Entropy Stability and TeCNO Computation of Entropy Measure-Valued Solutions

Eitan Tadmor

Center for Scientific Computation and Mathematical Modeling (CSCAMM)
Department of Mathematics, Institute for Physical Science & Technology
University of Maryland

www.cscamm.umd.edu/tadmor

$\star$ with U. Fjordholm, R. Käppeli, S. Mishra, W.-G. Zhong

Numerical Approximations of Hyperbolic Systems with Source Terms and Applications

Cortona, Italy, June 14-20 2015

Epilogue. Perfect derivatives and conservative differences

$$\underbrace{u_x}_{\displaystyle\downarrow} \quad \rightsquigarrow \quad \int_a^b u_x\,dx = \text{boundary terms of } u$$

$$\frac{u_{\nu+1} - u_{\nu-1}}{2\Delta x} \quad \rightsquigarrow \quad \sum \left(\frac{u_{\nu+1} - u_{\nu-1}}{2\Delta x} \right) \Delta x = \text{boundary terms}$$

$$\underbrace{u u_x}_{\displaystyle\downarrow} \quad \rightsquigarrow \quad \int_a^b \overbrace{u u_x}^{\frac{1}{2}(u^2)_x}\,dx = \text{boundary terms of } u$$

$$u_\nu \left(\frac{u_{\nu+1} - u_{\nu-1}}{2\Delta x} \right) \rightsquigarrow \overbrace{\sum \left(\frac{u_\nu u_{\nu+1} - u_{\nu-1} u_\nu}{2\Delta x} \right)}^{\text{telescoping sum}} \Delta x = \text{quadratic boundary terms}$$

- but . . . $\underbrace{u^3 u_x}_{\displaystyle\downarrow} \quad \rightsquigarrow \quad \int_a^b \overbrace{u^3 u_x}^{\frac{1}{4}(u^4)_x}\,dx = \text{quartic boundary terms of } u$

$$u_\nu^3 \left(\frac{u_{\nu+1} - u_{\nu-1}}{2\Delta x} \right) \rightsquigarrow \sum \overbrace{\left(\frac{u_\nu^3 u_{\nu+1} - u_{\nu-1} u_\nu^3}{2\Delta x} \right)}^{\text{no perfect deriv.}} \Delta x \quad \mapsto \quad \text{no cancellation}$$

Epilogue. Perfect derivatives and conservative differences

$$(\star) \qquad \text{Set} \quad u_x \approx \frac{3}{4\Delta x}\left(\frac{u_{\nu+1}^4 - u_\nu^4}{u_{\nu+1}^3 - u_\nu^3} - \frac{u_\nu^4 - u_{\nu-1}^4}{u_\nu^3 - u_{\nu-1}^3}\right)$$

$$\sum \frac{3}{4\Delta x}\left(\frac{u_{\nu+1}^4 - u_\nu^4}{u_{\nu+1}^3 - u_\nu^3} - \frac{u_\nu^4 - u_{\nu-1}^4}{u_\nu^3 - u_{\nu-1}^3}\right)\Delta x \quad \mapsto \quad \text{boundary terms of } u$$

$$\sum \frac{3}{4\Delta x} u_\nu^3 \left(\frac{u_{\nu+1}^4 - u_\nu^4}{u_{\nu+1}^3 - u_\nu^3} - \frac{u_\nu^4 - u_{\nu-1}^4}{u_\nu^3 - u_{\nu-1}^3}\right)\Delta x =$$

$$= -\sum \frac{3}{4\Delta x}\left(u_{\nu+1}^3 - u_\nu^3\right)\left(\frac{u_{\nu+1}^4 - u_\nu^4}{u_{\nu+1}^3 - u_\nu^3}\right)\Delta x \;\mapsto\; \text{boundary terms of } u^4$$

- How do we come up with $(\star)$?
- Can we conserve general multipliers $\eta'(u)u_x = \eta(u)_x$
- Applications — entropic solution for nonlinear conservation laws

Strong, weak and measure valued solutions

- Euler equations with pressure law $p := (\gamma - 1)\left(E - \frac{\rho}{2}(u^2 + v^2)\right)$:

$$\frac{\partial}{\partial t}\begin{bmatrix} \rho \\ \rho u \\ \rho v \\ E \end{bmatrix} + \frac{\partial}{\partial x_1}\begin{bmatrix} \rho u \\ \rho u^2 + p \\ \rho uv \\ u(E+p) \end{bmatrix} + \frac{\partial}{\partial x_2}\begin{bmatrix} \rho v \\ \rho uv \\ \rho v^2 + p \\ v(E+p) \end{bmatrix} = 0$$

- Nonlinear conservation laws: $\mathbf{u}_t + \nabla_{\mathbf{x}} \cdot \mathbf{f}(\mathbf{u}) = 0$

balance of conservative variables $\mathbf{u}$ over spatial variables $\mathbf{x} = (x_1, x_2, \dots)$

- Strong solutions – pointwise values $\mathbf{u}(\mathbf{x}, t)$
- Weak solutions – give up the certainty in pointvalues

Instead – observe the cell averages $\overline{\mathbf{u}}(\mathbf{x}, t) := \dfrac{1}{\Delta \mathbf{x}} \displaystyle\int_{\mathbf{x}-\Delta\mathbf{x}/2}^{\mathbf{x}+\Delta\mathbf{x}/2} \mathbf{u}(\mathbf{y}, t)d\mathbf{y}$

$$\frac{\overline{\mathbf{u}}(\mathbf{x}, t+\Delta t) - \overline{\mathbf{u}}(\mathbf{x}, t)}{\Delta t} + \frac{1}{\Delta \mathbf{x}}\left[\int_{\tau=t}^{t+\Delta t} \mathbf{f}(\mathbf{u}(\mathbf{x}+\frac{\Delta \mathbf{x}}{2}, \tau))d\tau - \int_{\tau=t}^{t+\Delta t} \dots(\mathbf{x}-\frac{\Delta \mathbf{x}}{2})d\tau\right] = 0$$

- Computation of cell averages $\overline{\mathbf{u}}(\mathbf{x}_\nu) \rightsquigarrow \overline{\mathbf{u}}_\nu$: $\dfrac{d}{dt}\overline{\mathbf{u}}_\nu(t) + \dfrac{\mathbf{f}_{\nu+\frac{1}{2}} - \mathbf{f}_{\nu-\frac{1}{2}}}{\Delta \mathbf{x}} = 0$

Weak solutions and entropy stability

$$\left\langle \eta'(\mathbf{u}),\ \mathbf{u}_t + \nabla_{\mathbf{x}} \cdot \mathbf{f}(\mathbf{u}) = 0 \right\rangle \to \overbrace{\eta(\mathbf{u})_t}^{\text{entropy}} + \overbrace{\left\langle \eta'(\mathbf{u}), \nabla_{\mathbf{x}} \cdot \mathbf{f}(\mathbf{u}) \right\rangle}^{\text{perfect derivatives?}} = 0$$

- $\eta(\mathbf{u})$ is an entropy iff $\boxed{\left\langle \eta'(\mathbf{u})\ ,\ \nabla_{\mathbf{x}} \cdot \mathbf{f}(\mathbf{u}) \right\rangle = \nabla_{\mathbf{x}} \cdot F(\mathbf{u})}$

- Entropy stability: $\eta(\mathbf{u})_t + \nabla_{\mathbf{x}} \cdot F(\mathbf{u}) \begin{cases} = 0 \\ \leqslant 0 \end{cases}$

- Euler equations – specific entropy $S = \ln(p\rho^{-\gamma})$:

$$\overbrace{(-\rho S)}^{\eta(\mathbf{u})}{}_t + \nabla_{\mathbf{x}} \cdot \overbrace{(-\rho \mathbf{u} S)}^{F(\mathbf{u})} \begin{cases} = 0 \\ \leqslant 0 \end{cases}$$

