec{p}\cdot\nabla_{\vec{x}}\, w - \nabla_{\vec{x}}\, V(\vec{x})\cdot\nabla_{\vec{p}}\, w = 0$$

for $w=\phi^i$, $i=1,\ldots,n$, and $w=f$

Initial data:

$$\phi^i(\vec{x},\vec{p},0) = p^i - \partial_{x^i} S_0(\vec{x}), \quad i=1,\ldots,n$$
$$f(\vec{x},\vec{p},0) = \rho_0(\vec{x}),$$

- Compute observables involving $\mathcal{I}_2$ type integrals

$$\bar{\rho}(\vec{x},t) = \int_{\mathbb{R}^n} f(\vec{x},\vec{p},t)\,\Pi_{i=1}^n\delta(\phi^i(\vec{x},\vec{p},t))\,d\vec{p},$$
$$\bar{v}^i(\vec{x},t) = \frac{1}{\bar{\rho}(\vec{x},t)}\int_{\mathbb{R}^n} p^i f(\vec{x},\vec{p},t)\,\Pi_{i=1}^n\delta(\phi^i(\vec{x},\vec{p},t))\,d\vec{p}, \quad i=1,\ldots,n.$$

One-dimensional example (Example 6.1 of Liu, Osher, Tsai)

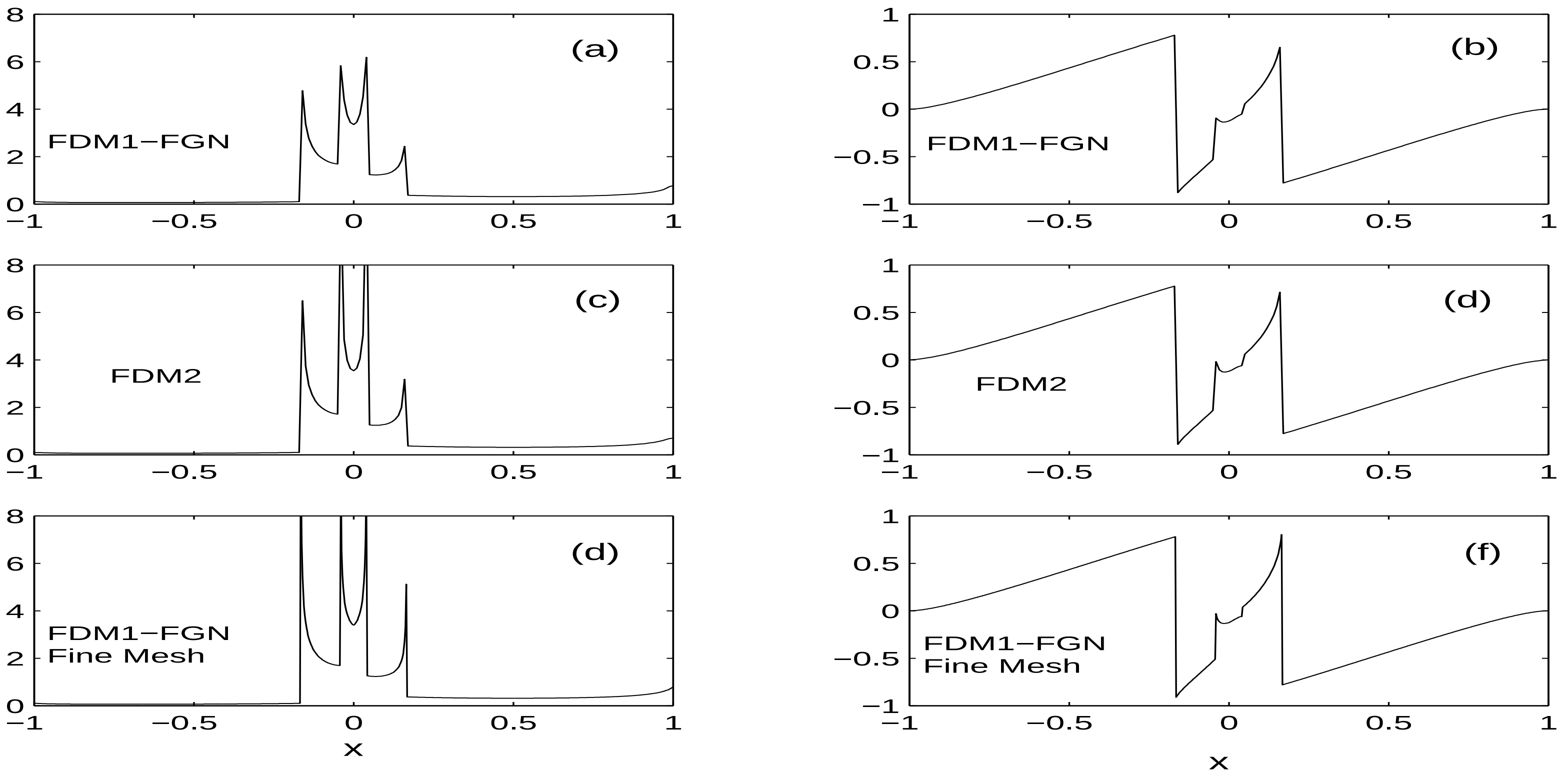


Figure 2: Example 9. Observables at $t = .625$ computed using FDM algorithms. Plots on the left show $\bar{\rho}^h$, and plots on the right show $\bar{v}^h$.

One-dimensional example (Example 6.1 of Liu, Osher, Tsai)

