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Title: Machine Learning Optimal Flux-Limiters for Hydrodynamic Calculations

Author(s): Chiodi, Robert Michael
McKerns, Michael
Livescu, Daniel

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Los Alamos NATIONAL LABORATORY

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Robert Chiodi, Michael McKerns, Daniel Livescu

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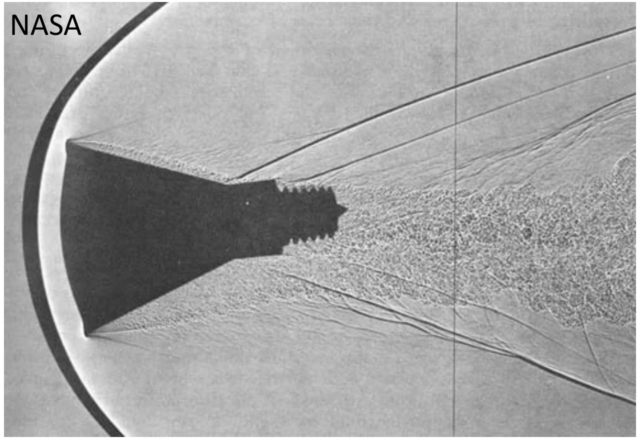
Importance of Compressible Flows



Euler Equations in 1D

- The Euler equations govern inviscid flow

$$\frac{\partial \vec{U}}{\partial t} + \frac{\partial F(\vec{U})}{\partial x} = 0$$

$$\vec{U} = [\rho, \rho u, E]^T; \;\; F(\vec{U}) = [\rho u, \rho u^2 + p, u(E + P)]^T$$

- An equation of state relates the internal energy and density to pressure

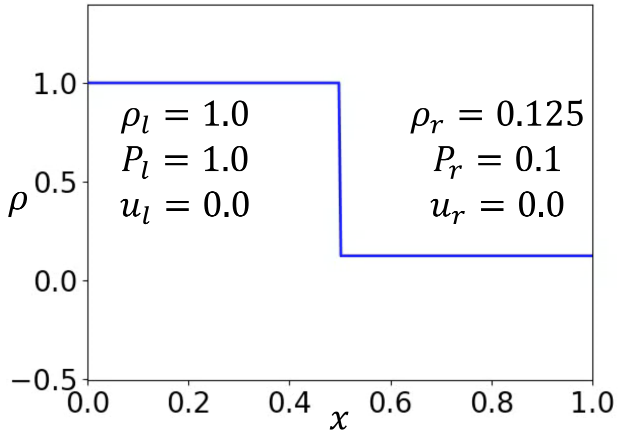
$$e(\rho, P) = \frac{P}{\rho(\gamma - 1)}$$

Compressible CFD and Slope-Limiters

- Numerically solving the Euler equations requires taking derivatives over discontinuities (shocks)

- Naïve approaches to taking these derivatives lead to ringing and numerical instabilities

- Many approaches have been developed for this
  - Slope-limiters
  - Flux-limiters
  - WENO/ENO schemes