- Computation – impose the entropy stability requirement

$$\frac{d}{dt}\eta(\overline{\mathbf{u}}_\nu(t)) + \frac{F_{\nu+\frac{1}{2}} - F_{\nu-\frac{1}{2}}}{\Delta \mathbf{x}} \begin{cases} = 0 \\ \leqslant 0 \end{cases}$$

Kelvin-Helmholtz instability

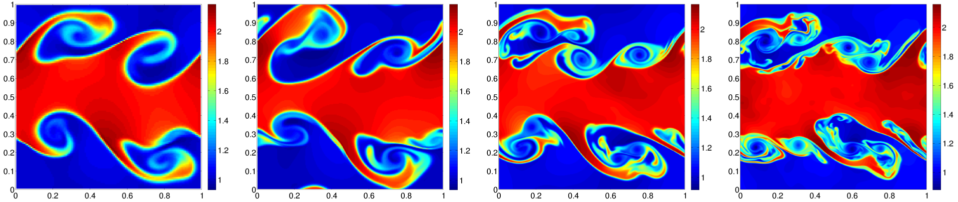
- initial state of three layers $\mathbf{u}_0(\mathbf{x}) = \begin{cases} \mathbf{u}_L, & H_1 \leqslant x_2 < H_2 \\ \mathbf{u}_R, & 0 \leqslant x_2 \leqslant H_1 \text{ or } H_2 \leqslant x_2 \leqslant 1 \end{cases}$

  fixed $\mathbf{u}_{L,R}$; perturbed interface $H_j(\mathbf{x},\omega) = \frac{j}{2} - \frac{1}{4} + \epsilon Y_j(\mathbf{x},\omega), \quad j = 1,2$

- $\epsilon = 0$: $\mathbf{u}_L \mathbf{1}(x_2)_{[\frac{1}{4},\frac{3}{4}]} + \mathbf{u}_R \mathbf{1}(x_2)_{[0,\frac{1}{2}]\cup[\frac{3}{4},1]}$ is an entropic steady state
- Perturbed state — $\mathbf{u}_0(\mathbf{x},\omega) = \mathbf{u}_L \mathbf{1}(x_2)_{[H_1,H_2]} + \mathbf{u}_R \mathbf{1}(x_2)_{[0,H_1]\cup[H_2,1]}$:

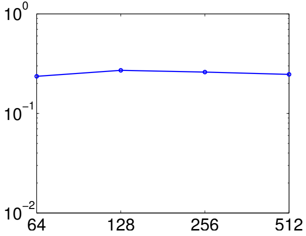
$$Y_j(\mathbf{x},\omega) = \sum_n a_n(\omega)\cos(b_n(\omega) + 2n\pi x_1) \quad \sum a_n = 1 \quad \text{so that} \quad |\epsilon Y_j| \leqslant \epsilon$$

- Lack of convergence: Fix ω and keep mesh refinement... ρ_ϵ, $\epsilon = 0.01$:

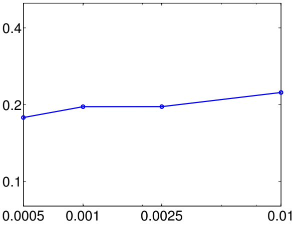


(a) 128^2 (b) 256^2 (c) 512^2 (d) 1024^2

The notion of entropic weak solution is not enough ($d > 1$)



(e) L^1 rates vs. number of gridpoints with $\epsilon = 0.01$



(f) L^1 error with respect to ϵ, at a fixed 1024^2 mesh

Figure: L^1 differences in density ρ at time $t = 2$ for the Kelvin-Helmholtz problem

"Just because we cannot prove that compressible flows with prescribed initial values exist doesn't mean that we cannot compute them" [Lax 2007]

- The question is what information is encoded in our computations?

Answer: Young measures and measure valued solutions

- Recall about weak convergence: $\mathbf{u}_n \rightharpoonup \mathbf{u}_\infty$ and $\mathbf{f}(\mathbf{u}_n) \rightharpoonup \mathbf{f}_\infty$
  What is the relation $\mathbf{f}_\infty$ and $\mathbf{f}(\mathbf{u}_\infty)$?

- $\mathbf{f}_\infty(\mathbf{x}, t)$ depends <u>linearly and positively</u> on $\mathbf{f}$: hence $\mathbf{f}_\infty(\mathbf{x}, t) = \langle \nu_{\mathbf{x},t}, \mathbf{f} \rangle$

- Complete description in terms of Young measure $\nu_{\mathbf{x},t}$

Certainty: strong convergence with Dirac Mass $\nu_{\mathbf{x},t} = \delta_{\mathbf{u}_\infty(\mathbf{x},t)} \rightsquigarrow \mathbf{f}_\infty = \mathbf{f}(\mathbf{u}_\infty)$

- Entropy measure valued (EMV) solutions: $\mathbf{u}(\mathbf{x}, t) \rightsquigarrow \nu_{\mathbf{x},t}$:

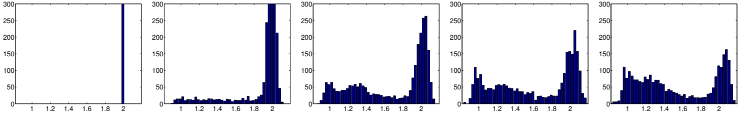
$$\begin{aligned} \mathbf{u}_t + \nabla_\mathbf{x} \cdot \mathbf{f}(\mathbf{u}) = 0 \quad &\rightsquigarrow \quad \partial_t \langle \nu_{\mathbf{x},t}, id \rangle + \nabla_\mathbf{x} \cdot \langle \nu_{\mathbf{x},t}, \mathbf{f} \rangle = 0 \\ \eta(\mathbf{u})_t + \nabla_\mathbf{x} \cdot F(\mathbf{u}) \leqslant 0 \quad &\rightsquigarrow \quad \partial_t \langle \nu_{\mathbf{x},t}, \eta \rangle + \nabla_\mathbf{x} \cdot \langle \nu_{\mathbf{x},t}, F \rangle \leqslant 0 \end{aligned}$$

- $\nu_{\mathbf{x},t}$ is the (weighted) probability of having the value $\langle \nu_{\mathbf{x},t}, \mathbf{u} \rangle$ at that point

- With certainty: $\nu_{\mathbf{x},t} = \delta_{\mathbf{u}(\mathbf{x},t)}$ (back to weak solutions)

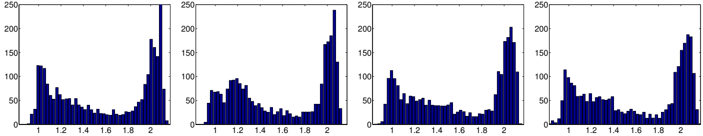
- Measure valued solutions –
  give up the certainty in a given solution
  Instead – observe averages in configuration space

Ron DiPerna

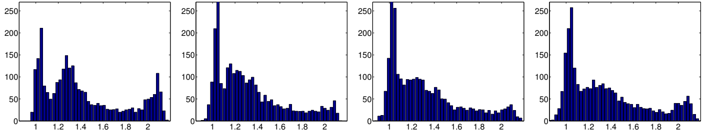


(a) $t = 0$ (b) $t = 0.5$ (c) $t = 1$ (d) $t = 1.5$ (e) $t = 2$

Figure: The approximate PDF for density ρ at $x = (0.5, 0.7)$.



(a) nx = 128 (b) nx = 256 (c) nx = 512 (d) nx = 1024



(e) nx = 128 (f) nx = 256 (g) nx = 512 (h) nx = 1024

Figure: The approximate PDF for density ρ at the points $x = (0.5, 0.7)$ (first row) and $x = (0.5, 0.8)$ (second row) a series of meshes.

