Learning Thermodynamically Stable and Galilean Invariant PDEs for Non-equilibrium Flows

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Problem

- Consider BGK Boltzmann kinetic model in 1D:

$$\frac{\partial f}{\partial t} + \xi \frac{\partial f}{\partial x} = \frac{1}{\varepsilon}(f_M - f), \quad (1)$$

Here $f = f(x, t, \xi)$ is a distribution function with $\xi \in \mathbb{R}$ the particle velocity, and f_M is the Maxwellian

$$f_M = f_M(\xi; \rho, v, T) = \frac{\rho}{(2\pi T)^{1/2}} \exp\left(-\frac{(\xi - v)^2}{2T}\right)$$

with

$$\rho = \int_{\mathbb{R}} f d\xi, \quad \rho v = \int_{\mathbb{R}} \xi f d\xi, \; \rho T = \int_{\mathbb{R}} (\xi - v)^2 f d\xi. \quad (2)$$

Knudsen number: $Kn = \varepsilon = \frac{\lambda}{L}$ with λ mean free path, L representative physical length scale

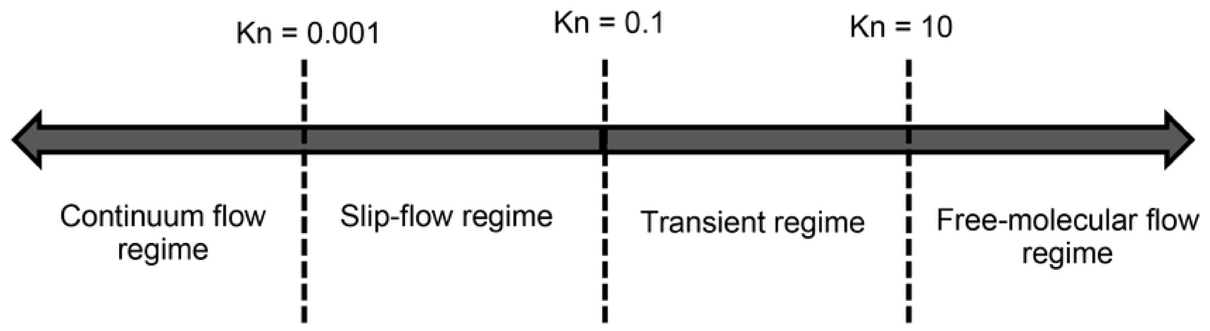


Figure 1: modeling gas dynamics

- multiply by 1, ξ and $\xi^2/2$, integrate over ξ, we derive fluid flows with the conservation laws of mass, momentum and energy:

$$\begin{aligned} \partial_t \rho + \nabla \cdot (\rho v) &= 0, \\ \partial_t (\rho v) + \nabla \cdot (\rho v v + P) &= 0, \\ \partial_t E + \nabla \cdot (E v + q + P v) &= 0. \end{aligned} \quad (3)$$

Here ρ is the fluid density, $v \in \mathbb{R}^d$ is the velocity, $E = \rho e + \frac{1}{2}\rho |v|^2$ is the total energy with e the specific internal energy, P is the pressure tensor, and q represents the heat flux.

- For 1D kinetic model, we derive equation of state

$$p = 2\rho e \quad (4)$$

Therefore, only heat flux q is an extra variable.

- Our goal: close (3) and discover new constitutive laws from data generated by kinetic model (instead of empirical laws)

CDF theory

Conservation-Dissipation Formalism (CDF) [3]:

- Assume that the non-equilibrium system is governed by first-order PDEs (hyperbolic balance laws)

$$\partial_t U + \sum_{j=1}^{d} \partial_{x_j} F_j(U) = Q(U), \quad (5)$$

where

$$U = \begin{pmatrix} u \\ v \end{pmatrix}, \quad F_j(U) = \begin{pmatrix} f_j(U) \\ g_j(U) \end{pmatrix}, \quad Q(U) = \begin{pmatrix} 0 \\ q(U) \end{pmatrix}.$$

with the structure stability constrain:

(i) There is a strictly concave smooth function $\eta = \eta(U)$, called entropy (density), such that the matrix product $\eta_{UU} F_{jU}$ is symmetric for each j and for all U under consideration.

(ii) There is a positive definite matrix $M = M(U)$, called dissipation matrix, such that the non-zero source can be written as $q(U) = M(U)\eta_v(U)$.