Shock Tube Problem

We will focus on slope limiters

Compressible CFD and Slope-Limiters

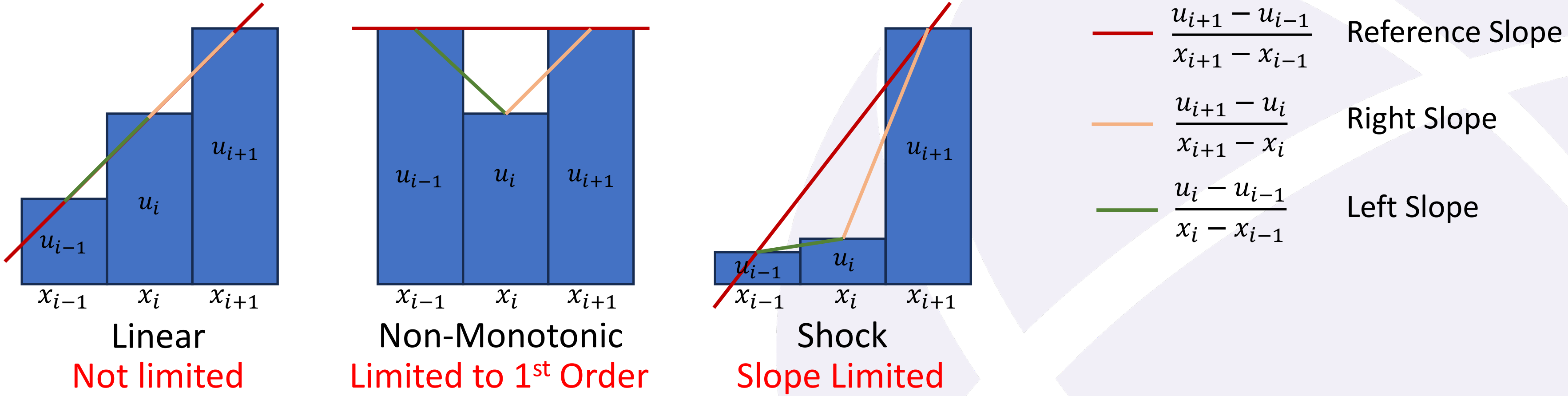
- Semi-discrete inviscid 1D Euler equation

$$\frac{d\vec{U}_i}{dt} + \frac{1}{\Delta x_i}\left[\vec{F}\left(\vec{U}_{i+\frac{1}{2}}\right) - \vec{F}\left(\vec{U}_{i-\frac{1}{2}}\right)\right] = 0$$

- The Riemann solver for $\vec{F}$ depends on reconstructed values $\vec{U}_{i+\frac{1}{2},\, l}$, $\vec{U}_{i+\frac{1}{2},\, r}$
- **Slope-limiters** control the order of the reconstruction
  - Dependent on local smoothness $r_i = \frac{\rho_i - \rho_{i-1}}{\rho_{i+1} - \rho_i}$
- For smooth regions, high-order reconstruction used. Near shocks, revert to zeroth order interpolation

$$\vec{U}_{i+\frac{1}{2},\, l} = \vec{U}_i, \qquad \vec{U}_{i+\frac{1}{2},\, r} = \vec{U}_{i+1}$$