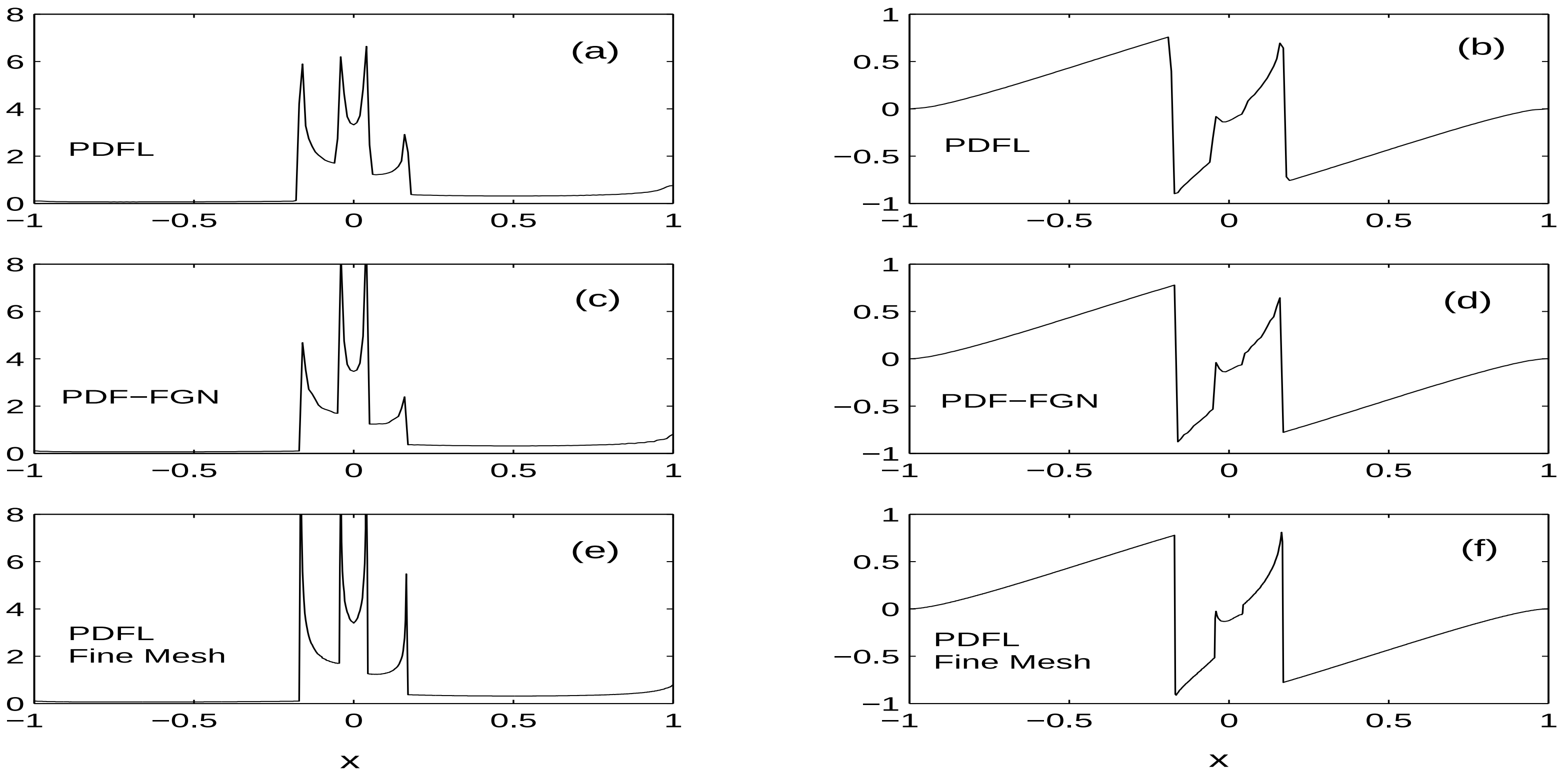


Figure 3: Example 9. Observables at $t = .625$ computed using PDF algorithms. Plots on the left show $\bar{\rho}^h$, and plots on the right show $\bar{v}^h$.

Two-dimensional example (Example 6.3 of Liu, Osher, Tsai)