Computing Entropy Measure Valued (EMV) solutions

$\star$ Trilogy of talks; this one is the SOURCE TERM for computing EMVs ...

. . . .

- (Formally) arbitrarily high-order of accuracy;
- Entropy stability;
- Essentially non-oscillatory in the presence of discontinuities;
- Convergence for linear systems;
- How to realize (the configuration space of) EMVs?
- Computationally efficient;

The class of the entropy Conservative Non-Oscillatory (TeCNO) schemes[1] which compute "faithful" samples required for the ensemble of EMVs

[1] U. Fjordholm, S. Mishra, ET, Arbitrarily high-order accurate entropy stable schemes ...., SINUM 2012

Entropy inequality: PDEs $\to$ numerical approximations

$$\left\langle \eta'(\mathbf{u}),\ \mathbf{u}_t + \mathbf{f}(\mathbf{u})_x \right\rangle = 0 \quad \overset{\langle \eta'(\mathbf{u}),\ \mathbf{f}(\mathbf{u})_x \rangle = F(\mathbf{u})_x}{\Longrightarrow} \quad \eta(\mathbf{u})_t + F(\mathbf{u})_x \left\{ \begin{array}{l} = 0 \\ \leqslant 0 \end{array} \right.$$

- Semi-discrete approximations:

$$\frac{d}{dt}\overline{\mathbf{u}}_\nu(t) + \frac{1}{\Delta x}\left[\mathbf{f}_{\nu+\frac{1}{2}} - \mathbf{f}_{\nu-\frac{1}{2}}\right] = 0 \quad \mathbf{f}_{\nu+\frac{1}{2}} = \mathbf{f}(\overline{\mathbf{u}}_{\nu-p+1}, \ldots, \overline{\mathbf{u}}_{\nu+p})$$

- Entropy conservative discretization — given η find $\mathbf{f}^*$ s.t.

$$\frac{d}{dt}\overline{\mathbf{u}}_\nu(t) + \frac{\mathbf{f}^*_{\nu+\frac{1}{2}} - \mathbf{f}^*_{\nu-\frac{1}{2}}}{\Delta x} = 0 \overset{?}{\Longrightarrow} \frac{d}{dt}\eta(\overline{\mathbf{u}}_\nu(t)) + \frac{F_{\nu+\frac{1}{2}} - F_{\nu-\frac{1}{2}}}{\Delta x} \left\{ \begin{array}{l} = 0 \\ \leqslant 0 \end{array} \right.$$

Does $\boxed{\left\langle \eta'(\overline{\mathbf{u}}_\nu)\ ,\ \mathbf{f}^*_{\nu+\frac{1}{2}} - \mathbf{f}^*_{\nu-\frac{1}{2}} \right\rangle \overset{?}{\longrightarrow} F_{\nu+\frac{1}{2}} - F_{\nu-\frac{1}{2}}}$

so that $\Longrightarrow \quad \sum_\nu \eta(\overline{\mathbf{u}}_\nu(t))\Delta x \left\{ \begin{array}{c} = \\ \leqslant \end{array} \right\} \sum_\nu \eta(\overline{\mathbf{u}}_\nu(0))\Delta x$

Entropy variables and entropy conservative schemes

- Fix an entropy $\eta(\mathbf{u})$. Set Entropy variables: $\mathbf{v} \equiv \mathbf{v}(\mathbf{u}) := \eta'(\mathbf{u})$.

⊙ Convexity of $\eta(\cdot)$, $\mathbf{u} \leftrightarrow \mathbf{v}$ is 1-1: $\mathbf{v}_\nu = \eta'(\overline{\mathbf{u}}_\nu)$ (NOTE – we drop the $\overline{\{\bullet\}}$)

$$\frac{d}{dt}\overline{\mathbf{u}}_\nu(t) = -\frac{1}{\Delta x}\left[\mathbf{f}^*_{\nu+\frac{1}{2}} - \mathbf{f}^*_{\nu-\frac{1}{2}}\right], \quad \mathbf{f}_{\nu+\frac{1}{2}} = \mathbf{f}(\mathbf{v}_{\nu-p+1}, \ldots, \mathbf{v}_{\nu+p})$$

- Entropy conservation: $\left\langle \eta'(\overline{\mathbf{u}}_\nu)\, ,\, \mathbf{f}^*_{\nu+\frac{1}{2}} - \mathbf{f}^*_{\nu-\frac{1}{2}} \right\rangle \stackrel{?}{=} F_{\nu+\frac{1}{2}} - F_{\nu-\frac{1}{2}}$

$$\overbrace{\left\langle \mathbf{v}_\nu\, ,\, \mathbf{f}^*_{\nu+\frac{1}{2}} - \mathbf{f}^*_{\nu-\frac{1}{2}} \right\rangle}^{\text{perfect difference}} \quad \text{if and only if} \quad \overbrace{\left\langle \mathbf{v}_{\nu+1} - \mathbf{v}_\nu\, ,\, \mathbf{f}^*_{\nu+\frac{1}{2}} \right\rangle}^{\text{perfect difference}}:$$

- Entropy conservative: $\boxed{\left\langle \mathbf{v}_{\nu+1} - \mathbf{v}_\nu, \mathbf{f}^*_{\nu+\frac{1}{2}} \right\rangle = \psi(\mathbf{v}_{\nu+1}) - \psi(\mathbf{v}_\nu)}$

- Entropy flux potential: $\psi(\mathbf{v}) := \left\langle \mathbf{v}\, ,\, \mathbf{f}(\mathbf{v}) \right\rangle - F(\mathbf{u}(\mathbf{v}))$

⋆ The scalar case: $\eta'(u)f(u)_x = (\ldots)_x$ - all convex η's are entropies

#1. Scalar examples: $f^{*}_{\nu+\frac{1}{2}} = \dfrac{\psi(v_{\nu+1}) - \psi(v_\nu)}{v_{\nu+1} - v_\nu}$

- Toda flow: $u_t + (e^u)_x = 0$ with Exp entropy pair: $(e^u)_t + (e^{2u})_x = 0$

$\eta(u) = v(u) = e^u,\ F(u) = \frac{1}{2}e^{2u}$ and potential $\psi(v) := vf - F = \frac{1}{2}v^2$

$\rightsquigarrow$ Entropy-conservative flux:

$$f^{*}_{\nu+\frac{1}{2}} = \frac{\psi(v_{\nu+1}) - \psi(v_\nu)}{v_{\nu+1} - v_\nu} = \frac{\frac{1}{2}v^2_{\nu+1} - \frac{1}{2}v^2_\nu}{v_{\nu+1} - v_\nu} = \frac{1}{2}(v_\nu + v_{\nu+1}) = \frac{1}{2}\left[e^{u_\nu} + e^{u_{\nu+1}}\right]$$

Toda flow: $\displaystyle \frac{d}{dt}\overline{u}_\nu(t) = -\frac{e^{u_{\nu+1}(t)} - e^{u_{\nu-1}(t)}}{2\Delta x} \rightsquigarrow \frac{d}{dt}\sum e^{\overline{u}_\nu(t)}\Delta x = Const.$

- Inviscid Burgers: $u_t + (\frac{1}{2}u^2)_x = 0$ quadratic entropy $(\dfrac{1}{2}u^2)_t + (\dfrac{1}{3}u^3)_x = 0$

$\eta(u) = \dfrac{u^2}{2},\ v(u) = u,\ F(u) = \dfrac{u^3}{3}$ and potential $\psi(v) := vf - F = \frac{1}{6}u^3$

$\rightsquigarrow$ Entropy conservative "$\frac{1}{3}$-rule":

$$\frac{d}{dt}\overline{u}_\nu(t) = -\frac{2}{3}\left[\frac{u^2_{\nu+1} - u^2_{\nu-1}}{4\Delta x}\right] - \frac{1}{3}\left[u_\nu\frac{u_{\nu+1} - u_{\nu-1}}{2\Delta x}\right] \rightsquigarrow \sum \overline{u}^2_\nu(t)\Delta x = Const.$$

#2. Linear equations

- Linear transport: How to discretize u_x such that $u_t + au_x = 0$ conserves the balance of quartic perfect derivatives $\left(u^4\right)_t + \left(au^4\right)_x = 0$?