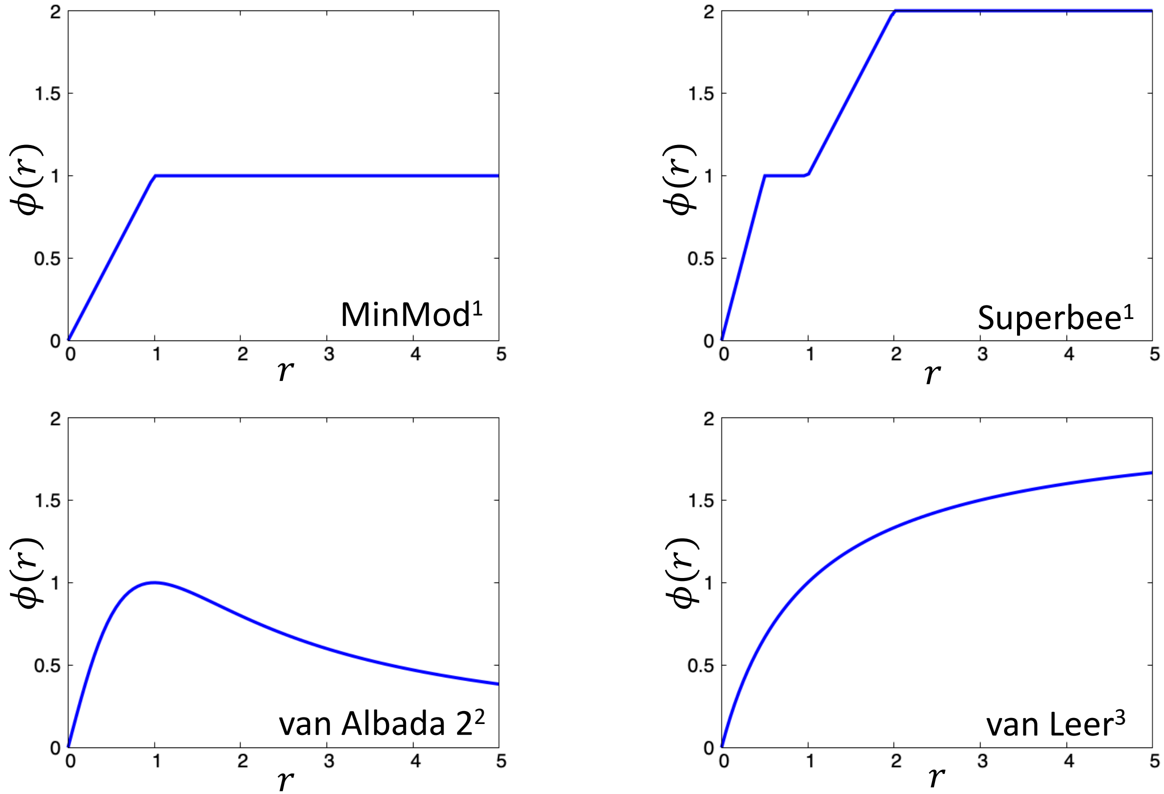
Compressible CFD and Slope-Limiters



Need to find limited slopes s to perform reconstruction

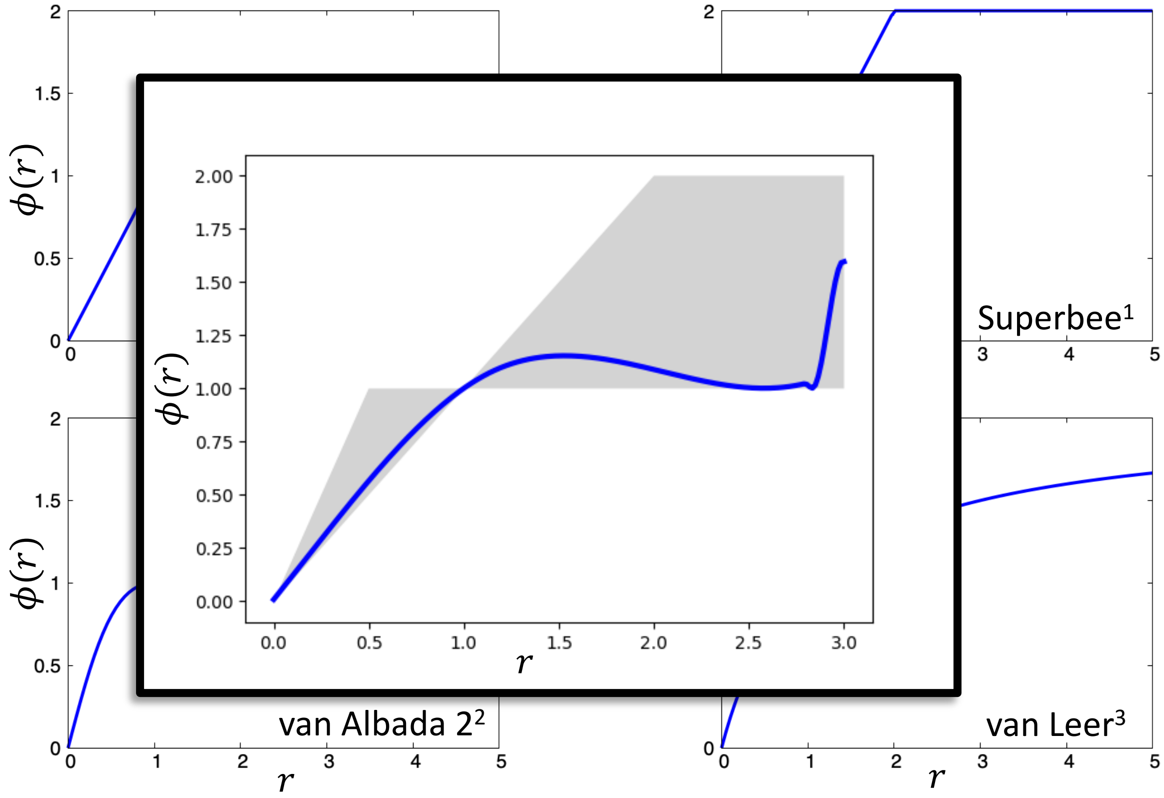
$r_i = \frac{u_i - u_{i-1}}{u_{i+1} - u_i}$, $s = \frac{u_{i+1} - u_i}{x_{i+1} - x_i}\phi(r)$, with $\phi(r)$ being the non-linear slope limiter function