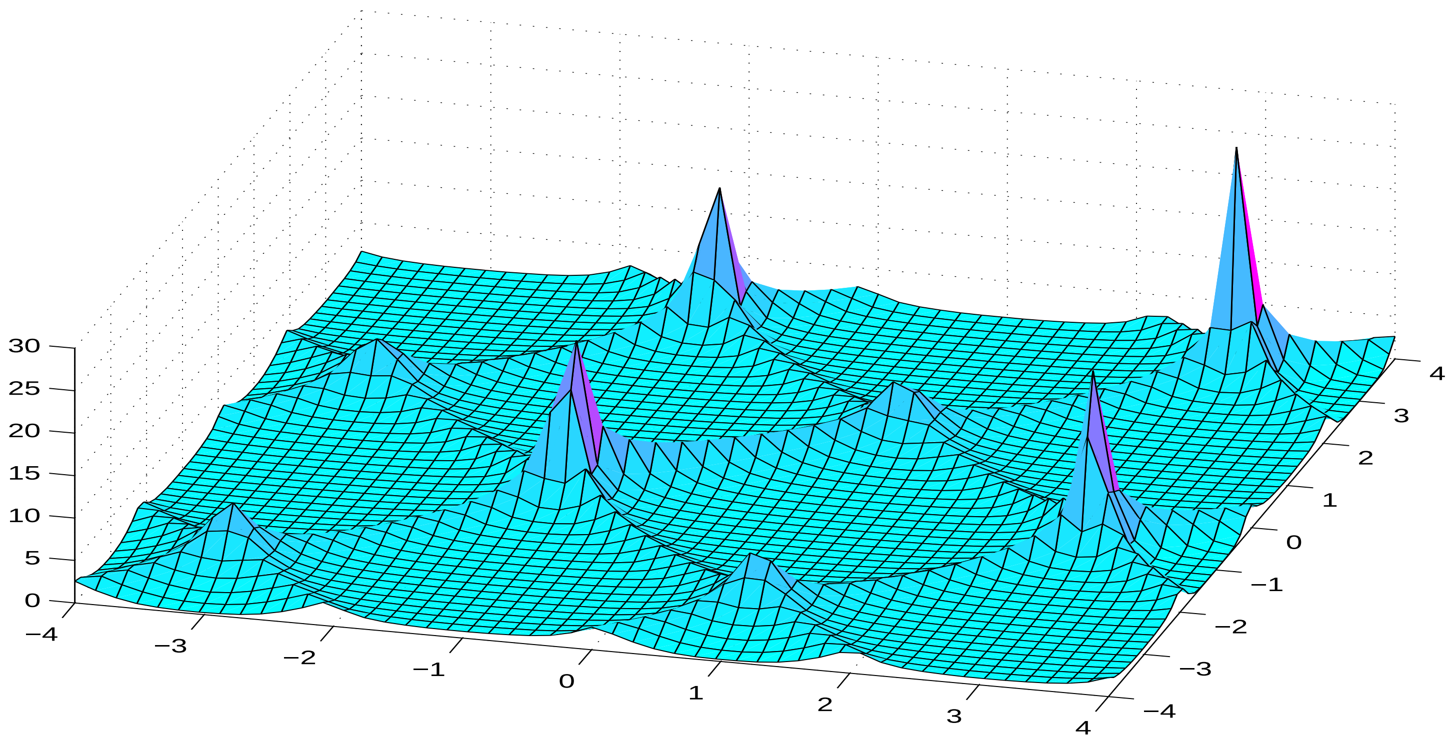


Figure 4: Example 11. Averaged density $\bar{\rho}^h$ at $t = 6.9$. The spikes represent caustics, i.e., points where $\det \nabla\vec{\phi} = 0$.