$(\star)$ Set $u_{x|x=x_\nu} \approx \dfrac{3}{4\Delta x}\left(\dfrac{u^4_{\nu+1}-u^4_\nu}{u^3_{\nu+1}-u^3_\nu} - \dfrac{u^4_\nu - u^4_{\nu-1}}{u^3_\nu - u^3_{\nu-1}}\right)$

$$\sum \frac{3}{4\Delta x}\left(\frac{u^4_{\nu+1}-u^4_\nu}{u^3_{\nu+1}-u^3_\nu} - \frac{u^4_\nu - u^4_{\nu-1}}{u^3_\nu - u^3_{\nu-1}}\right)\Delta x \quad \mapsto \quad \text{boundary terms of } u$$

$$\sum \frac{3}{4\Delta x}u^3_\nu\left(\frac{u^4_{\nu+1}-u^4_\nu}{u^3_{\nu+1}-u^3_\nu} - \frac{u^4_\nu - u^4_{\nu-1}}{u^3_\nu - u^3_{\nu-1}}\right)\Delta x =$$

$$= -\sum \frac{3}{4\Delta x}\left(u^3_{\nu+1}-u^3_\nu\right)\left(\frac{u^4_{\nu+1}-u^4_\nu}{u^3_{\nu+1}-u^3_\nu}\right)\Delta x \ \mapsto \text{quartic boundary terms}$$

- Derivation of $(\star)$: conservative differences of u_x <u>and</u> $4u^3u_x = \left(u^4\right)_x$:

$\eta(u) = u^4,\ v = 4u^3,\ f(u) = au,\ F = au^4$ and $\psi(u) = 3au^4$

$$\rightsquigarrow \qquad u_x \approx \frac{f^*_{\nu+\frac{1}{2}} - f^*_{\nu-\frac{1}{2}}}{\Delta x}, \qquad f^*_{\nu+\frac{1}{2}} = \frac{\Delta\psi_{\nu+\frac{1}{2}}}{\Delta v_{\nu+\frac{1}{2}}} = \frac{3}{4}\frac{u^4_{\nu+1}-u^4_\nu}{u^3_{\nu+1}-u^3_\nu}$$

#3. Second order accuracy

- The u^4 entropy conservative flux is 2nd-order accurate:

$$f^{*}_{\nu+\frac{1}{2}} = \frac{3}{4}\frac{u^4_{\nu+1}-u^4_{\nu}}{u^3_{\nu+1}-u^3_{\nu}}: \quad \frac{f^{*}_{\nu+\frac{1}{2}} - f^{*}_{\nu-\frac{1}{2}}}{2\Delta x} \text{ is 2nd-order approximation of } u_x$$

$$f^{*}_{\nu+\frac{1}{2}} = \frac{\Delta\psi}{\Delta u} = \frac{3}{4}\frac{u^4_{\nu+1}-u^4_{\nu}}{u^3_{\nu+1}-u^3_{\nu}} \approx \frac{3}{4}\cdot\frac{8u^3_{\nu+\frac{1}{2}}\frac{\Delta x}{2}u_x}{6u^2_{\nu+\frac{1}{2}}\frac{\Delta x}{2}u_x} \approx u_{\nu+\frac{1}{2}}$$

- The general case: express the flux in the "viscosity form"

"viscosity form": $f_{\nu+\frac{1}{2}} = \frac{1}{2}\left(f_\nu + f_{\nu+1}\right) - \frac{1}{2}D_{\nu+\frac{1}{2}}(u_{\nu+1}-u_\nu)$

$$\frac{d}{dt}\overline{u}_\nu(t) = -\overbrace{\left[\frac{f(u_{\nu+1})-f(u_{\nu-1})}{2\Delta x}\right]}^{\text{2nd order centered differencing}} + \frac{1}{2\Delta x}\overbrace{\left[D_{\nu+\frac{1}{2}}\Delta u_{\nu+\frac{1}{2}} - D_{\nu-\frac{1}{2}}\Delta u_{\nu-\frac{1}{2}}\right]}^{\Delta x^2 (Du_x)_x}$$

- <u>2nd-order</u>: $f^{*}_{\nu+\frac{1}{2}} \quad \rightsquigarrow \quad D^{*}_{\nu+\frac{1}{2}} := \frac{1}{8}\left(\int_{\xi=-1}^{1}(1-\xi^2)f''(u_{\nu+\frac{1}{2}})d\xi\right)\cdot\Delta u_{\nu+\frac{1}{2}}$

$\rightsquigarrow$ The entropy-conservative flux is 2nd-order accurate

#4. Beyond second-order accuracy

- Weak formulation (semi-discrete) in terms of entropy variables: $v(\cdot, t)$

$$\frac{d}{dt}u(v) + f(v)_x = 0 \rightsquigarrow \int_{I_\nu} \Big\langle \varphi(x)\,,\ \frac{d}{dt}u(v) \Big\rangle dx = \int_{I_\nu} \Big\langle \frac{\partial}{\partial x}\varphi(x)\,,\ f(v) \Big\rangle dx$$

- [ET 1986] Finite-element discretization: $v \longrightarrow \hat{v}(x,t) = \sum_j v_j(t)\hat{H}_j(x)$:

$$\varphi(x) = \hat{H}_\nu(x) \rightsquigarrow \int_{x_{\nu-1}}^{x_{\nu+1}} \frac{\partial}{\partial x}\hat{H}_\nu(x) f\left(\sum_j v_j(t)\hat{H}_j(x)\right) dx = -\Big(f^*_{\nu+\frac{1}{2}} - f^*_{\nu-\frac{1}{2}}\Big)$$

- Replace piecewise linear with high-order elements $\rightsquigarrow$ higher-order
- [LeFloch & Rohde 2000] Richardson extrapolation for higher-order fluxes

Third-order entropy conservative flux $f^{**}_{\nu+\frac{1}{2}}$:

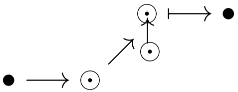
$$f^{**}_{\nu+\frac{1}{2}} = \int_{-1}^{1} f\Big(v_{\nu+\frac{1}{2}}(\xi)\Big) d\xi - \frac{1}{12}\Big[Q^{**}_{\nu+\frac{3}{2}}\Delta v_{\nu+\frac{3}{2}} - R^{**}_{\nu+\frac{1}{2}}\Delta v_{\nu+\frac{1}{2}}\Big]$$

$\rightsquigarrow$ Computation – entropy conservative fluxes to <u>any order of accuracy</u>

#5. Systems: $\left\langle \mathbf{v}_{\nu+1} - \mathbf{v}_\nu \, , \, \mathbf{f}^{*}_{\nu+\frac{1}{2}} \right\rangle = \psi(\mathbf{v}_{\nu+1}) - \psi(\mathbf{v}_\nu)$

- Choice of path: N linearly independent directions $\left\{\mathbf{r}^j\right\}_{j=1}^{N}$

$\odot$ Intermediate states $\left\{\mathbf{v}^j_{\nu+\frac{1}{2}}\right\}_{j=1}^{N}$:



Starting with $\mathbf{v}^1_{\nu+\frac{1}{2}} = \mathbf{v}_\nu$, and followed by $(\Delta \mathbf{v}_{\nu+\frac{1}{2}} \equiv \mathbf{v}_{\nu+1} - \mathbf{v}_\nu)$

$$\mathbf{v}^{j+1}_{\nu+\frac{1}{2}} = \mathbf{v}^{j}_{\nu+\frac{1}{2}} + \left\langle \ell^j, \Delta \mathbf{v}_{\nu+\frac{1}{2}} \right\rangle \mathbf{r}^j, \; j = 1, 2, \ldots, N \quad (\mathbf{v}^{N+1}_{\nu+\frac{1}{2}} = \mathbf{v}_{\nu+1})$$

- [ET 2003] The conservative scheme $\dfrac{d}{dt}\overline{\mathbf{u}}_\nu(t) = -\dfrac{1}{\Delta x}\left[\mathbf{f}^{*}_{\nu+\frac{1}{2}} - \mathbf{f}^{*}_{\nu-\frac{1}{2}}\right]$

$$\boxed{\mathbf{f}^{*}_{\nu+\frac{1}{2}} = \sum_{j=1}^{N} \frac{\psi\left(\mathbf{v}^{j+1}_{\nu+\frac{1}{2}}\right) - \psi\left(\mathbf{v}^{j}_{\nu+\frac{1}{2}}\right)}{\left\langle \ell^j, \Delta \mathbf{v}_{\nu+\frac{1}{2}} \right\rangle} \ell^j}$$

is entropy conservative: $\left\langle \mathbf{v}_{\nu+1} - \mathbf{v}_\nu \, , \, \mathbf{f}^{*}_{\nu+\frac{1}{2}} \right\rangle = \psi(\mathbf{v}_{\nu+1}) - \psi(\mathbf{v}_\nu)$

#6. Entropy conservative Euler scheme (with W.-G. Zhong)

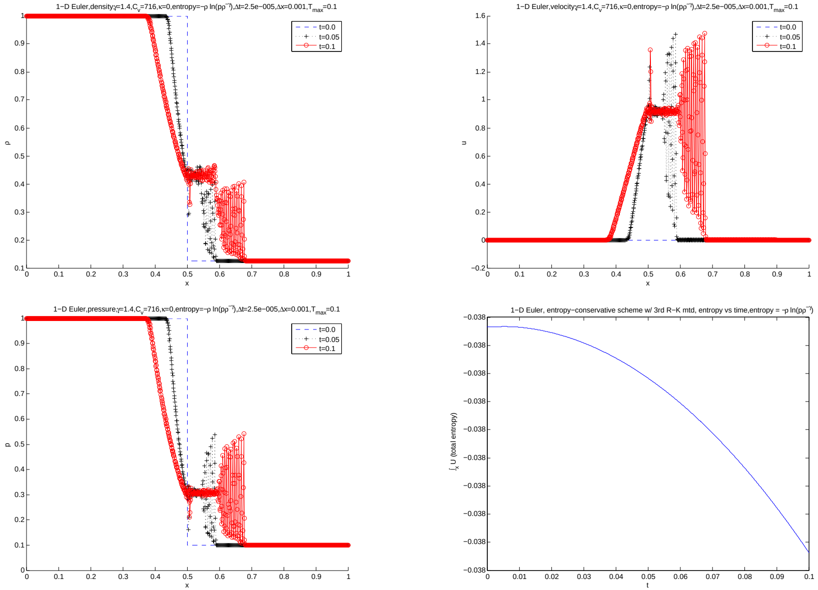
$$\mathbf{f}^{*}_{\nu+\frac{1}{2}} = \sum_{j=1}^{N} \frac{\psi\left(\mathbf{v}^{j+1}_{\nu+\frac{1}{2}}\right) - \psi\left(\mathbf{v}^{j}_{\nu+\frac{1}{2}}\right)}{\left\langle \boldsymbol{\ell}^{j}, \Delta\mathbf{v}_{\nu+\frac{1}{2}} \right\rangle} \boldsymbol{\ell}^{j}$$

- Entropy function: $\eta(\mathbf{u}) = -\rho S$
- Euler entropy variables: $\mathbf{v}(\mathbf{u}) = \eta_{\mathbf{u}}(\mathbf{u}) = \begin{bmatrix} -E/e - S + \gamma + 1 \\ q/\theta \\ -1/\theta \end{bmatrix}$
- Euler entropy flux potential $\psi(\mathbf{v}) = \langle \mathbf{v}\,,\, \mathbf{f} \rangle - F(\mathbf{u}) = (\gamma-1)m$
- path in phase-space:
- $\mathbf{v}^{0} = \mathbf{v}_{\nu}, \quad \mathbf{v}^{j+1} = \mathbf{v}^{j} + \langle \boldsymbol{\ell}^{j}, \Delta\mathbf{v}_{\nu+\frac{1}{2}} \rangle \mathbf{r}^{j}, \quad \mathbf{v}^{4} = \mathbf{v}_{\nu+1}$

  $\left\{\mathbf{r}^{j}\right\}_{j=1}^{3}$: three linearly independent directions in $\mathbf{v}$-space (Riemann path)

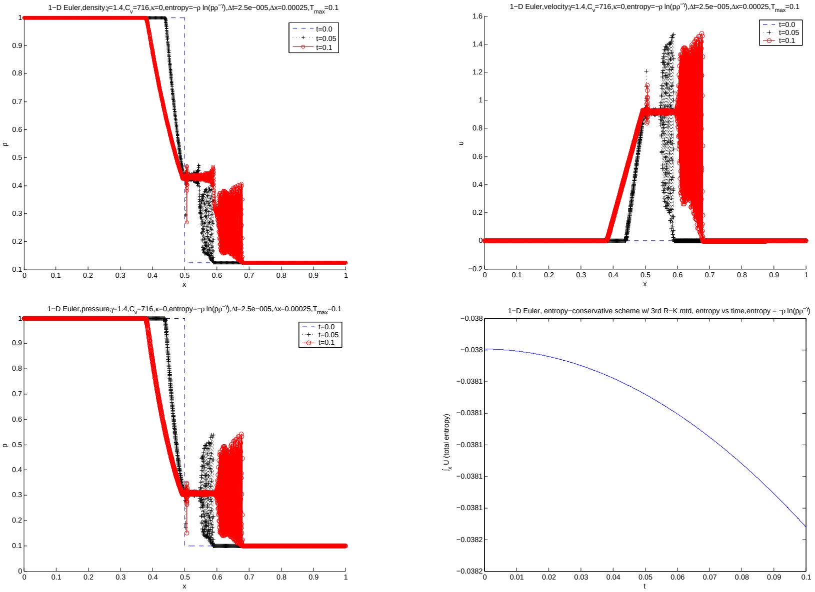
  $\left\{\boldsymbol{\ell}^{j}\right\}_{j=1}^{3}$: the corresponding orthogonal system

  $\left\{m^{j}\right\}_{j=1}^{3}$: intermediate values of the momentum along the path
- $$\mathbf{f}^{*}_{\nu+\frac{1}{2}} = (\gamma-1) \sum_{j=1}^{3} \frac{m^{j+1} - m^{j}}{\langle \boldsymbol{\ell}^{j}\,,\, \Delta\mathbf{v}_{\nu+\frac{1}{2}} \rangle} \boldsymbol{\ell}^{j}$$



Entropy conservative results for Euler's Sod problem:

density, velocity, pressure & entropy. 1000 spatial grids, $\eta(\mathbf{u}) = -\rho \ln\left(p\rho^{-\gamma}\right)$