Existing Slope-Limiters



1. Rho, 1986 2. Kermani, 2003 3. van Leer, 1974

Existing Slope-Limiters

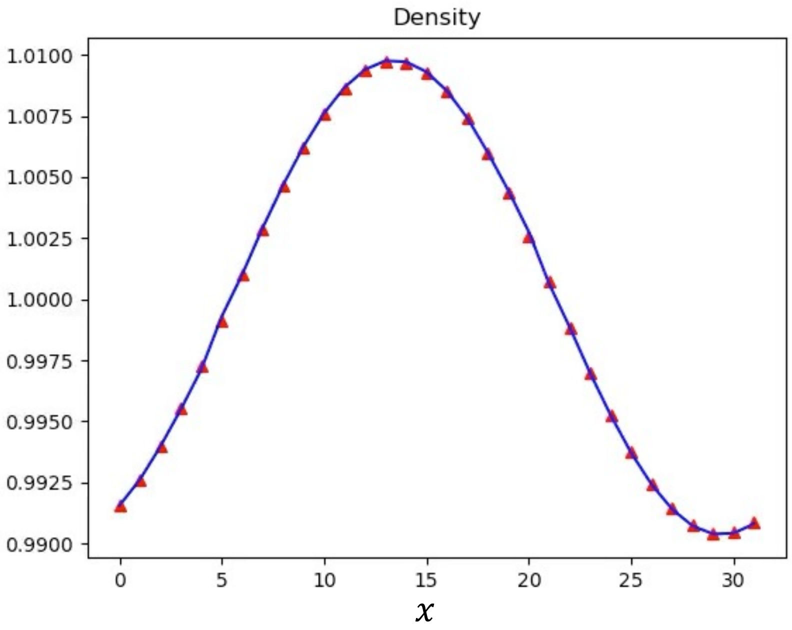


1. Rho, 1986 2. Kermani, 2003 3. van Leer, 1974

Approach for Finding Slope Limiter

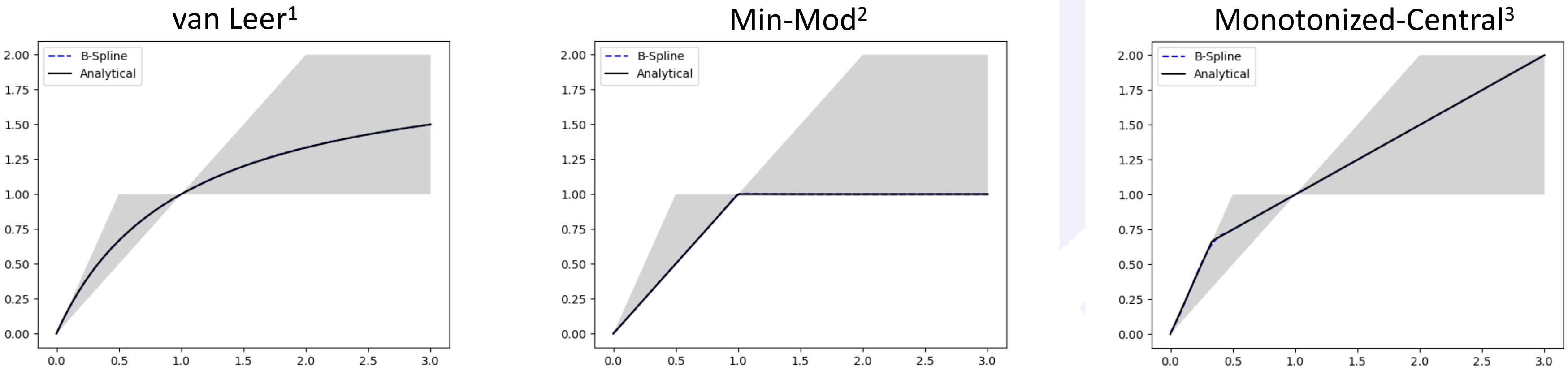
Simulation-Based

- Finite volume code used with HLLC Riemann solver, slope-limited PLM reconstruction, and RK2 time advancement
- Trained by evaluating single-step pointwise errors for two configurations
  1. Self-Steepening Sine-Waves:
     A sine-wave that grows into a shock due to properties of the Euler equations
  2. Shock-Tubes:
     Riemann problem with jump in density and pressure



