SAND2012-4983P

A New Peridynamic Inspired Approach for a Nonlocal, Nonlinear Conservation Law

Nonlocal Continuum Models for Diffusion, Mechanics, and Other Applications

Statistical and Applied Mathematical Sciences Institute

June 25-29 2012

Michael Parks

Computing Research Center

Sandia National Laboratories

Qiang Du

Dept. of Mathematics

Penn State University

Jim Kamm, Rich Lehoucq

Computing Research Center

Sandia National Laboratories

SAND2012-XXXXP

Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

Peridynamics & Nonlocal Advection

- Peridynamics provides a nonlocal framework for elasticity that naturally admits discontinuous solutions (e.g., fracture)

- Expand peridynamics-based simulation capabilities to include impact, energetic materials, etc. Couple mass, momentum, and energy balance equations with more complex material response.

- Goals:
  - Understand relation between nonlinear advection and peridynamics
  - Develop a peridynamic-inspired approach for nonlocal nonlinear advection that captures "shock-like" behavior

- Nonlocal advection not novel; many others have explored nonlocal variants of classical advection
  - Nonlocal wavespeed, integral operators (Hilbert transform), fractional differential operators, generalized flux, nonlocal regularization, nonlocal convection diffusion (Ignat & Rossi)*

Sandia National Laboratories

* L. I. Ignat and J. D. Rossi. A nonlocal convection-diffusion equation. J. Funct. Anal., 251:399-437, 2007.

Classical (Local) Advection

- Classical (local) advection is well-understood. Many, many papers, textbooks, etc.
- Conservation law (f is flux function):

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0$$

- Simple examples:
  - $f(u) = cu$ $\rightarrow$ linear advection
  - $f(u) = u^2/2$ $\rightarrow$ Burgers equation
- Linear advection
  - Initial condition propagated along characteristic
  - $u(x,t) = u_0(x-ct)$

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = 0$$

- Burgers' equation
  - Exact solution via Cole-Hopf transform
  - Inviscid Burgers' equation exhibits shocks in finite time (crossing characteristics)
  - Viscid Burgers' equation regularizes solution. No shocks possible!

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0$$

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}$$

Sandia National Laboratories

Nonlocal Advection

- Posit the integro-differential equation

$$\frac{\partial u}{\partial t} + \int_{x-\varepsilon}^{x+\varepsilon} \psi\left(\frac{u(y,t)+u(x,t)}{2}\right)\varphi(y,x)dy = 0 \qquad (x,t) \in \mathbb{R} \times (0,\infty)$$

$$u(x,0) = g(x) \qquad x \in \mathbb{R}$$

- Points (x,y) interact directly and nonlocally
- Maximum interaction distance ε (peridynamic horizon)
- Kernel is antisymmetric:

$$\varphi(y,x) = -\varphi(x,y)$$

- Contrast with peridynamic models of solids, where kernel is *symmetric*
- The kernel is (usually) translation invariant:

$$\varphi(y,x) = \varphi(y - x) = \varphi(\xi)$$

- Requirement for consistency with classical (local) advection equation:

$$\lim_{\xi \to 0} \varphi(\xi) = - \frac{\partial \delta}{\partial x}$$

(in distributional sense)

- Contrast with peridynamic models of solids, where this limit (usually) gives δ

Sandia National Laboratories

Relation to Local Advection

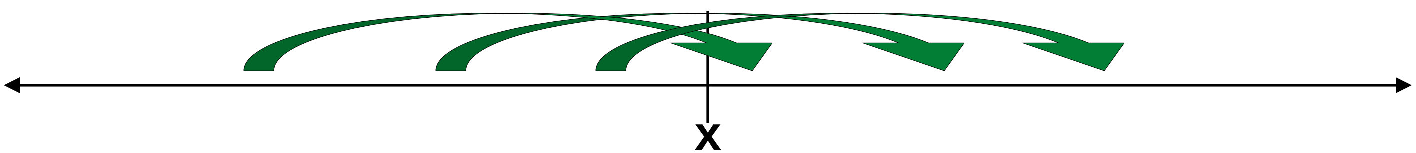
- Compare forms of equations

$$\frac{\partial u}{\partial t} + \int_{x-\varepsilon}^{x+\varepsilon} \psi\left(\frac{u(y,t)+u(x,t)}{2}\right)\varphi(y,x)\,dy = 0$$

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} f(u) = 0$$

"gradient of flux"

- What is the nonlocal flux through a surface? (e.g., through x?)



