Numerics for Hyperbolic Conservation Laws with Help from Entropy

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Thanks to Carl Zinner

13 Moments and Entropy

Synopsis: In thin air

Thermodynamically Admissible 13 Moment Equations from the Boltzmann Equation

Hans Christian Öttinger
Phys. Rev. Lett. **104**, 120601 (2010)
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In a sufficiently rarefied gas, the tools of standard hydrodynamics, namely, the Navier-Stokes-Fourier equations (based on Newton's second law applied to fluid motion), no longer apply. On the other hand, tracking the statistics of individual molecules, as is done in Boltzmann's kinetic equation approach, is computationally prohibitive.

Writing in *Physical Review Letters*, Hans Christian Öttinger at the ETH in Zurich, Switzerland, strengthens a description of rarefied gas flow that is intermediate between these two extremes. Previous work showed that Boltzmann's kinetic equation can yield a set of 13 moment equations that describe the momentum of the gas and heat flux within it. In his work, Öttinger looks to the laws of nonequilibrium thermodynamics to provide the necessary constraints on the equations. For example, entropy is conserved in reversible processes and standard hydrodynamics is recovered in the limiting case.

The results could advance efforts—particularly those based on numerical calculations—to describe the kinetics of nonequilibrium gases. These calculations are important for understanding gas flow in the smallest of channels—as in microfluidics—and aerodynamics of satellites and space stations in the outer limits of our atmosphere. – *Jessica Thomas*

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Why 13 Moment Equations?

Balance equations for mass, momentum, and energy (5)

Equation for the traceless symmetric pressure tensor (5)

Equation for the heat flux (3)

The Trick for Getting an Entropy

$$\pi = \langle (\boldsymbol{p} - \langle \boldsymbol{p} \rangle)(\boldsymbol{p} - \langle \boldsymbol{p} \rangle) \rangle$$

$$\boldsymbol{Q} = \langle (\boldsymbol{p} - \langle \boldsymbol{p} \rangle)(\boldsymbol{p} - \langle \boldsymbol{p} \rangle)(\boldsymbol{p} - \langle \boldsymbol{p} \rangle) \rangle$$

How to form a third-moment vector?

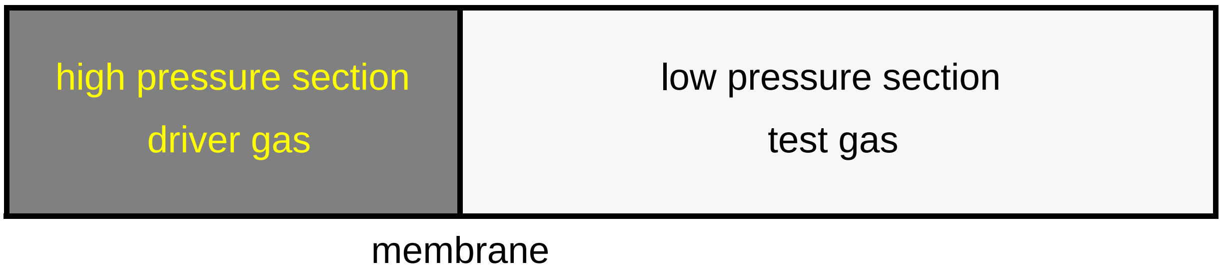
usually: $\lambda = \boldsymbol{Q}:\mathbf{1}$

better: $\boldsymbol{q} = \boldsymbol{Q}:\pi^{-1}$

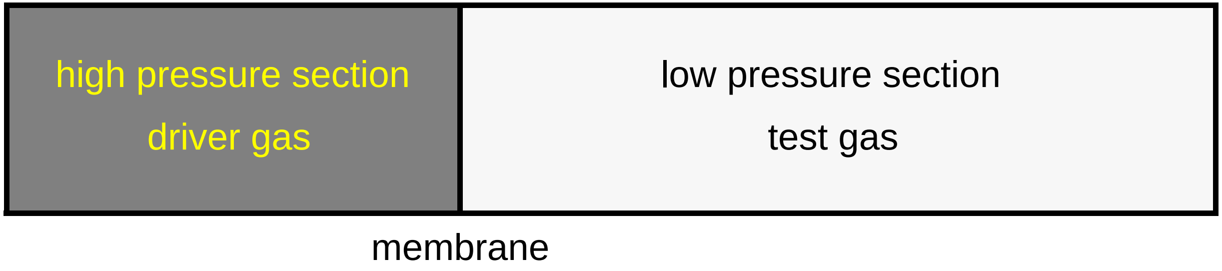
Scalar: $\varphi = \boldsymbol{q} \cdot \pi^{-1} \cdot \boldsymbol{q}$