Two-dimensional example (Example 6.3 of Liu, Osher, Tsai)

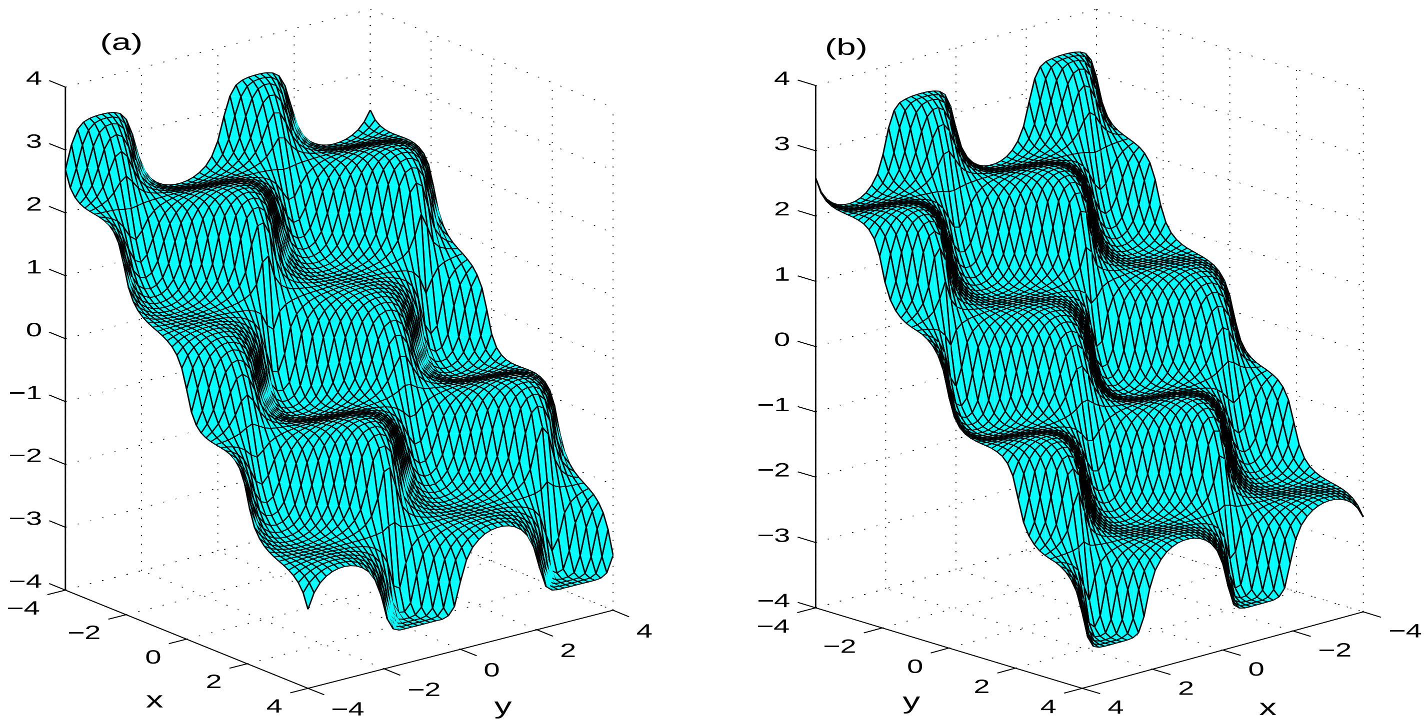


Figure 5: Example 11. Averaged velocities at $t = 6.9$. (a) $\bar{v}^{1,h}$ and (b) $\bar{v}^{2,h}$.