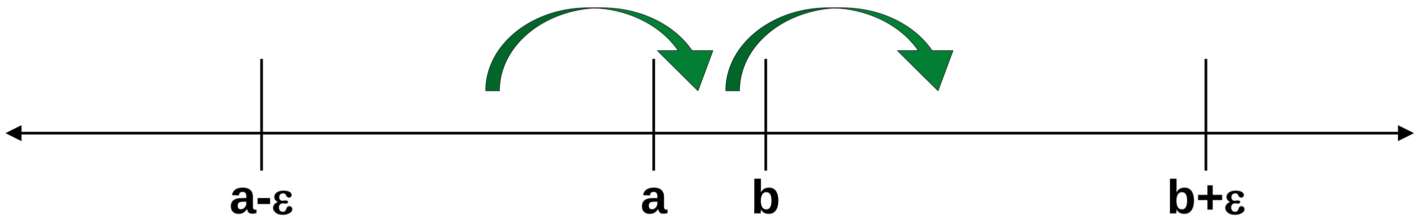
$$f_{NL}(x) = \int_0^{\varepsilon}\int_0^{\varepsilon - z} \psi\left(\frac{u(x+y,t)+u(x-z,t)}{2}\right)\varphi(x+y,x-z)\,dy\,dz$$

- Flux carried by infinite number of nonlocal interactions passing through x
  - Many have derived this expression before; See [1,2,3].
  - Under assumptions, Noll's lemma [4] can be used to derive flux function.
- Under assumptions, nonlocal equation converges to local equation as $\varepsilon \to 0$.

[1] Silling, Zimmerman, and Abeyaratne, Deformation of a Peridynamic Bar, J. Elasticity. 73:173-190, 2003.
[2] Bobaru and Duangpanya, The peridynamic formulation for transient heat conduction, Int. J. Heat Mass Transfer. 53: 4047-4059, 2010.
[3] Lehoucq and Silling, Force flux and the peridynamic stress tensor, J. Mech. Phys. Solids. 56:1566-1577, 2008.
[4] Noll, Die herleitung der grundgleichungen der thermomechanik der kontinua aus der statistischen mechanik. J. Ration. Mech. Anal. 4:627–646, 1955.

Conservation Law

- Conservation: Instantaneous change in u over [a,b] is balanced by flux in/out of [a,b]



- Integrate nonlocal advection equation over [a,b] for some a<b

$$\frac{\partial}{\partial t}\int_a^b u(x,y)dx+\int_a^b\int_{x-\varepsilon}^{x+\varepsilon}\psi\left(\frac{u(y,t)+u(x,t)}{2}\right)\varphi(y,x)dydx=0$$

- Re-write as

$$\frac{\partial}{\partial t}\int_a^b u(x,y)dx+\int_a^b\int_{a-\varepsilon}^{a}\psi\left(\frac{u(y,t)+u(x,t)}{2}\right)\varphi(y,x)dydx$$

Flux from [a,b] to [a-ε] through a

$$+\int_a^b\int_b^{b+\varepsilon}\psi\left(\frac{u(y,t)+u(x,t)}{2}\right)\varphi(y,x)dydx$$

Flux from [a,b] to [b+ε] through b

$$+\int_a^b\int_a^b\psi\left(\frac{u(y,t)+u(x,t)}{2}\right)\varphi(y,x)dydx=0$$

This term is zero (antisymmetry)

Sandia National Laboratories

Nonlocal Linear One-Way Wave Equation

- Let $\psi(u) = u$. This give the nonlocal equivalent of $u_t+u_x=0$.

$$\frac{\partial u}{\partial t} + \int_{x-\varepsilon}^{x+\varepsilon} u(y,t)\varphi(y,x)dy = 0$$

- Plug in traveling wave solution

$$u(x,t) = \exp\left(ik(x - c(k)t)\right)$$

to analyze speed of individual modes.

- For particular kernel, can show

$$c(k) = \frac{\sin^2(k\varepsilon/2)}{(k\varepsilon/2)^2} \leq 1$$

- Two important differences from local one-way wave equation
  - Nonlocal wavespeed varies with wavenumber
  - Nonlocal wavespeed slower than classical wavespeed

Nonlocal Burgers: Theory

- Nonlocal Burgers: $\psi(u) = u^2/2$
- Conservation:

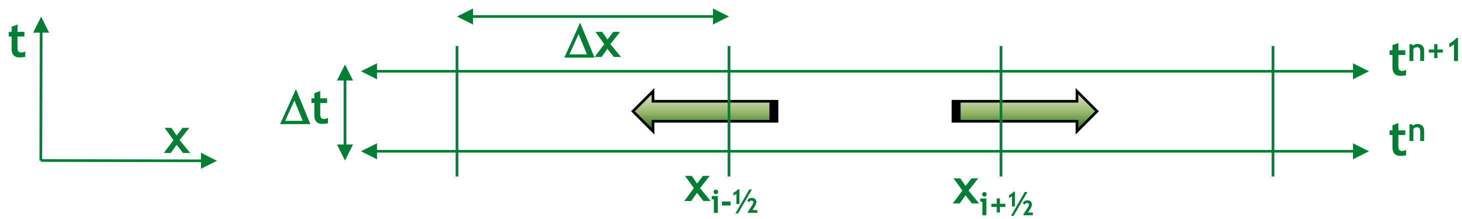
$$\frac{d}{dt}\int u(x,t)dx = 0 \qquad\qquad \frac{d}{dt}\int u^2(x,t)dx \neq 0$$