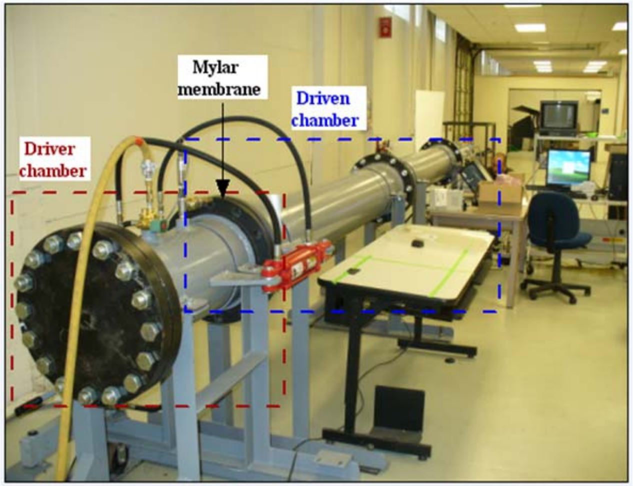
The Flow Problem

Shock Tube Problem



Shock Tube Problem





http://www.acoustics.org/press/159th/king01.jpg

The Equations

The Equations

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} \rho \\ \rho v_1 \\ \rho(v_1^2 + \Pi_{11} + 2\Pi_{22})/2 \\ \rho\Pi_{22}/2 \\ q_1 \end{bmatrix}$$

variables

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

free of derivatives

The Equations

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} \rho \\ \rho v_1 \\ \rho(v_1^2 + \Pi_{11} + 2\Pi_{22})/2 \\ \rho\Pi_{22}/2 \\ q_1 \end{bmatrix}$$

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

free of derivatives

$$f(u) = v_1 u + \begin{bmatrix} 0 \\ \rho\Pi_{11} \\ \rho v_1 \Pi_{11} + (\Pi_{11} + 2\Pi_{22})K \\ 0 \\ (\Pi_{11} + 2\Pi_{22})c/c' \end{bmatrix}$$

$$K = \frac{c\rho q_1}{1 + c' q_1^2/\Pi_{11}}$$

The Equations

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} \rho \\ \rho v_1 \\ \rho(v_1^2 + \Pi_{11} + 2\Pi_{22})/2 \\ \rho \Pi_{22}/2 \\ q_1 \end{bmatrix}$$

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

free of derivatives

$$g(u) = -\frac{1}{2\tau} \begin{bmatrix} 0 \\ 0 \\ 0 \\ \rho(\Pi_{22} - \Pi_{11})/3 \\ D_{11} q_1 \end{bmatrix}$$

The Equations

$$\begin{bmatrix} u_1 \\ u_2 \\ u_3 \\ u_4 \\ u_5 \end{bmatrix} = \begin{bmatrix} \rho \\ \rho v_1 \\ \rho(v_1^2 + \Pi_{11} + 2\Pi_{22})/2 \\ \rho \Pi_{22}/2 \\ q_1 \end{bmatrix}$$

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

free of derivatives

$$h(u) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ -\Pi_{22} J \\ -q_1 J/\rho \end{bmatrix}$$

$$J = \frac{\partial}{\partial x}\left(\frac{c \rho q_1}{1 + c' q_1^2/\Pi_{11}}\right) = \frac{\partial}{\partial x} K$$