Such kind of PDEs describe a large number of irreversible processes [2]

- kinetic models (moment closure systems, discrete-velocity kinetic models), chemically reactive flows/combustion, nonlinear optics, radiation hydrodynamics, compressible non-Newtonian fluid flows...

Our model

- introduce a new dissipative variable w and postulate (concave) entropy of the form

$$\eta = \eta(\rho, \rho v, E, \rho w; \varepsilon) = \rho s(\nu, e, w; \varepsilon) = \rho(s^{(\mathrm{eq})}(\nu, e) + s^{(\mathrm{neq})}(w; \varepsilon))$$

Here the equilibrium entropy $s^{(\mathrm{eq})}$ is

$$s^{(\mathrm{eq})} = s^{(\mathrm{eq})}(\nu, e) = -k_b \nu \int_{\mathbb{R}} f_M \ln f_M d\xi = k_b \left(\frac{1}{2}\ln e + \ln \nu\right) + C,$$

Then we compute evolution equation of η

$$\begin{aligned} \eta_t + \partial_x(v\eta) \equiv Ds &= s_\nu D\nu + s_e De + s_w Dw \\ &= \rho \partial_x v + \theta^{-1}(-\partial_x q - \rho\theta\partial_x v) + s_w Dw \\ &= -\theta^{-1}\partial_x q + s_w Dw \\ &= -\partial_x(\theta^{-1} q) + s_w Dw + q\partial_x \theta^{-1} \end{aligned}$$

with $\theta^{-1} := s_e$. This suggests that $\theta^{-1} q$ is entropy flux and $s_w Dw + q\partial_x\theta^{-1}$ is entropy production. Then choose the heat flux $q = s_w^{(\mathrm{neq})}(w; \varepsilon)$ and evolution equation for w:

$$\partial_t(\rho w) + \partial_x(\rho v w) + \partial_x \theta^{-1} = Mq$$

- Finally, we have the following balance laws

$$\begin{aligned} \partial_t \rho + \partial_x(\rho v) &= 0, \\ \partial_t(\rho v) + \partial_x(\rho v^2 + \rho\theta) &= 0, \\ \partial_t E + \partial_x(Ev + s_w^{(\mathrm{neq})} + \rho\theta v) &= 0, \\ \partial_t(\rho w) + \partial_x(\rho v w) + \partial_x \theta^{-1} &= M s_w^{(\mathrm{neq})} \end{aligned} \quad (6)$$

with $\theta = T$ and the freedoms $M = M(\rho, e, w; \varepsilon)$ and $s^{(\mathrm{neq})} = s^{(\mathrm{neq})}(w; \varepsilon)$.

This system satisfies the properties:

- conservation-dissipation principle (globally symmetrizable hyperbolic)
- Galilean invariant

Neural networks

- We use the variables $(\rho, \rho v, E, q)$ with $q = s_w^{(\mathrm{neq})}(w; \varepsilon)$ and rewrite the balance laws (6) as

$$\begin{aligned} \partial_t \rho + \partial_x(\rho v) &= 0, \\ \partial_t(\rho v) + \partial_x(\rho v^2 + \rho\theta) &= 0, \\ \partial_t E + \partial_x(Ev + q + \rho\theta v) &= 0, \\ \partial_t q + v\partial_x q + \frac{g}{\rho}\partial_x \theta^{-1} &= \frac{gMq}{\rho} \end{aligned} \quad (7)$$

with

$$g = s_{ww}^{(\mathrm{neq})}(w; \varepsilon) < 0.$$

Therefore, our task becomes to learn the negative function $g = g(q; \varepsilon)$ and the positive function $M = M(\rho, e, q; \varepsilon)$.

- Here we discretize the last equation in (7) as

$$q_j^{n+1} = q_j^n - \frac{\Delta t}{2\Delta x} v_j^n (q_{j+1}^n - q_{j-1}^n) - \frac{\Delta t}{2\Delta x} \frac{g_j^n}{\rho_j^n}\left((\theta_{j+1}^n)^{-1} - (\theta_{j-1}^n)^{-1}\right) + \Delta t \left(\frac{gMq}{\rho}\right)_j^n, \quad (8)$$

By writing the above equation in the abstract form

$$q_j^{n+1} = \mathcal{S}[g, M](V_{j-1}^n, V_j^n, V_{j+1}^n; \Delta t, \Delta x) \quad (9)$$

with $V = (\rho, v, E, q)$, we define our loss function as the mean squared error (MSE):

$$\mathcal{L} = \sum_{\text{training data}} |q_j^{n+1} - \mathcal{S}[g, M](V_{j-1}^n, V_j^n, V_{j+1}^n; \Delta t, \Delta x)|^2. \quad (10)$$