Two-dimensional example (Example 6.3 of Liu, Osher, Tsai)

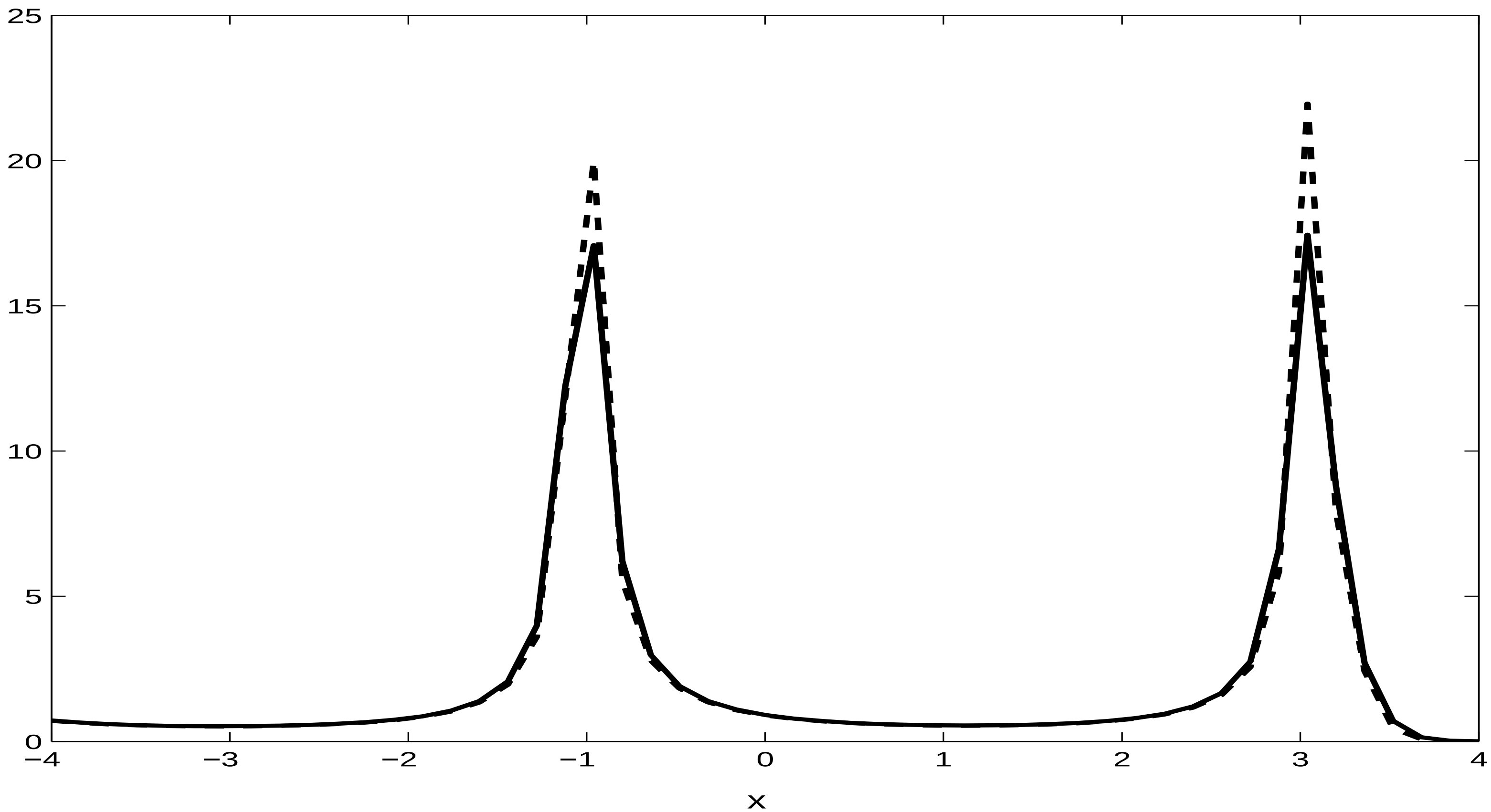


Figure 6: Example 11. Averaged density $\bar{\rho}^h$ at $t = 6.9$, $y = -.96$. FDM1 (solid line) and FDM1-FGN (dashed line).