- Well-Posedness:
  - Assume $\varphi \in L^1(-\varepsilon, \varepsilon)$, $g \in H^1(R)$. Then, there exists a time interval (0, T) such that the nonlocal Burgers equation has a unique solution. Moreover, let (0, T) be the maximum time interval on which such a solution exists. Then, $\limsup_{t \to T} \|u(\cdot,t)\|_{L^\infty} = \infty$.
- Consequences:
  - If we start with smooth data, solution maintains H^1 regularity so long as it is pointwise bounded in space and time. Moreover, only finite-time blow-up can cause loss of H^1 regularity of the solution.
  - If $\varphi \in L^1$ and initial data smooth, solution maintains H^1 regularity for positive horizon. There is no shock formation with an L^1 kernel!
  - Contrast with local Burgers, where initial smooth data can lead to shock
    - Addition of viscosity forbids shock formation in local case
    - L^1 kernel forbids shock formation in nonlocal case (no additional regularization needed)

Sandia National Laboratories

Nonlocal Lax-Friedrichs Discretization (1)

- Discretize space & time into cells $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ and intervals $[t^n, t^{n+1}]$
- The flux out of cell i is the flux out of $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ through $x_{i-\frac{1}{2}}$ and $x_{i+\frac{1}{2}}$



- Flux out of $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ through $x_{i+\frac{1}{2}}$ (expression for $x_{i-\frac{1}{2}}$ similar)

$$f_{[x_{i-\frac{1}{2}},x_{i+\frac{1}{2}}]}\left(x_{i+\frac{1}{2}},t\right)=\int_{0}^{\Delta x}\int_{0}^{\varepsilon-z}\psi\left(\frac{u(x+y,t)+u(x-z,t)}{2}\right)\varphi(x+y,x-z)\,dydz$$

- Convervative numerical scheme: Change in u over cell $[x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$ in time interval $[t^n, t^{n+1}]$ must be balanced by flux over that cell over that time interval

$$\int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\left(u(x,t^{n+1})-u(x,t^{n})\right)dx+\int_{t_n}^{t_{n+1}}\left(f_{[x_{i-\frac{1}{2}},x_{i+\frac{1}{2}}]}\left(x_{i-\frac{1}{2}},t\right)+f_{[x_{i-\frac{1}{2}},x_{i+\frac{1}{2}}]}\left(x_{i+\frac{1}{2}},t\right)\right)dt=0$$

Nonlocal Lax-Friedrichs Discretization (2)

- Define

$$\bar{u}_i^n \approx \frac{1}{\Delta x}\int_{x_{i-½}}^{x_{i+½}} u(x,t^n)dx$$

$$\bar{F}_{i+½}^n \approx \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} f_{[x_{i-½},x_{i+½}]}\left(x_{i+½},t\right)dt$$

$$\bar{F}_{i-½}^n \approx \frac{1}{\Delta t}\int_{t^n}^{t^{n+1}} f_{[x_{i-½},x_{i+½}]}\left(x_{i-½},t\right)dt$$

- This gives

$$\bar{u}_i^{n+1} = \bar{u}_i^n - \frac{\Delta t}{\Delta x}\left(\bar{F}_{i+½}^n + \bar{F}_{i-½}^n\right)$$

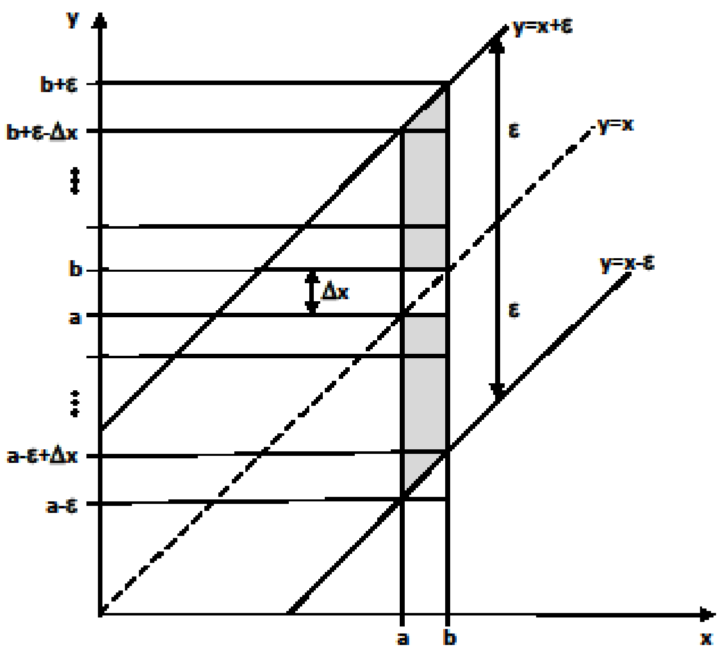
- This is the nonlocal equivalent of FTCS (unconditionally unstable)
- Stabilization produces nonlocal Lax-Friedrichs:

$$\bar{u}_i^{n+1} = \frac{\bar{u}_{i+1}^n + \bar{u}_{i-1}^n}{2} - \frac{\Delta t}{\Delta x}\left(\bar{F}_{i+½}^n + \bar{F}_{i-½}^n\right)$$

Nonlocal Lax-Friedrichs Discretization (3)