Entropy conservative density, velocity, pressure & entropy w/4000 spatial grids, $\eta(\mathbf{u}) = -\rho \ln\left(p\rho^{-\gamma}\right)$

- Does not "enforce" physical solution with numerical viscosity

#7. Another entropy conservative flux for Euler eqs

- [Ismail & Roe & 2009] 2D Euler eqs $\mathbf{u}_t + \mathbf{f_x} + \mathbf{g_y} = 0$:

Express an entropy conservative flux $\mathbf{f}^*_{\nu+\frac{1}{2}} := (\mathbf{f}^1, \mathbf{f}^2, \mathbf{f}^3, \mathbf{f}^4)^\top$

in terms of $\mathbf{z} := \sqrt{\dfrac{\rho}{p}} \begin{bmatrix} 1 \\ u \\ v \\ p \end{bmatrix}$ and the averages $\begin{cases} \bar{z}_{\nu+\frac{1}{2}} & := & \frac{1}{2}(z_\nu + z_{\nu+1}) \\ z^{ln}_{\nu+\frac{1}{2}} & := & \dfrac{\Delta z_{\nu+\frac{1}{2}}}{\Delta \log(z)_{\nu+\frac{1}{2}}} \end{cases}$

$$
\begin{aligned}
\mathbf{f}^1_{\nu+\frac{1}{2}} &= (\bar{z}_2)_{\nu+\frac{1}{2}} (z_4)^{ln}_{\nu+\frac{1}{2}} \\
\mathbf{f}^2_{\nu+\frac{1}{2}} &= \frac{(\bar{z}_4)_{\nu+\frac{1}{2}}}{(\bar{z}_1)_{\nu+\frac{1}{2}}} + \frac{(\bar{z}_2)_{\nu+\frac{1}{2}}}{(\bar{z}_1)_{\nu+\frac{1}{2}}} \mathbf{f}^1_{\nu+\frac{1}{2}} \\
\mathbf{f}^3_{\nu+\frac{1}{2}} &= \frac{(\bar{z}_3)_{\nu+\frac{1}{2}}}{(\bar{z}_1)_{\nu+\frac{1}{2}}} \mathbf{f}^1_{\nu+\frac{1}{2}} \\
\mathbf{f}^4_{\nu+\frac{1}{2}} &= \frac{1}{2(\bar{z}_1)_{\nu+\frac{1}{2}}} \left(\frac{\gamma+1}{\gamma-1} \frac{1}{(z_1)^{ln}_{\nu+\frac{1}{2}}} \mathbf{f}^1_{\nu+\frac{1}{2}} + (\bar{z}_2)_{\nu+\frac{1}{2}} \mathbf{f}^2_{\nu+\frac{1}{2}} + (\bar{z}_3)_{\nu+\frac{1}{2}} \mathbf{f}^3_{\nu+\frac{1}{2}} \right)
\end{aligned}
$$

satisfies the algebraic compatibility relation

$$
\langle \mathbf{v}_{\nu+1} - \mathbf{v}_\nu, \mathbf{f}^*_{\nu+\frac{1}{2}} \rangle = \psi(\mathbf{v}_{\nu+1}) - \psi(\mathbf{v}_\nu)
$$

#8. The question of entropy stability – entropy dissipation

- Entropy conservation: $\eta(\mathbf{u})_t + \nabla_{\mathbf{x}} \cdot F(\mathbf{u}) = 0$

- Entropy decay due to shock discontinuities (Lax):

$$\eta(\mathbf{u})_t + \nabla_{\mathbf{x}} \cdot F(\mathbf{u}) \leqslant 0$$

- Entropy decay is balanced by perfect derivatives:

$$\int \eta(\mathbf{u}(\mathbf{x}, t_2))d\mathbf{x} \leqslant \int \eta(\mathbf{u}(\mathbf{x}, t_1))d\mathbf{x}, \quad t_2 > t_1$$

- Q. How much entropy decay "$\leqslant$" is enough?
- A. "physically relevant" entropy decay:
  - Entropy conservative Euler vs. entropy decay in Navier-Stokes
  - Entropy dissipation by numerical viscosity ...
  - while keeping high-resolution, non-oscillatory: TeCNO
  - Lack of uniqueness; entropy measure-valued solutions

#9. Entropy balance in Navier-Stokes (NS) eq's

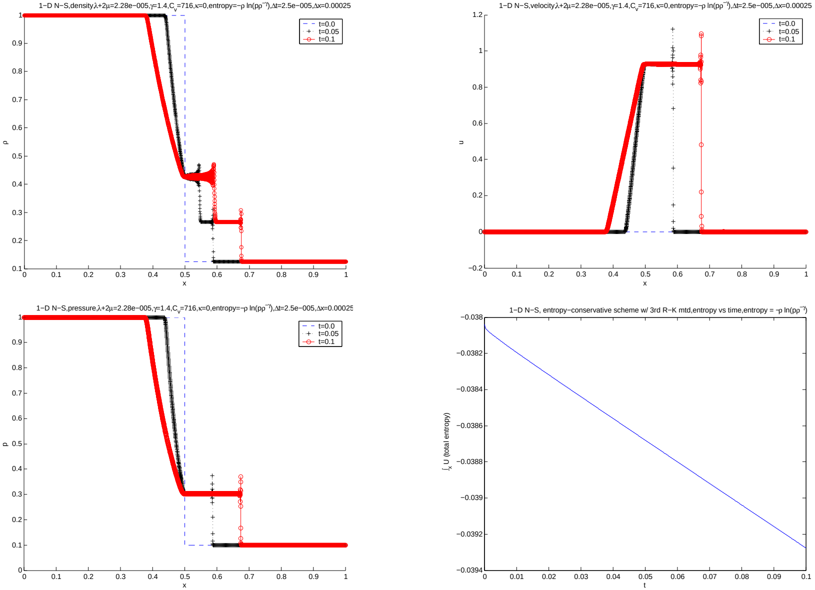
- A semi-discrete scheme of NS equations $\mathbf{u}_t + \mathbf{f}(\mathbf{u})_x = \epsilon \mathbf{d}(\mathbf{u})_{xx}$

$$\left\langle \eta(\overline{\mathbf{u}}_\nu) \rightsquigarrow \mathbf{v}_\nu \,, \frac{d}{dt}\overline{\mathbf{u}}_\nu(t) + \frac{1}{\Delta x}\left(\mathbf{f}^*_{\nu+\frac{1}{2}} - \mathbf{f}^*_{\nu-\frac{1}{2}}\right) = \frac{\epsilon}{\Delta x}\left(\frac{\mathbf{d}_{\nu+1} - \mathbf{d}_\nu}{\Delta x} - \frac{\mathbf{d}_\nu - \mathbf{d}_{\nu-1}}{\Delta x}\right) \right\rangle$$

- Entropy-conservative flux $\mathbf{f}^*_{\nu+\frac{1}{2}}$: $\left\langle \mathbf{v}_{\nu+1} - \mathbf{v}_\nu, \mathbf{f}^*_{\nu+\frac{1}{2}} \right\rangle = \Delta\psi_{\nu+\frac{1}{2}}$
- Euler eq's: entropy conservation $\displaystyle \frac{d}{dt}\sum_\nu \eta(\overline{\mathbf{u}}_\nu(t))\,\Delta x = 0$
- NS eqs: $\displaystyle \frac{d}{dt}\sum_\nu \eta(\overline{\mathbf{u}}_\nu(t))\,\Delta x = -\frac{\epsilon}{\Delta x}\sum_\nu \left\langle \Delta\mathbf{v}_{\nu+\frac{1}{2}},\, \Delta\mathbf{d}_{\nu+\frac{1}{2}} \right\rangle \leqslant 0$