Numerical Integration

Help from Entropy

Consider the redundant balance equation for the entropy,

$$s = s(u_1, u_2, u_3, u_4, u_5)$$

$$\frac{\partial}{\partial t}s + \frac{\partial}{\partial x}v_1 s = \sigma(u) - c''J$$

$$\sigma(u) = \ldots\left[(\Pi_{11} + 2\Pi_{22})\left(\frac{1}{\Pi_{11}} + \frac{2}{\Pi_{22}}\right) - 9\right] + \ldots\frac{q_1^2}{\Pi_{11}}$$

Help from Entropy

Consider the redundant balance equation for the entropy,

$$s = s(u_1, u_2, u_3, u_4, u_5)$$

$$\frac{\partial}{\partial t}s + \frac{\partial}{\partial x}v_1 s = \sigma(u) - c'' J$$

Treat J as additional unknown

Equation for J (for implicit Euler scheme),

j: discrete space

n: discrete time

$$\frac{s(u_j^{n+1}) - s(u_j^n)}{\Delta t} + \frac{[v_1 s(u)]_{j+1}^n - [v_1 s(u)]_j^n}{\Delta x} = \sigma(u_j^{n+1}) - c'' J_j^{n+1}$$

simplified

Results

naive

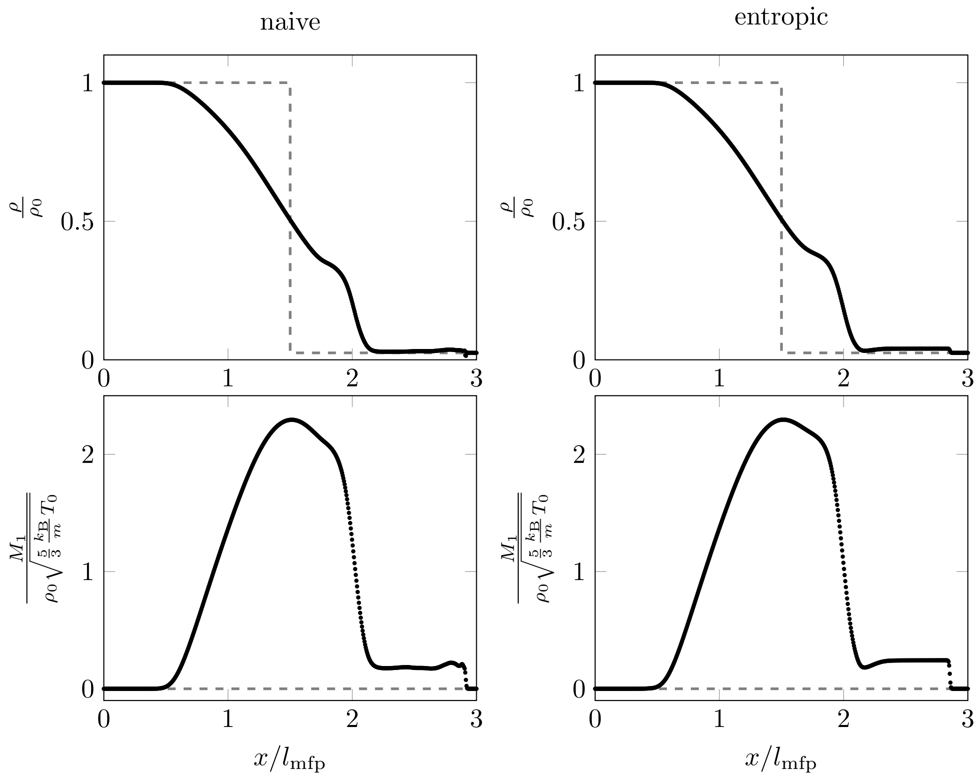


Fig. 7.2: Comparison of the naive and entropic schemes for density and momentum. Simulation results for $N = 600$, $\lambda = 0.025$ and $\epsilon = 1$. The dashed line shows the initial conditions, the dots represent the grid point values.