- Suppose (for convenience) that $r\,\Delta x = \varepsilon$, r an integer.
- Quadrature (midpoint in space):

$$\left(f_{[x_{i-1/2},x_{i+1/2}]}\left(x_{i-1/2},t\right)+f_{[x_{i-1/2},x_{i+1/2}]}\left(x_{i+1/2},t\right)\right)=\sum_{j=-r}^{j=r}\omega_j\psi\left(\frac{u(x_{i+j},t)+u(x_i,t)}{2}\right)\varphi(x_{i+j},x_i)\left(\Delta x\right)^2$$



$$\omega_j=\begin{cases}0 & j=0\\ 1 & j=\pm1,\ldots,\pm(r-1)\\ \frac{1}{2} & j=-r,r\end{cases}$$

- Stability analysis: Let $\psi(u)=u,\ \varphi(y,x)=\frac{1}{\varepsilon^2}\begin{cases}1 & y>x\\ 0 & y=x\\ -1 & y<x\end{cases}$
- Then $\Delta t<\frac{2r}{r+1}\Delta x$

Sandia National Laboratories

Nonlocal Burgers: Computational Results

- There are two primary nondimensional length scales:
  - ε/L Ratio of PD length scale to problem length scale
  - $\varepsilon/\Delta x$ Ratio of PD horizon to cell size
- So, perform two independent studies: ε-refinement and Δx refinement

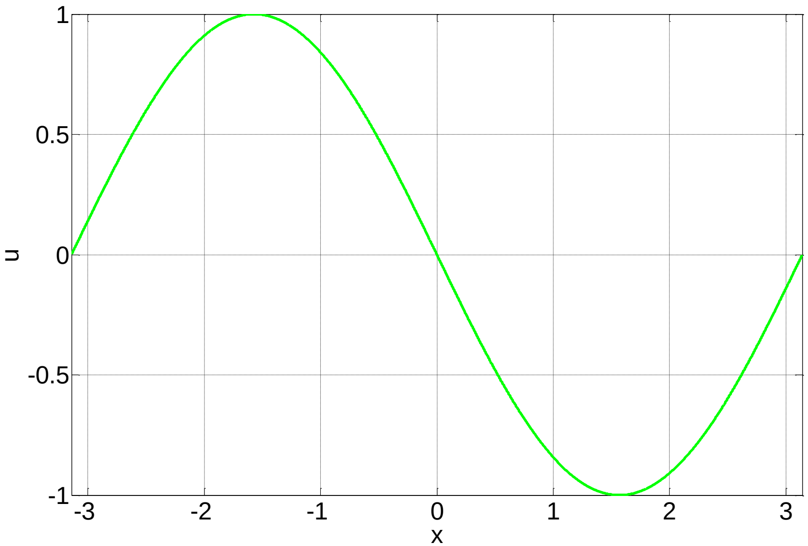
- Let $\Delta t/\Delta x = 2/c$ fixed, c = 80. (i.e., artificial viscosity same for all experiments)
  - $\min(\varepsilon/L) \approx 0.004$ (small horizon)
  - $\max(\varepsilon/L) \approx 0.1$ (large horizon)
  - $\min(\varepsilon/\Delta x) \approx 16$
  - $\max(\varepsilon/\Delta x) \approx 256$
  - The horizon is typically 3× the mesh spacing in PD solid mechanics. In these numerical experiments, nonlocality is well-resolved

	Δx-refinement study					ε-refinement study			
N	2000	4000	8000	16000	32000	10000	10000	10000	10000
Δx	3.14e-3	1.57e-3	7.86e-4	3.93e-4	1.97e-4	6.28e-4	6.28e-4	6.28e-4	6.28e-4
ε	5.02e-2	5.02e-2	5.02e-2	5.02e-2	5.02e-2	1.26e-2	6.28e-2	1.57e-1	3.14e-1
ε/L	1.60e-2	1.60e-2	1.60e-2	1.60e-2	1.59e-2	4.00e-3	2.00e-2	5.00e-2	1.00e-1
$\varepsilon/\Delta x$	16	32	64	128	256	20	100	250	500

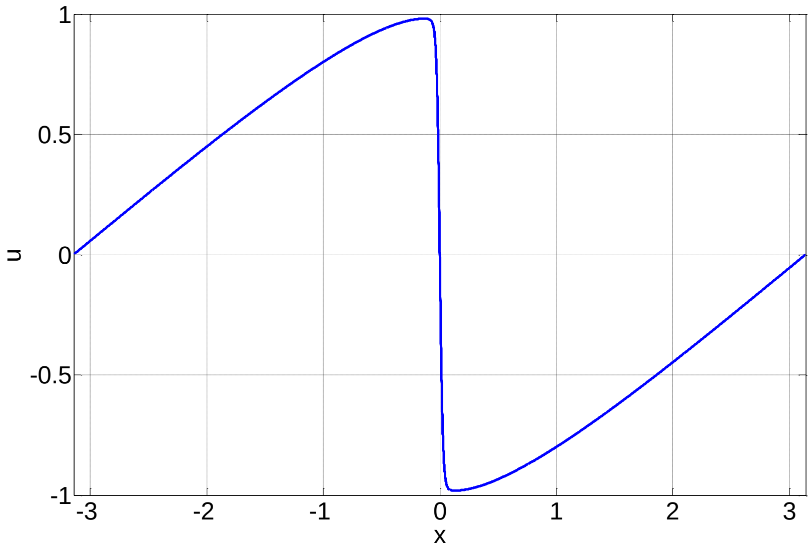
Sandia National Laboratories

Nonlocal Burgers: Sine IC

- ❑ Domain: $-\pi \leq x < \pi$; N cells with $\Delta x = L/N$; $L = \pi$.
- ❑ Boundary conditions: $u(x + kL, t) = u(x,t)$; $k \in Z^+$
- ❑ Initial condition: $u_0 = -\sin(x)$