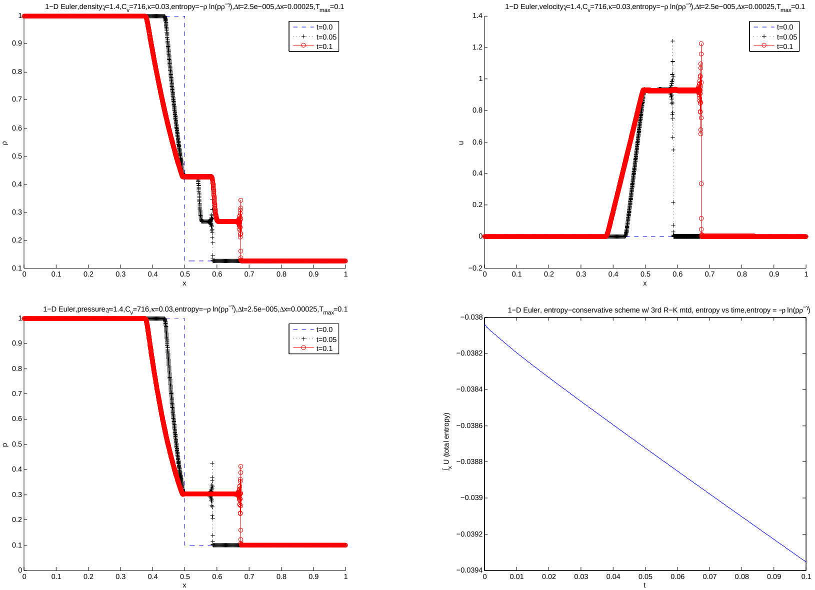
$\star$ $\displaystyle \frac{d}{dt}\sum_\nu (-\rho_\nu S_\nu)\Delta x =$

$$\overbrace{-(\lambda+2\mu)\sum_\nu \left(\frac{\Delta q_{\nu+\frac{1}{2}}}{\Delta x}\right)^2 \overline{\left(\frac{1}{\theta}\right)}_{\nu+\frac{1}{2}} \Delta x}^{viscosity} \overbrace{-\kappa \sum_\nu \left(\frac{\Delta\theta_{\nu+\frac{1}{2}}}{\Delta x}\right)^2 \widetilde{\left(\frac{1}{\theta}\right)}^2_{\nu+\frac{1}{2}} \Delta x}^{heat\ \ conduction} \leqslant 0$$



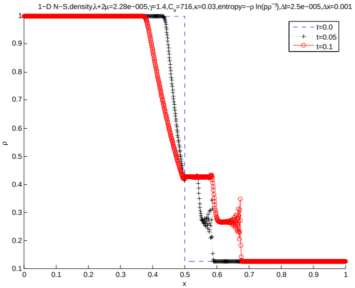
Navier-Stokes equations for Sod's problem:

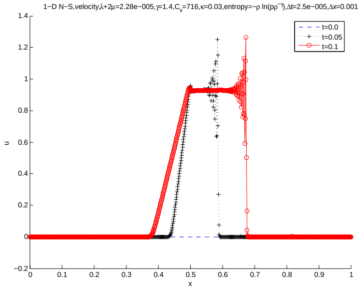
viscosity but no heat conduction; 4000 spatial grids. $\eta(\mathbf{u}) = -\rho \ln \left(p\rho^{-\gamma} \right)$

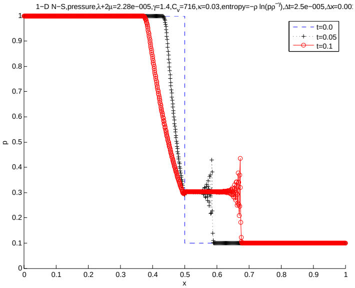


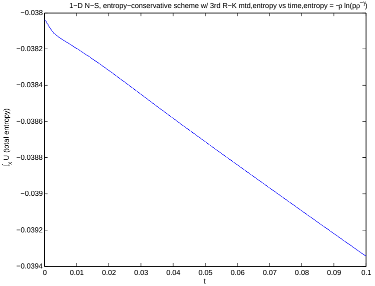
Entropy conservative results for Sod's problem:

heat conduction but no viscosity; 4000 spatial grids. $\eta(\mathbf{u}) = -\rho \ln\left(p\rho^{-\gamma}\right)$



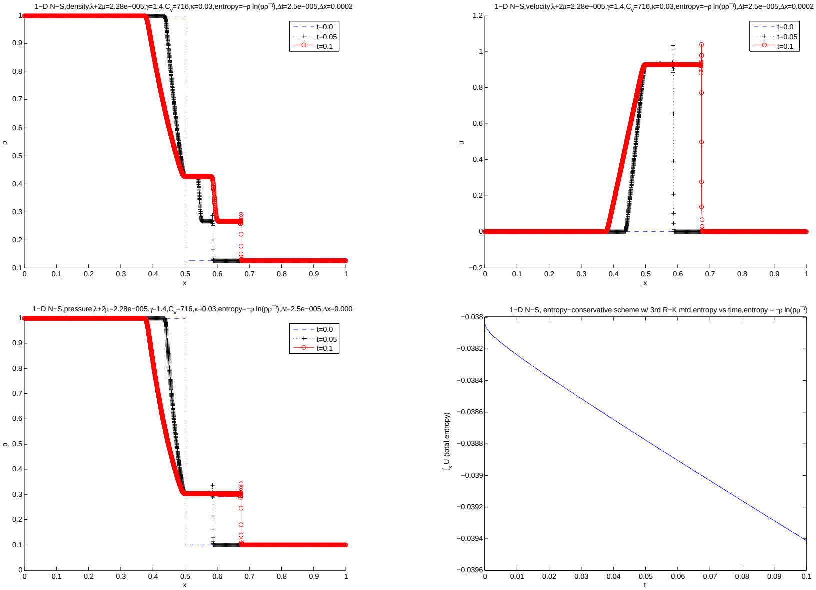






Navier-Stokes equations Sod problem:

both viscosity and heat conduction; 1000 spatial grids, $\eta(\mathbf{u}) = -\rho \ln \left(p\rho^{-\gamma} \right)$



Navier-Stokes equations Sod problem:

viscosity and heat conduction; 4000 spatial grids, $\eta(\mathbf{u}) = -\rho \ln \left(p\rho^{-\gamma} \right)$

#10. TeCNO: Arbitrarily high-order entropy stable schemes

- Set numerical viscosity $\mathbf{f}_{\nu+\frac{1}{2}} = \mathbf{f}^{*}_{\nu+\frac{1}{2}} - \dfrac{1}{2} D_{\nu+\frac{1}{2}}(\mathbf{v}_{\nu+1} - \mathbf{v}_{\nu})$ such that

  $\mathbf{f}^{*}_{\nu+\frac{1}{2}}$ is high order and $\mathbf{f}_{\nu+\frac{1}{2}}$ entropy stable: $\left\langle \Delta\mathbf{v}_{\nu+\frac{1}{2}}, D_{\nu+\frac{1}{2}} \Delta\mathbf{v}_{\nu+\frac{1}{2}} \right\rangle < 0$

- Any $D_{\nu+\frac{1}{2}} > 0$ will do for entropy dissipation but ...

  To overcome first order accuracy: $D_{\nu+\frac{1}{2}} \sim \left| \Delta\mathbf{v}_{\nu+\frac{1}{2}} \right|^{p-1}$; non-oscillatory?

