Level Set Methods for Tracking Discontinuities in Conservation Laws

Tariq Aslam

http://home.lanl.gov/aslam

Los Alamos National Laboratory
Group DX-1: Detonation Science and Technology

Collaborators:
LANL: John Bdzil
UCLA: Ron Fedkiw, Stan Osher
Outline

• Motivation for sharp shocks in DNS
• Review of Level Set and Ghost Fluid Methods
• Shock “tracking” using level set methods
  • Scalar equations
  • Euler equations
Motivation - 1

• Interest in direct simulation of detonation

Mass: \[ (\rho)_t + (\rho u)_x + (\rho v)_y = 0 \]

\( x \)-Momentum: \[ (\rho u)_t + \left( \rho u^2 + p \right)_x + (\rho uv)_y = 0 \]

\( y \)-Momentum: \[ (\rho v)_t + \left( \rho uv \right)_x + \left( \rho v^2 + p \right)_y = 0 \]

Energy: \[ (E)_t + (uE + up)_x + (vE + vp)_y = 0 \]

Rate Law: \[ (\rho \lambda)_t + (\rho u \lambda)_x + (\rho v \lambda)_y = \rho R(\rho, \rho, \lambda) \]

E.O.S.: \[ E = \frac{p}{\gamma - 1} - \rho Q \lambda + \frac{\rho}{2} \left( u^2 + v^2 \right) \]
Detonation Structure - shock followed reaction zone:

- ZND Theory
  - 1D, Steady
  - Finite reaction after shock
  - Conservation determines $D_n$
  - Minimum steady propagation speed, $D_{CJ}$
• Properties of Shock Capturing solution

- Start-up errors propagate along characteristics from shock
- Shock is "smeared" over a few cells - artificial ignition criteria
- Location and Speed of shock wave is not explicitly in solution
Motivation - 4

• Detonation Shock Dynamics and DNS issues

• Need accurate DNS to validate $O(\varepsilon)$ theory, $D_n(\kappa)$

• Need to have accurate intrinsic shock information for higher order theories ($D_n$, $DD_n /Dt$, $\kappa$, $D_{n,\xi\xi}$)

• Need to accurately model HE/inert interaction
Motivation - 5

- Difficult to measure 1st derivative from a DNS
What is a level set?

Interface is represented by (in 2-D)

\[ \psi(x, y, t) = 0 \]

and

\[ \psi(x, y, t) < 0 \]

“inside” interface and

\[ \psi(x, y, t) > 0 \]

“outside” interface.

\[ \hat{n} = \frac{\vec{\nabla} \psi}{|\vec{\nabla} \psi|} \]

\[ \frac{D\psi}{Dt} = 0 \]

\[ \frac{\partial\psi}{\partial t} + \vec{u} \cdot \vec{\nabla} \psi = 0 \]
Advantages of Level Set representation

- Same grid as physical problem, no extra data structures
- Use standard Hamilton-Jacobi solvers (TVD, ENO, etc.)
- Topology changes are handled easily
How do we use Level Sets for treating discontinuities? Ghost Fluid Method.

Key idea: Represent a Discontinuous function, $u$, with 2 smooth functions, $u_1$ and $u_2$, and a level set field function, $\psi$.

$$u_{\text{real}} = \begin{cases} u_1 & \text{if } \psi < 0 \\ u_2 & \text{if } \psi \geq 0 \end{cases} \quad u_{\text{ghost}} = \begin{cases} u_1 & \text{if } \psi \geq 0 \\ u_2 & \text{if } \psi < 0 \end{cases}$$

$\psi=0$ is discontinuity locus.

Working with smooth functions is advantageous computationally.
Example: Ghost Fluid Method for Multi-material Hydrodynamics

\( \rho \) vs \((x,y)\)

\( \rho_1 \) and \(\rho_2\) vs \((x,y)\)

\( \psi \) vs \((x,y)\)

Air Shock Collapse of He bubble, Numerical Schlieren ala Quirk
Level Sets for Tracking Discontinuities in Scalar Equations

• Use Level Set function for separating “shocked” and “un-shocked” material

• Solve 1D (normal) Riemann Problem between 2 states for all x, and calculate shock speed, s. Careful of shock entropy condition:

\[ f'(u_l) \geq s \geq f'(u_r) \]