Initial Condition



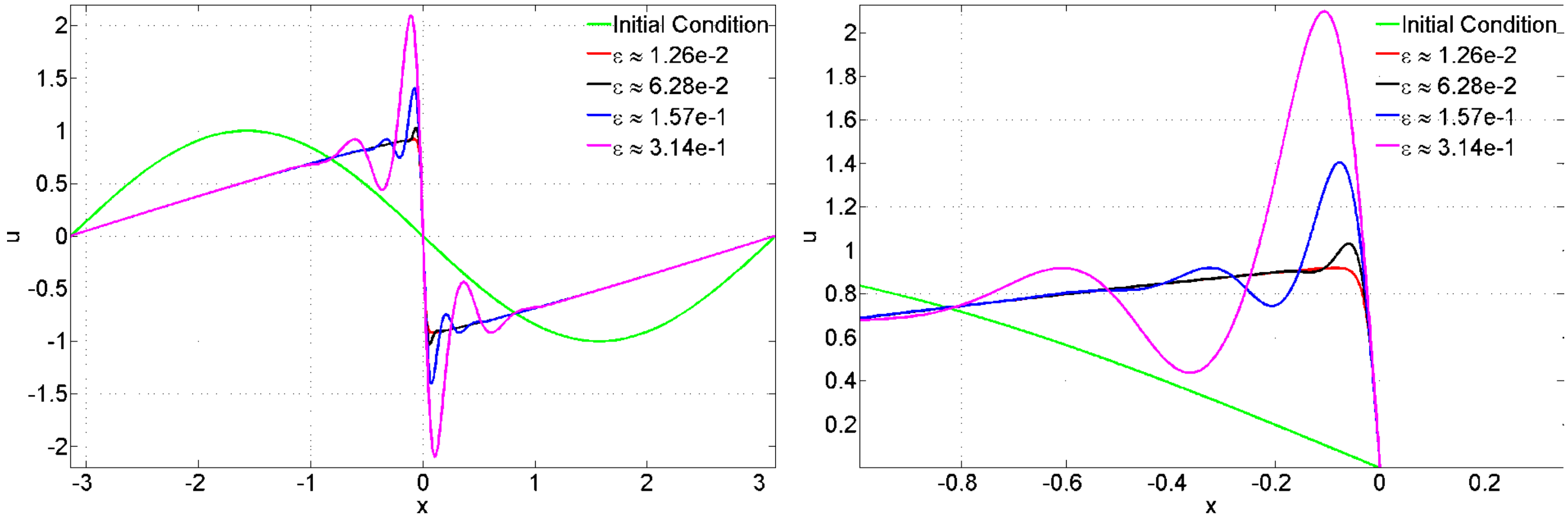
Local Lax-Friedrichs at t=1.5

- ❑ Compare with analytical and numerical for local Burgers' equation
  - ❑ Sinusoid IC leads to shock formation at x=0, t=1. N-wave develops as $t \to \infty$.

Sandia National Laboratories

Nonlocal Burgers: Sine IC

- ε-refinement study (for $\Delta x \approx 6.28e\text{-}4$) (fine mesh)



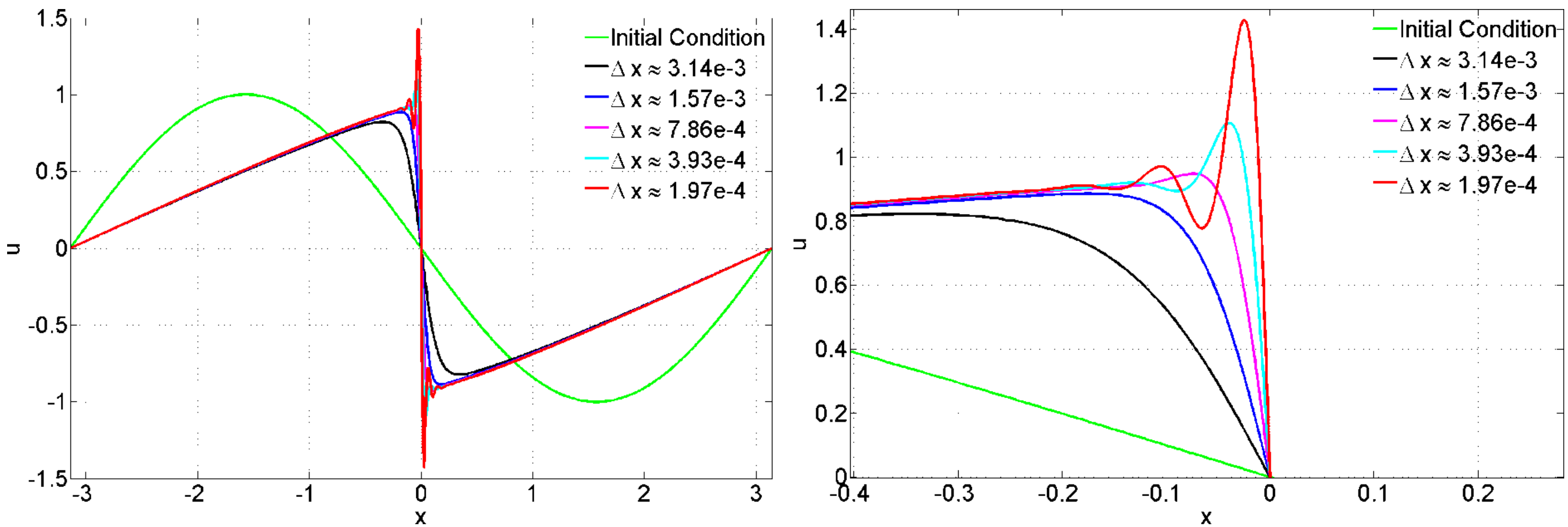
- For small ε, results qualitatively similar to N-wave
- Additional oscillations for larger ε