Representation of Slope Limiter

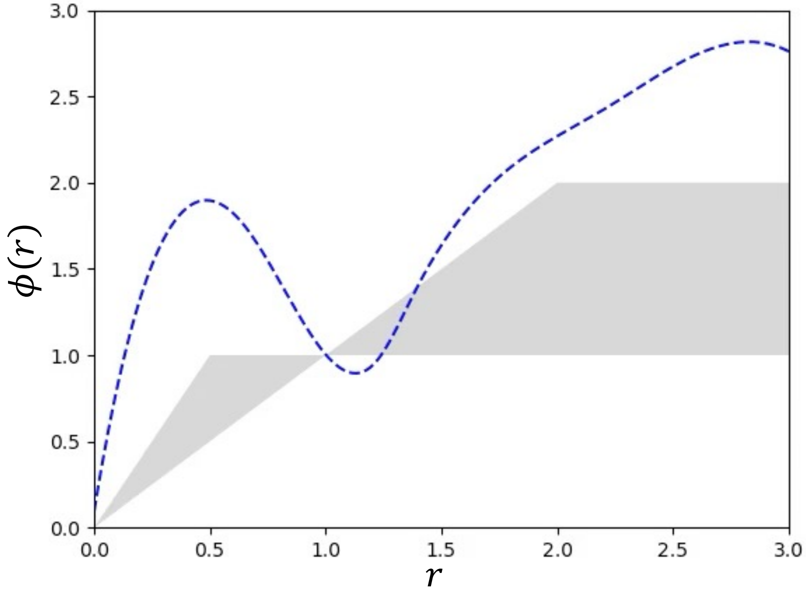
Slope limiter is parametrized as a cubic B-Spline with 6 knots

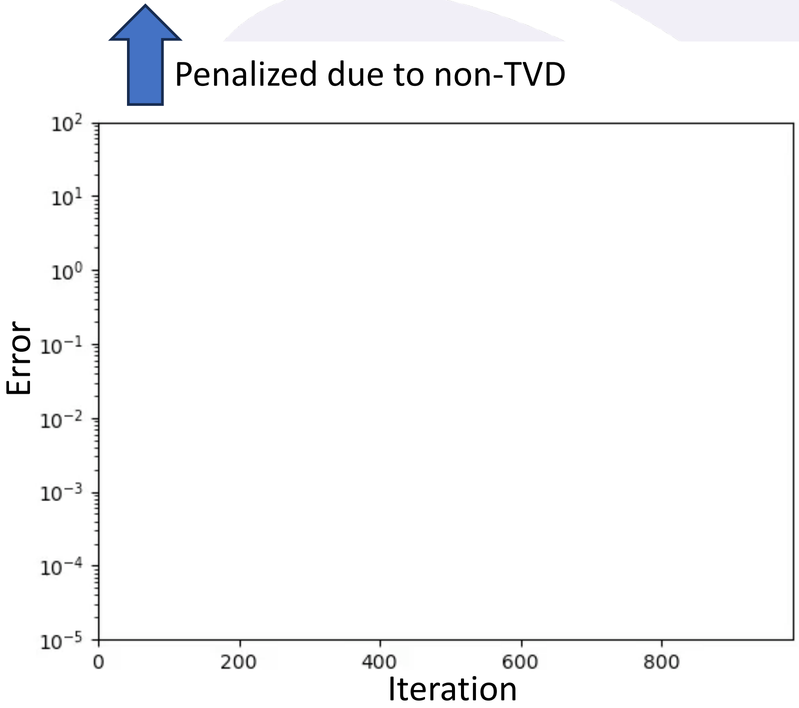


$$\phi(r)_{TVD} = \begin{cases} r \leq \phi(r) \leq 2r, & 0 \leq r < 1 \\ \phi(r) = 1, & r = 1 \\ 1 \leq \phi(r) \leq r, & 1 < r \leq 2 \\ 1 \leq \phi(r) \leq 2, & r > 2 \end{cases}$$