• Solve Scalar equations in both states

• Advect level set function at shock speed, s.
Justification of Method

• Justification stems from shock entropy condition

Characteristics flow into (through) shock
(from real region to ghost region)

\[ f'(u_l) \geq s \geq f'(u_r) \]
Example 1: Burgers’ Equation

Level Set

Standard form:  Tracking form:

\[ u_t + \left( \frac{u^2}{2} \right)_x = 0 \]

\[
\begin{align*}
(u_1)_t + \left( \frac{u_1^2}{2} \right)_x &= 0 \\
(u_2)_t + \left( \frac{u_2^2}{2} \right)_x &= 0 \\
\psi_t + s\psi_x &= 0 \\
s = \begin{bmatrix} f(u) \\ u \end{bmatrix} &= \frac{u_1 + u_2}{2}
\end{align*}
\]

Note, \( u_1 \) and \( u_2 \) are constrained in the ghost region to satisfy entropy condition.
Example 1: Burgers’ Equation

Initial conditions:
\[ u = \begin{cases} 
1 - \cos(\pi x), & x < 1 \\
\frac{1}{4}, & x > 1 
\end{cases} \]

\[ u_2 = 1 - \cos(\pi x) \]

\[ u_1 = \frac{1}{4} \]

\[ \psi = x - 1 \]
Example 2: 2D Burgers’ Equation

Standard form:

\[ u_t + \left( \frac{u^2}{2} \right)_x + \left( \frac{u^2}{2} \right)_y = 0 \]

Level Set Tracking form:

\[
\begin{align*}
(u_1)_t + & \left( \frac{u_1^2}{2} \right)_x + \left( \frac{u_1^2}{2} \right)_y = 0 \\
(u_2)_t + & \left( \frac{u_2^2}{2} \right)_x + \left( \frac{u_2^2}{2} \right)_y = 0 \\
\psi_t + & \vec{s} \cdot \nabla \psi = 0 \\
\vec{s} = & \begin{bmatrix} f(u) \\ u \end{bmatrix} \vec{i} + \begin{bmatrix} g(u) \\ u \end{bmatrix} \vec{j} = \frac{u_1 + u_2}{2} \vec{i} + \frac{u_1 + u_2}{2} \vec{j}
\end{align*}
\]
Initial conditions:

\[ u = \begin{cases} 1, & \text{if } r < 1/3 \\ 0, & \text{otherwise} \end{cases} \]

\[ r^2 = (x - 0.5)^2 + (y - 0.5)^2 \]

\[ u_1 = 1 \]

\[ u_2 = 0 \]

\[ \psi = \frac{1}{3} - |r| \]
Level Sets for Tracking Shock Waves

- Use Level Set function for separating “shocked” and “un-shocked” material
- Solve 1D (normal) Riemann Problem between 2 states, determine shock speed, check entropy condition and project shocked ghost state
- Solve Euler equations in both states
- Advect level set function with shock speed
Justification of Method

• Justification stems from shock entropy condition and projection of ghost states

• Projection forces the ghost state onto a 1D manifold, parameterized by shock speed and upstream state

\[ s_t + (u + c)_{\text{shock}} s_x = 0 \]
\[ \Rightarrow p(s), u(s), \rho(s) \]
Example: Ghost Region perturbation in inert planar Ma=3 shock

- Perturbations in Ghost Region travel faster than shock and do not influence real solution

\[ t=0 \]

\[ t=1.5 \]
Example: Steady Propagating Detonation

- Start-up errors are effectively removed
- Solution state is 2-5 times more accurate
- 1st order convergence for shock speed
Example: Pulsating Detonation

Example: Calculation of 1D unstable detonation

Physical parameters: $E=50$, $Q=50$, $\gamma=1.2$, $f=1.6$

Captured Shock
10 points per $L_{1/2}$

Level Set Tracked Shock
10 points per $L_{1/2}$
Example: Pulsating Detonation

Example: Calculation of 1D unstable detonation

Physical parameters: E=50, Q=50, γ=1.2, f=1.6

Captured Shock Velocity
2 resolutions

LST Shock Velocity
2 resolutions

Dn

5 pts per L1/2
10 pts per L1/2

0 8 16 24 32
time

Dn

5 pts per L1/2
10 pts per L1/2

0 8 16 24 32
time