- $\int u \, dx$ conserved; Numerical method is conservative (not shown here)
- $\int u^2 \, dx$ not conserved (artificial viscosity)

Sandia National Laboratories

Nonlocal Burgers: Sine IC

- Δx - refinement study (for $\varepsilon \approx 0.05$; $\varepsilon/L \approx 1.59\text{e-}2$) (small ε)

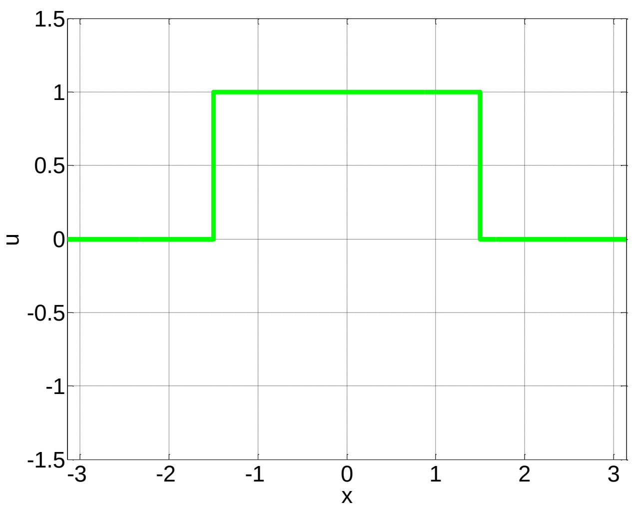


- Gibbs-like oscillations around shock-like feature

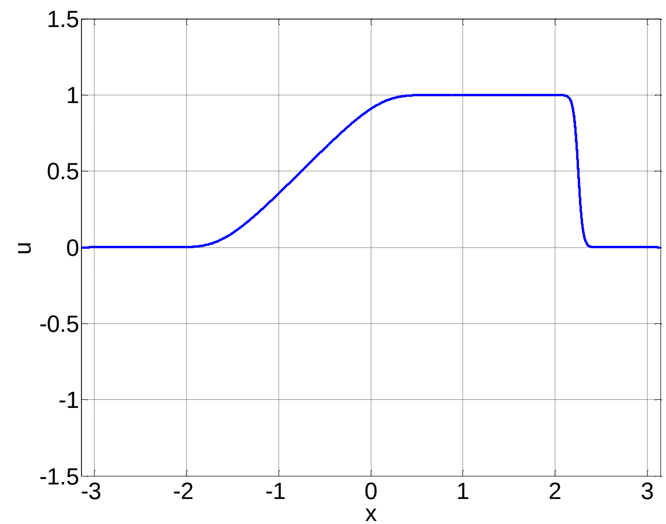
- $\int u \, dx$ conserved; Numerical method is conservative (not shown here)
- $\int u^2 \, dx$ not conserved (artificial viscosity)

Nonlocal Burgers: “Top Hat” IC

- Domain: $-\pi \leq x < \pi$; N cells with $\Delta x = L/N$; $L = \pi$.
- Boundary conditions: $u(x + 2kL, t) = u(x,t)$; $k \in$ ▯
- Initial condition: $u_0 = 1$ if $-1.5 \leq x < 1.5$; 0 elsewhere