- neural network structure:
two fully-connected neural networks to approximate $g = g(q; \varepsilon)$ and $M = M(\rho, \rho v, E, q; \varepsilon)$, softplus function is used in the output layer to ensure the positivity of M and $-g$

Data set

Two types of initial conditions:

- smooth: a convex combination of two Maxwellians with smooth macroscopic variables

$$f_{\mathrm{smooth}} = \alpha f_M(\xi; U_1) + (1 - \alpha) f_M(\xi; U_2)$$

Here the macroscopic variables $U_i = (\rho_i, v_i, T_i)$ for $i = 1, 2$ are the sine waves

$$\rho_i(x, 0) = a_{\rho,i}\sin(x + \psi_{\rho,i}) + b_{\rho,i}, \quad v_i(x, 0) = 0, \quad T_i(x, 0) = a_{T,i}\sin(x + \psi_{T,i}) + b_{T,i}.$$

- discontinuous: a convex combination of one Maxwellian with smooth macroscopic variables and another with Riemann problem

$$f_{\mathrm{shock}} = \alpha f_M(\xi; U_{\mathrm{smooth}}) + (1 - \alpha) f_M(\xi; U_{\mathrm{shock}})$$

with α sampled from $[0, 1]$.

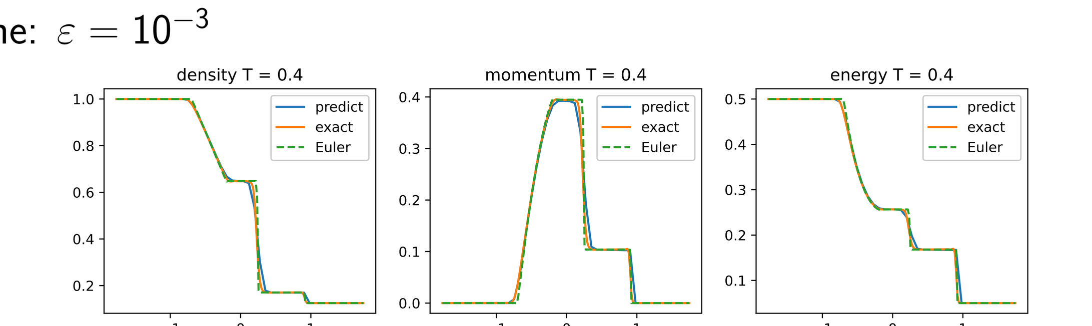
Numerical results

Accuracy in testing data:

- smooth solutions: relative errors is less than 3% for smooth solutions
- discontinuous solutions: relative errors is less than 6% for discontinuous solutions
- good generalization from smooth data (training) to discontinuous data

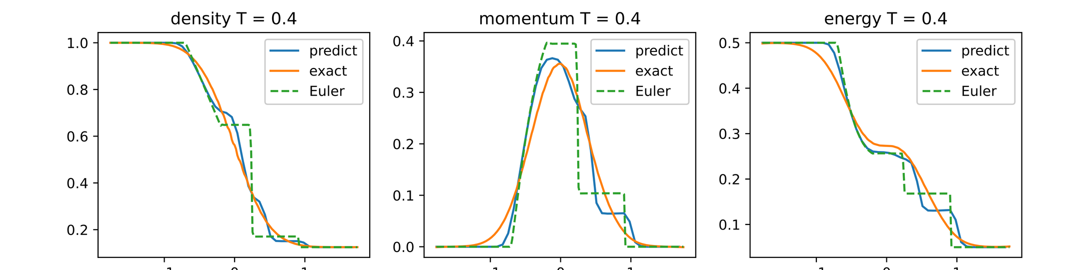
Sod shock tube problem:

- hydrodynamic regime: $\varepsilon = 10^{-3}$



our model agrees well with BGK model and also Euler equations.

- kinetic regime: $\varepsilon = 10$



our model behaves much better than Euler equations.

Conclusion

- What we have done [1]:
  - develop a method for learning interpretable and thermodynamically stable PDEs based on Conservation-dissipation Formalism
  - the learned PDEs satisfy the conservation-dissipation principle automatically (hyperbolic balance laws)
  - our model achieves good accuracy in a wide range of Knudsen numbers
  - good generalization from smooth data to discontinuous data
- Future work:
  - add more non-equilibrium variables to achieve better accuracy
  - generalization to multi-dimensional problems

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