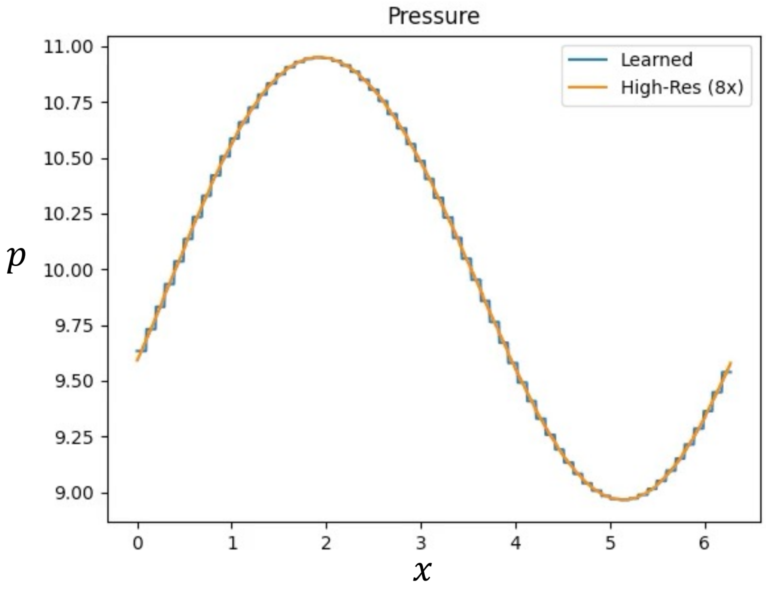
1. van Leer, 1974 2. Rho, 1986. 3. van Leer, 1977 4. Sweby, 1994

Found Slope Limiter





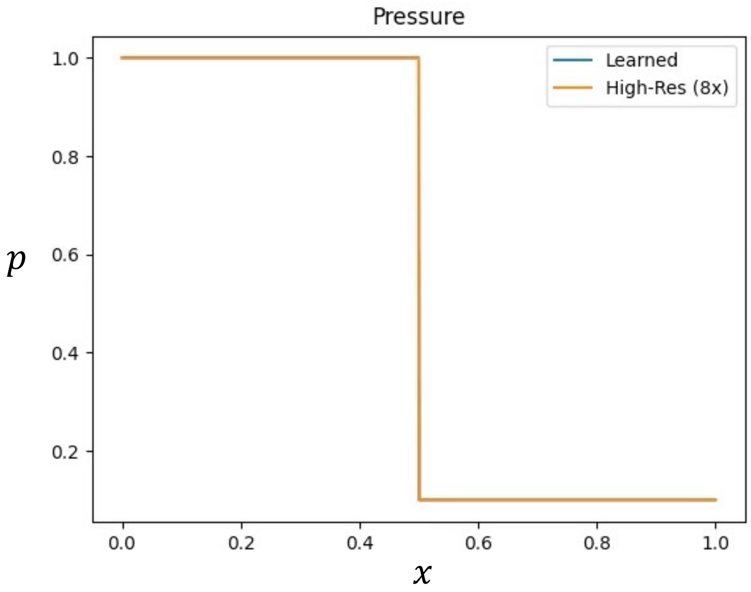
Example Sine-Wave Case



Error over randomized set of simulations

Method	Error
Learned	**1.782e-4**
van Leer	1.021e-3
Min Mod	7.382e-4
Superbee	3.076e-2
van Albada	5.584e-3
van Albada 2	3.177e-3
Monotonized Central	1.212e-2
UMIST	1.823e-3