Initial Condition

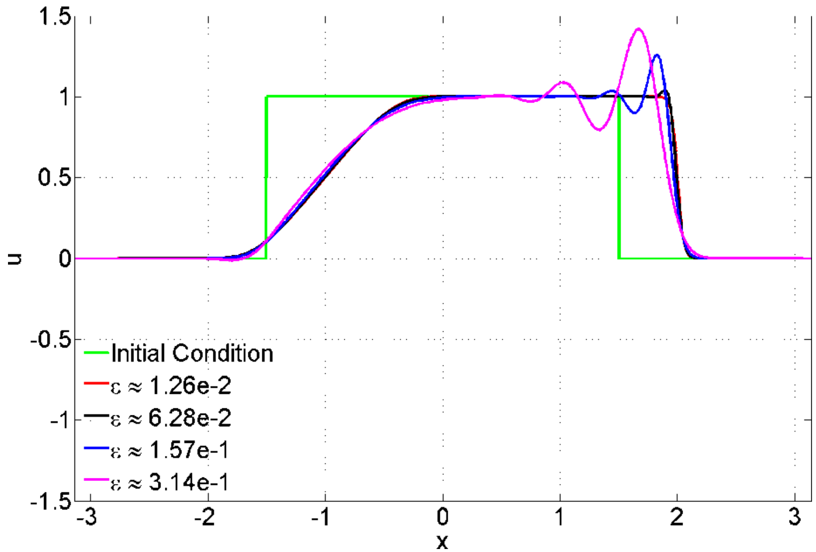


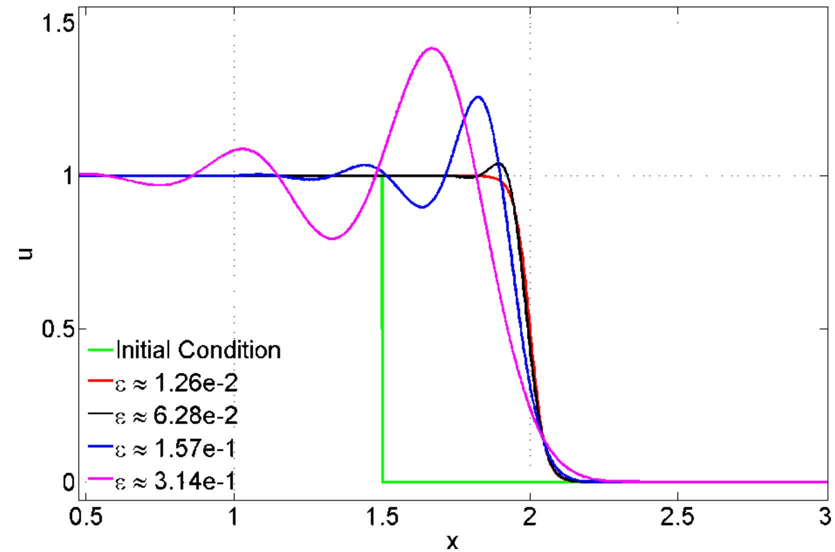
Local Lax-Friedrichs at t=1.5

- Compare with analytical and numerical for local Burgers’ equation
    - “Top Hat” IC leads to rarefaction (left) plus shock (right)

Nonlocal Burgers: “Top Hat” IC

- ε-refinement study (for $\Delta x \approx 6.28e\text{-}4$) (fine mesh)



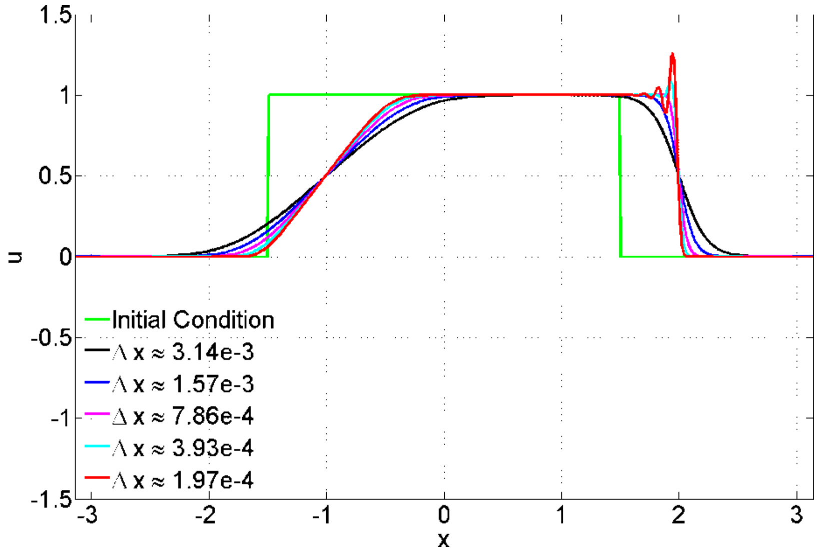


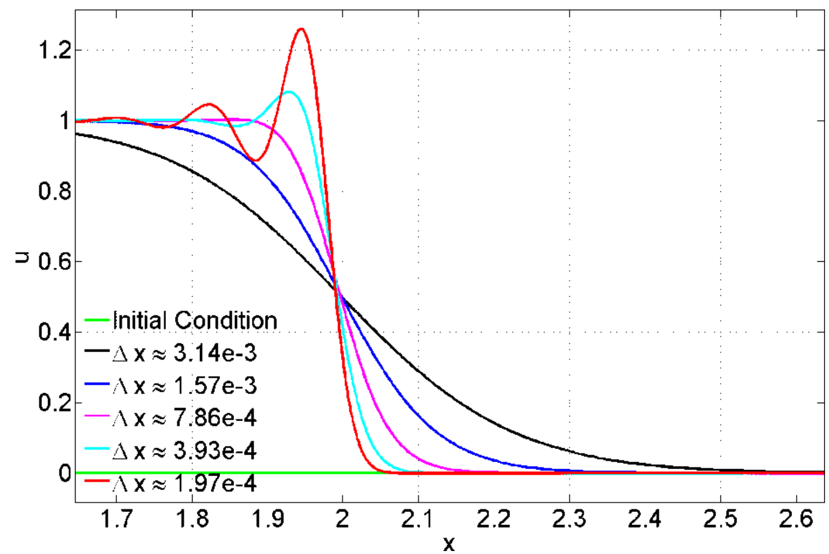
- For small ε, results qualitatively similar to classical results
- Additional oscillations around shock-like feature for larger ε