Two-dimensional example (Example 6.3 of Liu, Osher, Tsai)

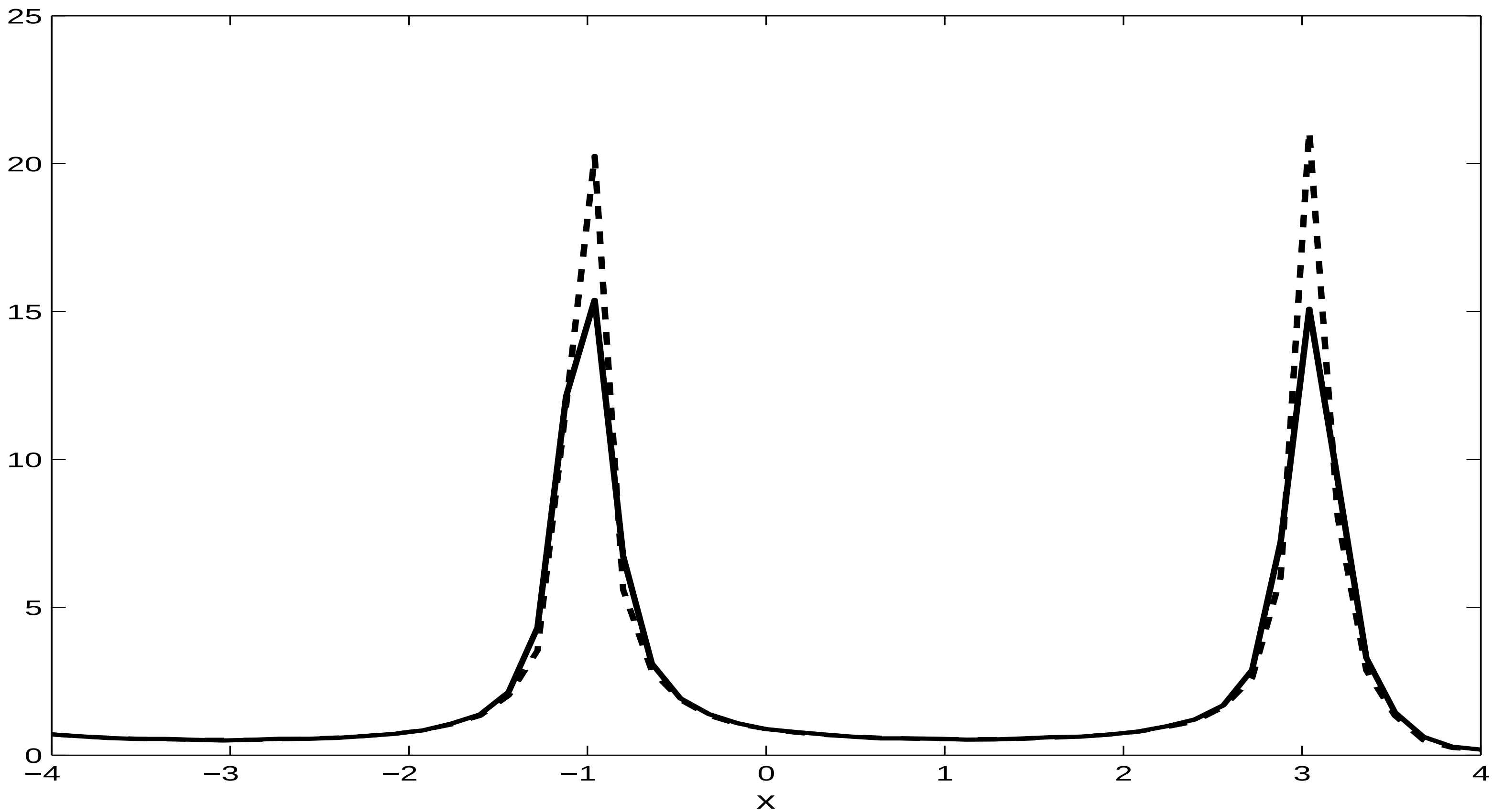


Figure 7: Example 11. Averaged density $\bar{\rho}^h$ at $t = 6.9$, $y = -.96$. PDFL (solid line) and PDF-FGN (dashed line).