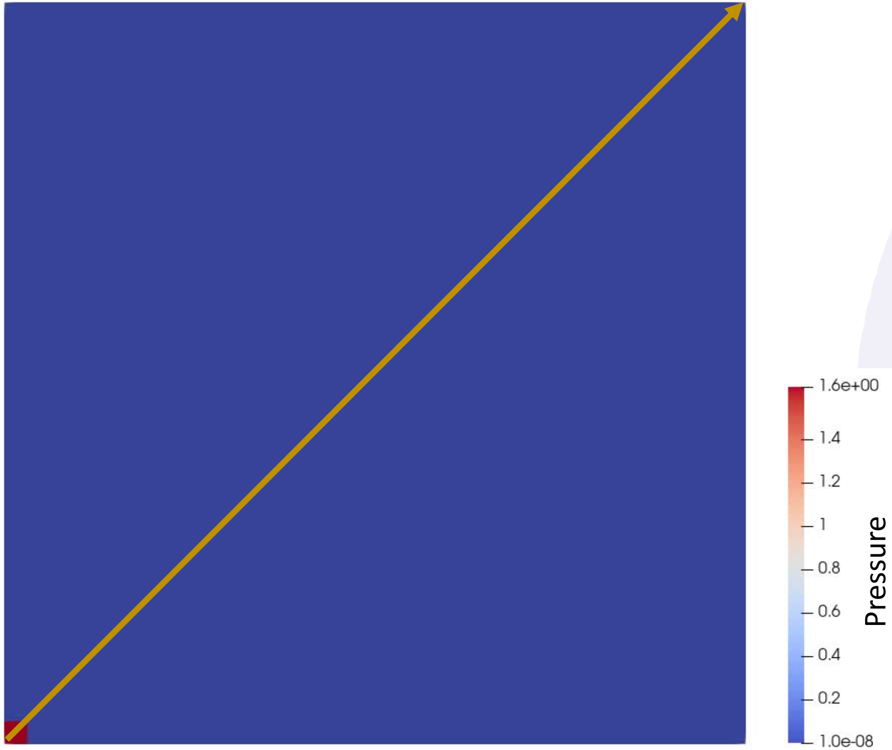
Example Shock Tube Case

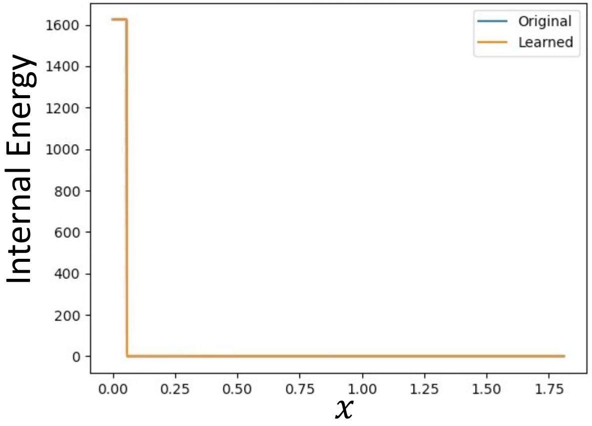


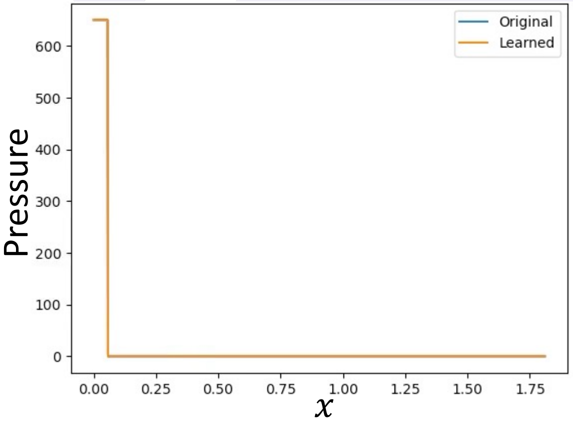
Error over randomized set of simulations

Method	Error
Learned	**2.422e-3**
van Leer	2.480e-3
Min Mod	2.438e-3
Superbee	2.476e-3
van Albada	2.522e-3
van Albada 2	2.508e-3
Monotonized Central	2.456e-3
UMIST	2.487e-3