- $\int u \, dx$ conserved; Numerical method is conservative (not shown here)
- $\int u^2 \, dx$ not conserved (artificial viscosity)

Nonlocal Burgers: “Top Hat” IC

- Δx - refinement study (for ε ≈ 0.05; ε/L ≈ 1.59e-2) (small ε)





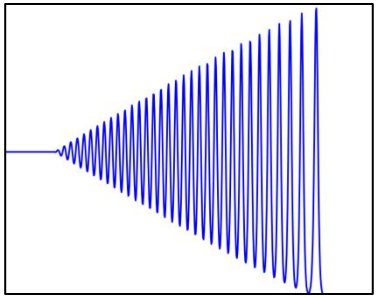
- Gibbs-like oscillations around shock-like feature

- ∫u dx conserved; Numerical method is conservative (not shown here)
- ∫u^2 dx not conserved (artificial viscosity)

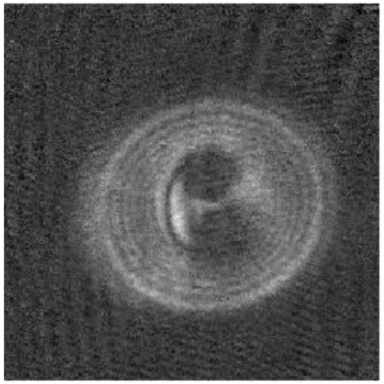
Relation to Dispersive Shocks (1)

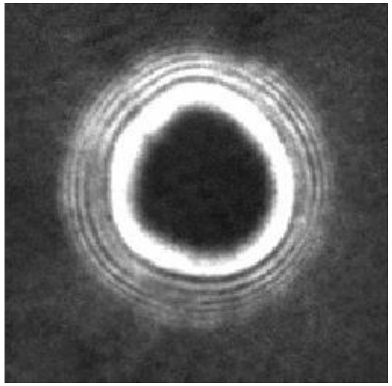
- The Korteweg–de Vries equation produces ***dispersive*** **shocks**[1]

$$\frac{\partial u}{\partial t} + 6u\frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3} = 0$$



- **Dispersive shocks appear (for example) in**
  - **Rotating Bose-Einstein condensate**
  - **Collisionless ion-acoustic shock waves observed from interaction of two plasmas**
  - **Optical wave breaking observed in propagation of light through nonlinear fiber**
  - **Propagation of intense electromagnetic wave through photorefractive medium**





Experimental absorption images of Bose-Einstein condensate blast wave [2]. The oscillatory ring structures correspond to dispersive shock waves.

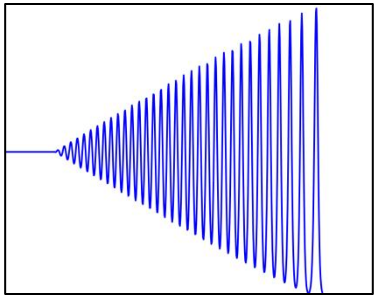
[1] Hoefer and Ablowitz, Dispersive Shock Waves, Scholarpedia, 4(11):5562, 2009.

[2] Hoefer, Ablowitz, Coddington, Cornell, Engels, and Schweikhard, Dispersive and classical shock waves in Bose-Einstein condensates and gas dynamics, Phys. Rev. A, 74:023623, 2006.

Relation to Dispersive Shocks (2)

- The Korteweg–de Vries equation produces *dispersive* shocks[1]

$$\frac{\partial u}{\partial t} + 6u\frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3} = 0$$



- Oscillatory solution reminiscent of solutions to nonlocal Burgers equation

- Compare with leading terms of Taylor series of nonlocal Burgers equation:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + \frac{60\varepsilon^2}{720}\frac{\partial^3 u}{\partial x^3} + \frac{90\varepsilon^2}{720}\left(\frac{\partial u}{\partial x}\right)\left(\frac{\partial^2 u}{\partial x^2}\right) + \cdots = 0$$

  - Leading terms match (up to scaling) with KdV
  - Reduces to local Burgers equation in limit as $\varepsilon \to 0$
- In nonlocal Burgers, no shocks possible for $\varepsilon > 0$ and $\varphi \in L^1$
  - Nonlocal Burgers provides additional regularity beyond KdV

[1] Hoefer and Ablowitz, Dispersive Shock Waves, Scholarpedia, 4(11):5562, 2009.

Sandia National Laboratories

Summary

- Peridynamic-inspired model for nonlocal, nonlinear advection
- Nonlocal flux and relation to classical flux
- Conservation law form
- Nonlocal one-way wave equation
- Nonlocal Burgers equation
  - Shocks not possible for $\varepsilon>0$ and $\varphi \in L^1$ for smooth data
- Nonlocal Lax-Friedrichs method
  - Computational results (sine IC, “top hat” IC)
- Relation to dispersive shock waves

- Papers, codes
  - www.sandia.gov/~mlparks; mlparks@sandia.gov