Two-dimensional example (Example 6.3 of Liu, Osher, Tsai)

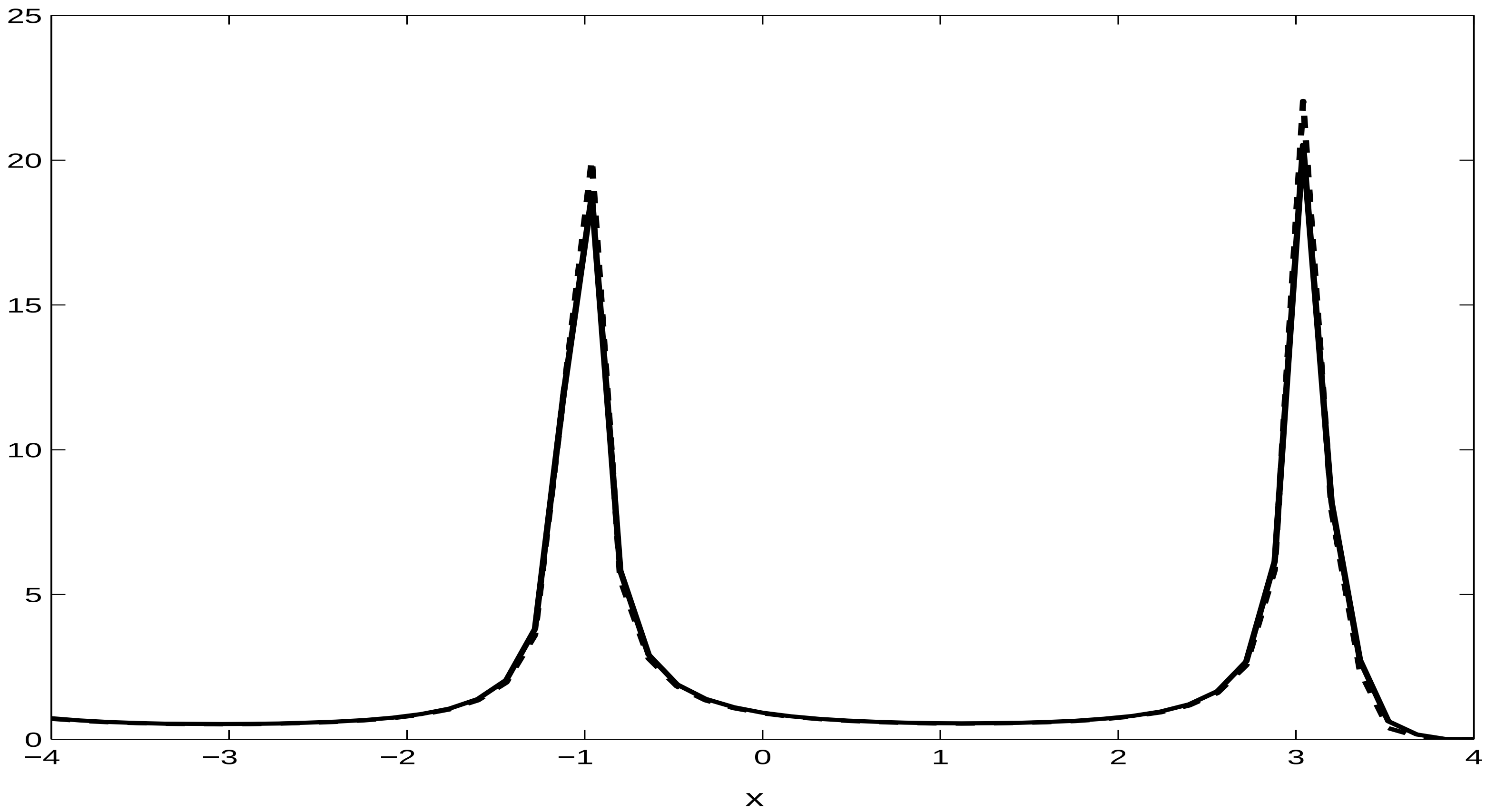


Figure 8: Example 11. Averaged density $\bar{\rho}^h$ at $t = 6.9$, $y = -.96$. FDM2 (solid line) and FDM2-FGN (dashed line).