Example 2D Sedov Case





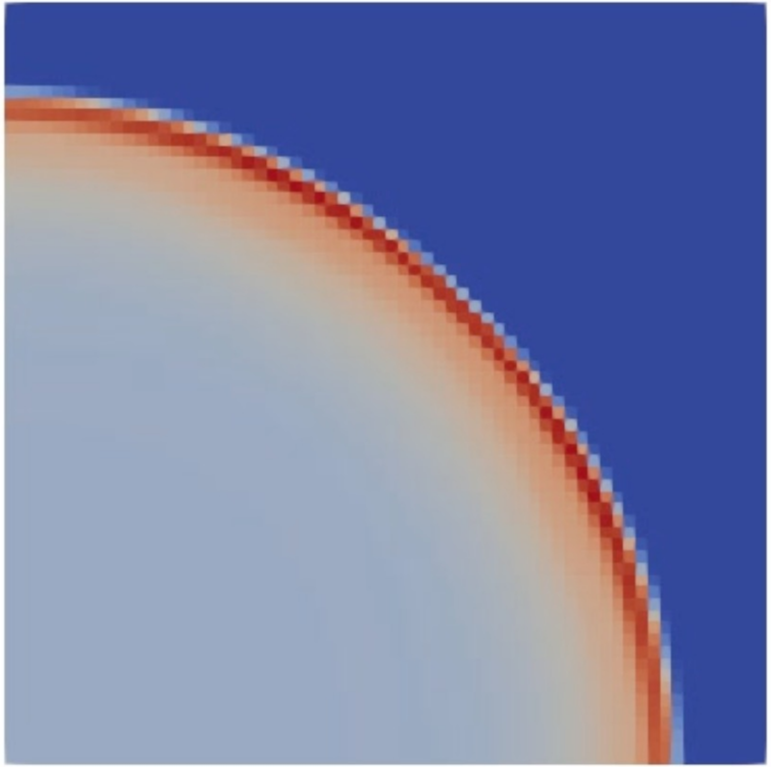


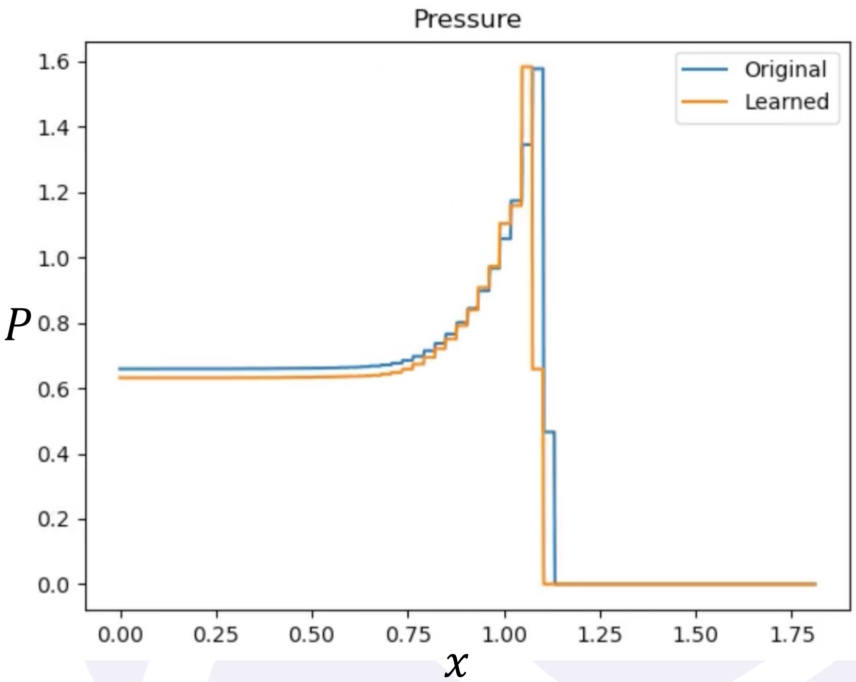
Conclusions

- Machine-learned slope limiters adopt strange forms but work well
- These slope-limiters performed as well as commonly used limiters for the range of test cases shown
- The computational cost of evaluating a B-Spline limiter tractable

Future Work

- Application to more complicated simulations (Taylor Green Vortex, Turbulence,)
- Use of methodology for other systems (Vlasov equation, MHD)





Pressure
Original
Learned
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
P
0.00
0.25
0.50
0.75
1.00
1.25
1.50
1.75
x

Computational Cost

No Limiter

Monotonized Central

Learned

Simulation	No Limiter (1st order)	Native Limiter (MC)	Learned Limiter
Sine	5.31e-01	5.33e-01	5.51e-01
Shock	6.14e-02	6.11e-02	6.10e-02
Sedov	7.61e-01	1.12e+00	1.26e+00