N = grid size

$\lambda = \frac{\Delta t}{\Delta x}$

ε = Knudsen number

Results

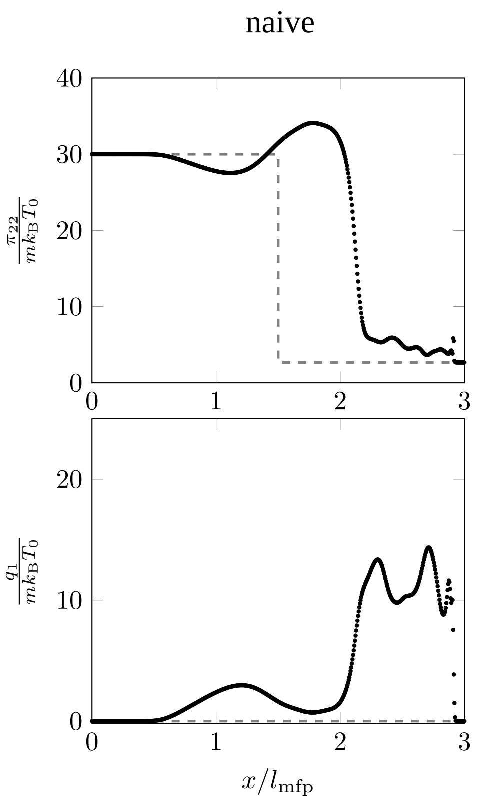


Fig. 7.3: Comparison of the naive and entropic schemes for the second moment tensor and third moment vector. Simulation results for $N = 600$, $\lambda = 0.025$ and $\epsilon = 1$.

Results

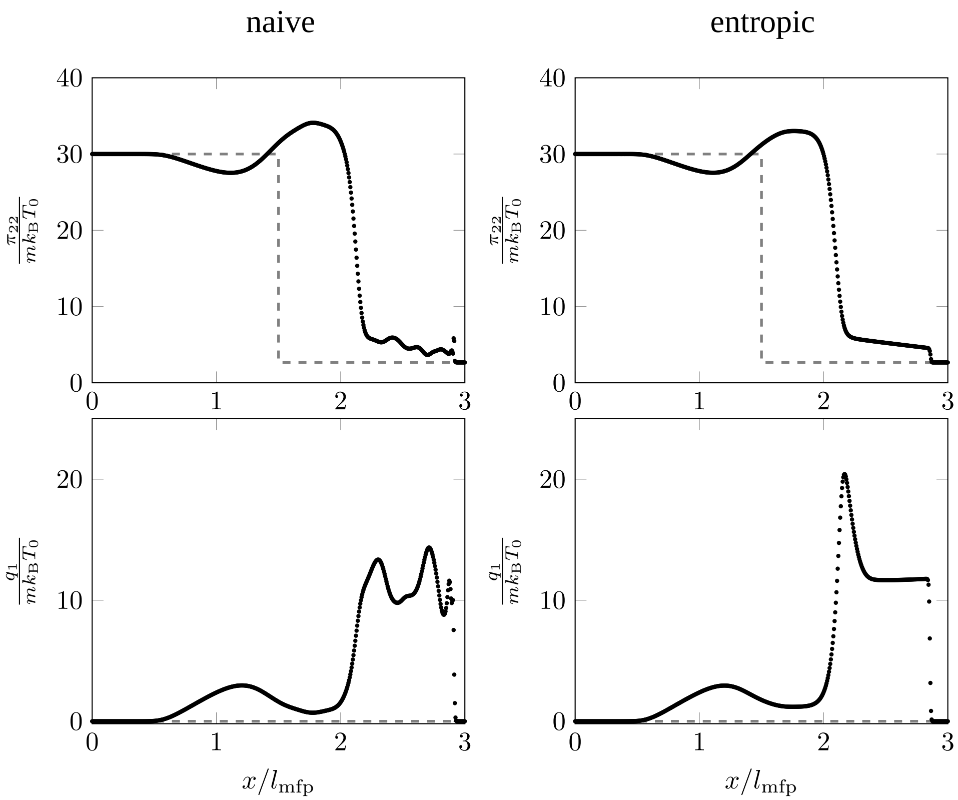


Fig. 7.3: Comparison of the naive and entropic schemes for the second moment tensor and third moment vector. Simulation results for $N = 600$, $\lambda = 0.025$ and $\epsilon = 1$.

Polymer Physics

Conclusions

- Equations with an entropy are better even for numerical solutions.
- Make proper use of entropy in developing numerical schemes!