Two-dimensional example (Example 6.3 of Liu, Osher, Tsai)

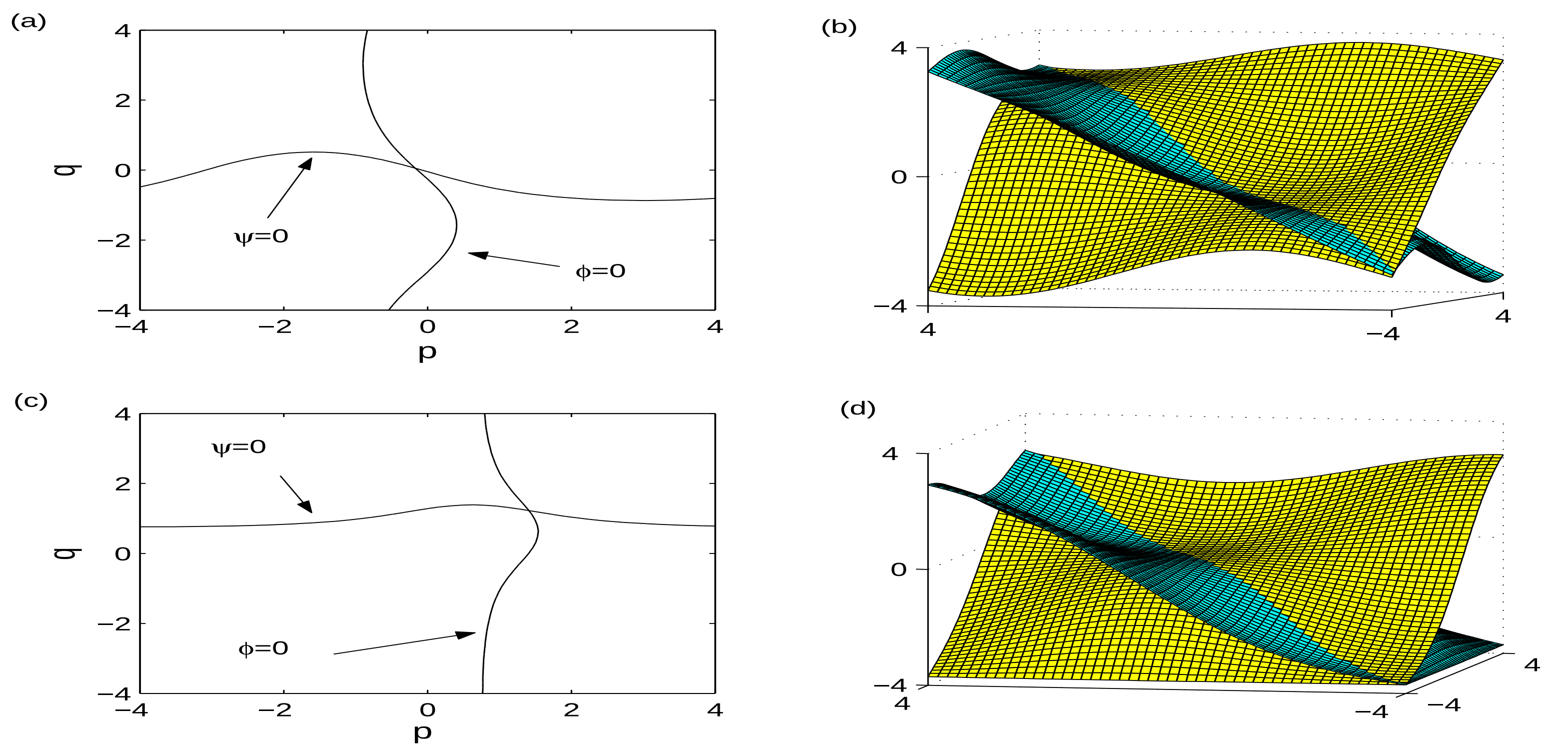


Figure 9: Zero level contours and level functions ϕ, ψ. Plots (a)&(b): $(x, y) = (.48, .48)$, not near any caustics. Plots (c)&(d): $(x, y) = (-1.12, -1.12)$, close to a caustic.