- A class of **arbitrarily** high-order entropy-stable schemes:

$$(\star) \qquad \mathbf{f}_{\nu+\frac{1}{2}} := \mathbf{f}^{*}(\mathbf{v})_{\nu+\frac{1}{2}} - \frac{1}{2} D_{\nu+\frac{1}{2}} \langle\!\langle \mathbf{v} \rangle\!\rangle_{\nu+\frac{1}{2}}, \quad \langle\!\langle \mathbf{v} \rangle\!\rangle_{\nu+\frac{1}{2}} := \mathbf{v}^{-}_{\nu+1} - \mathbf{v}^{+}_{\nu}$$

  Entropy stability requires $\left\langle \Delta\mathbf{v}_{\nu+\frac{1}{2}}, D_{\nu+\frac{1}{2}} \langle\!\langle \mathbf{v} \rangle\!\rangle_{\nu+\frac{1}{2}} \right\rangle < 0$

- Interface values $\mathbf{v}^{\pm}$: reconstructed by ENO (Harten, Engquist, Osher, Shu,..)

(*i*) ENO reconstruction is highly accurate: $D_{\nu+\frac{1}{2}} \langle\!\langle \mathbf{v} \rangle\!\rangle_{\nu+\frac{1}{2}} \sim \left| \Delta\mathbf{v}_{\nu+\frac{1}{2}} \right|^{p}$

(*ii*) It is **E**ssentially **N**on-**O**scillatory (hence the acronym...) ; and...

(*iii*) [FMT 2012] The sign property: $\mathrm{sign} \langle\!\langle v \rangle\!\rangle_{\nu+\frac{1}{2}} = \mathrm{sign}\, \Delta v_{\nu+\frac{1}{2}} \quad \rightsquigarrow \quad (\star)$!

Back to computation of entropy measure valued solutions

- EMV solutions $\nu_{\mathbf{x},t}$: $\partial_t \langle \nu_{\mathbf{x},t}, id\rangle + \nabla_{\mathbf{x}} \cdot \langle \nu_{\mathbf{x},t}, \mathbf{f}\rangle = 0$
- How to compute a realization of the Young measure $\nu_{\mathbf{x},t}$?
  Every Young measure can be realized as a law of random variable:
  $$\exists(\Omega, \Sigma, \mathbb{P}) : \quad \nu_{\mathbf{x},t}(E) = \mathbb{P}(\mathbf{u}(\mathbf{x}, t, \omega) \in E)$$
- **Initial data**: Realize the law of $\sigma_{\mathbf{x}} = \nu_{\mathbf{x},t=0}$ by a random field $\mathbf{u}_0(\mathbf{x}, \omega)$
  "Classical" case – atomic initial delta: $\sigma_{\mathbf{x}} = \delta_{\mathbf{u}_0(\mathbf{x})}$
  Beyond classical case – uncertainty in initial measurement (Mishra's talk)
- Compute the entropy measure valued solutions:
  To be well-defined, we need to make sure $\{\mathbf{u}(\cdot, t, \omega)\}$ form a measurable ensemble in the right space $(\Omega, \Sigma, \mathbb{P}) \mapsto (X, \mathcal{B}(X))$
  - ⊙ Scalar case – $X = L^1$ (Risebro, Schwab, Weber, ...)
  - ⊙ Systems – ?

Example Back to 2D Euler — realize steady KH as MC average:

$$\delta_{\mathbf{u}_0}(\mathbf{x}) = \mathbb{E}\mathbf{u}_0(\mathbf{x}, \omega) \approx \frac{1}{M}\sum_{k=1}^{M} \mathbf{u}_0^k(\mathbf{x}, \omega), \quad \mathbf{u}_0(\mathbf{x}, \omega) = \sum a_n \cos(b_n + 2n\pi x_1)$$

Computation of EMV solutions cont'd

- Evolution: compute the ensemble of entropic solutions

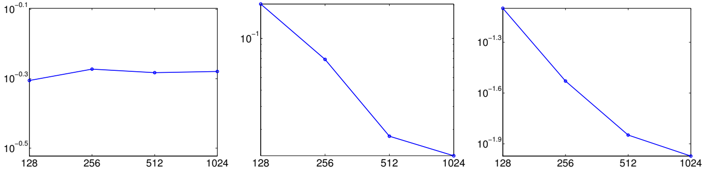
$$\mathbf{u}_0^{\Delta x,k}(\cdot,\omega) \mapsto \mathbf{u}^{\Delta x,k}(\cdot,t,\omega)$$

- Realize the EMVs by propagating the law of MC simulation

$$\nu_{\mathbf{x},t}^{\Delta x} = \frac{1}{M}\sum_{k=1}^{M}\delta_{\mathbf{u}^{\Delta x,k}(\mathbf{x},t,\omega)}, \quad \langle \nu_{\mathbf{x},t}^{\Delta x}, g\rangle = \frac{1}{M}\sum_{k} g(\mathbf{u}^{\Delta x,k}(\mathbf{x},t,\omega))$$

- MC slow convergence $\|\mathbb{E}\mathbf{u}^{\Delta x}(\cdot,t,\omega) - \mathbb{E}\mathbf{u}^{\Delta x,M}(\cdot,t,\omega)\| \lesssim M^{-1/2}$

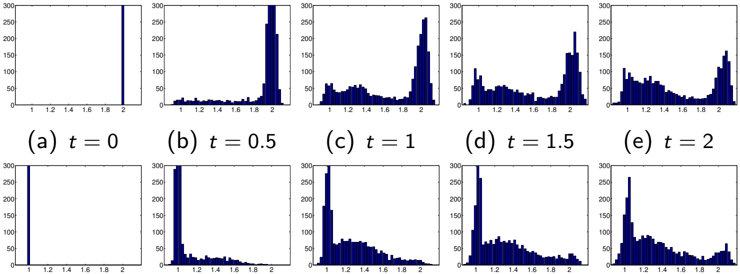
  Key point: Each ensemble was computed with $M = 400$ samples...!



(a) "Pointwise" (b) Mean (c) Variance

Figure: (a) The Cauchy rates at $t = 2$ for the density (y-axis) for a single sample of the Kelvin-Helmholtz problem, vs. different mesh resolutions (x-axis)

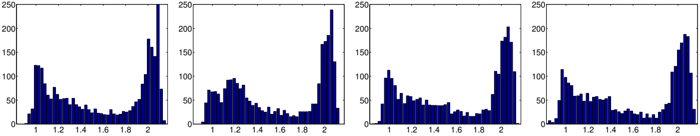
Computing entropy measure-valued solutions



(a) $t = 0$ (b) $t = 0.5$ (c) $t = 1$ (d) $t = 1.5$ (e) $t = 2$

(f) $t = 0$ (g) $t = 0.5$ (h) $t = 1$ (i) $t = 1.5$ (j) $t = 2$

Figure: The approximate PDF for density ρ at $x = (0.5, 0.7)$ (first row) and $x = (0.5, 0.8)$ (second row) on a grid of 1024^2 mesh points.



(a) $\mathrm{nx} = 128$ (b) $\mathrm{nx} = 256$ (c) $\mathrm{nx} = 512$ (d) $\mathrm{nx} = 1024$

Figure: The approximate PDF for density ρ at the points $x = (0.5, 0.7)$ (first row) and $x = (0.5, 0.8)$ (second row) a series of meshes.

TO BE CONTINUED...

• "The numerical viscosity of entropy stable schemes for systems of conservation laws. I", Math. Comp. 1987

• "Entropy stability theory for difference approximations of nonlinear conservation laws ...", Acta Numerica 2003.

• "Energy-preserving and stable approximations for the 2D SW eqs", Proc. of the Third Abel Symposium, 2008.

• "ENO reconstruction and ENO interpolation are stable", FoCM 2012

• "Arbitrarily high order accurate entropy stable ENO schemes for systems of conservation laws", SINUM 2012.

• "Construction of approximate entropy measure valued solutions for hyperbolic systems of conservation laws", ArXiv 1402.0909

THANK YOU