Structure Preserving Neural Networks: A Case Study in the Entropy Closure of the Boltzmann Equation

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Objectives

Accelerate numerical simluation of many-particle systems described by the Boltzmann moment equation:

- Employ convex neural networks to compute the minimal entropy closure
- Construct a hybrid neural-network accelerated numerical solver
- Analyze input and output space to control neural network errors
- Create an efficient data-generator - agnostic to specific simulation conditions

Introduction

The Boltzmann equation laid the foundation for statistical physics, and describes the evolution of one-particle probability density function $f(t,x,v)$, where $\{x \in \mathbb{R}^3, v \in \mathbb{R}^3\}$ are the coordinates in phase space, in a many-particle system

$$\partial_t f + v \cdot \nabla_x f = Q(f). \tag{1}$$

The linear collision operator $Q(f)$ describes interactions between particles and with the background medium. The high dimensionality yields tremendous challenges for large scale numerical solutions.

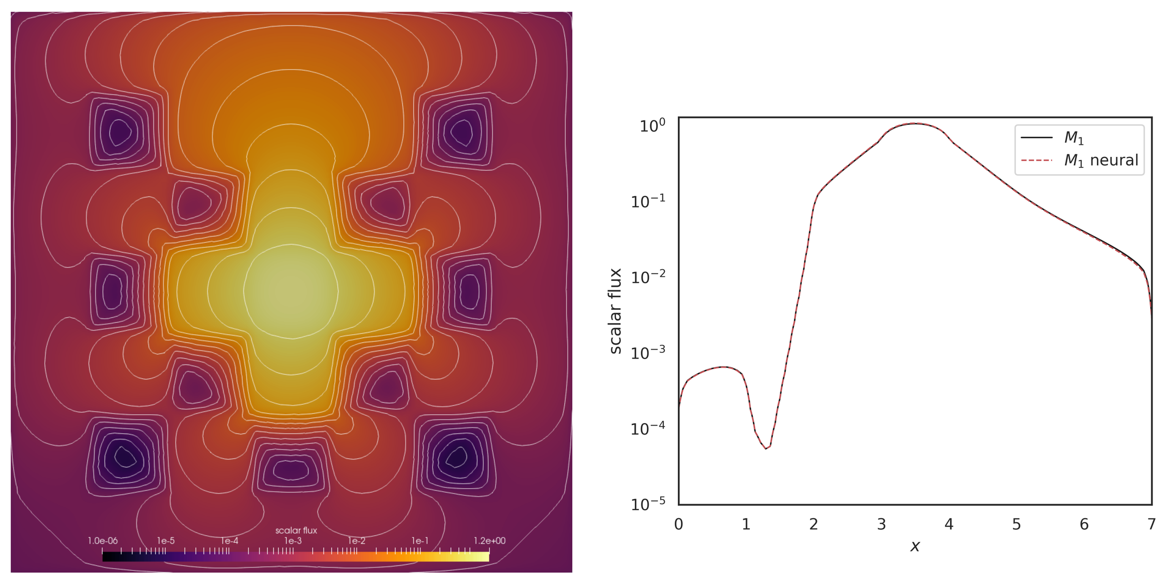

Figure 1:Neural network based nuclear reactor simulation (left), accuracy of the neural entropy at a cross section (right).

Moment Equations

Moment methods eliminate the dependency of the phase space on the velocity variable by computing the moment hierarchy of the Boltzmann equation

$$\partial_t u + \nabla_x \cdot \langle v m f\rangle = \langle m Q(f)\rangle\,, \tag{2}$$

where $u(t,x)$ is the moment vector and $m(v)$ is a vector of velocity dependent basis functions. The moment system (2) requires a closure due to the existence of high-order unclosed terms in the advection operator. The entropy closure [1],

$$h(u) = \min_{g\in F_m} \langle \eta(g)\rangle \quad \text{s.t. } u = \langle m g\rangle\,, \tag{3}$$

with minimizer f_u of Eq. (3) closes the moment system.
Minimal entropy closures are structurally beneficial for simulation, since they

- ensure hyperbolicity,
- dissipate physical entropy,
- conserve physical quantities, e.g. mass,
- ensure stability of the simulation.

Neural Entropy Closures

By the strong duality of the minimal entropy problem, we write at the optimal point (u, α_u) for the Lagrange multiplier α_u

$$h(u) = \alpha_u \cdot u - \langle \eta_*(\alpha_u \cdot m)\rangle\,. \tag{4}$$

Approximate this convex data-to-solution mapping by a input convex neural network $\mathcal{N}_\theta$ [2]

$$h(u) \approx \mathcal{N}_\theta(u), \qquad \alpha_u \approx \partial_u \mathcal{N}_\theta(u). \tag{5}$$

Close the equation with a reconstruction mapping

$$f_u = \eta'_*(\alpha_u \cdot m). \tag{6}$$

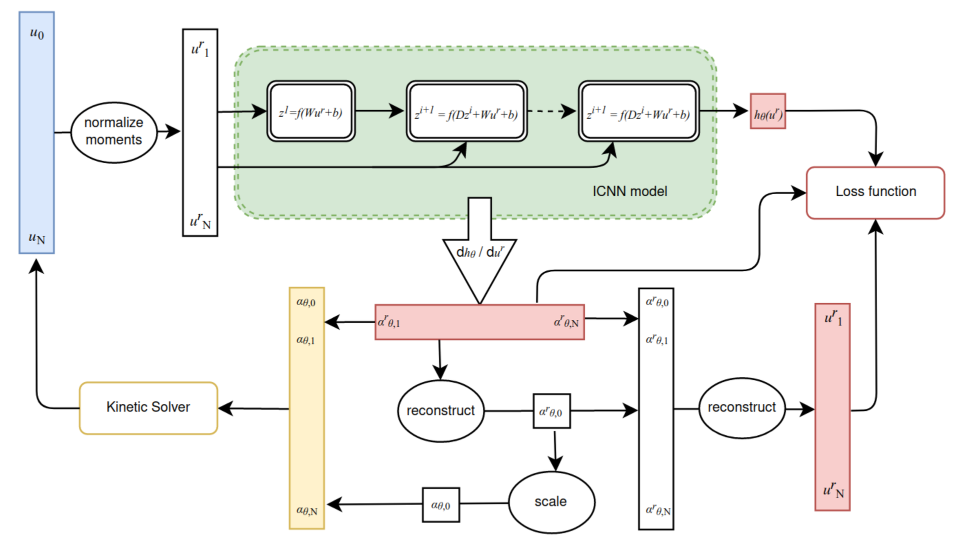

Figure 2:Interface of the neural network with the kinetic solver.

Data Sampling

The set of all moments corresponding to kinetic densities $f > 0$ is called the realizable set

$$\mathcal{R} = \{u : \langle m f\rangle = u,\ f \in F_m\}\,. \tag{7}$$

This gives full analytic control of the data and solution space.

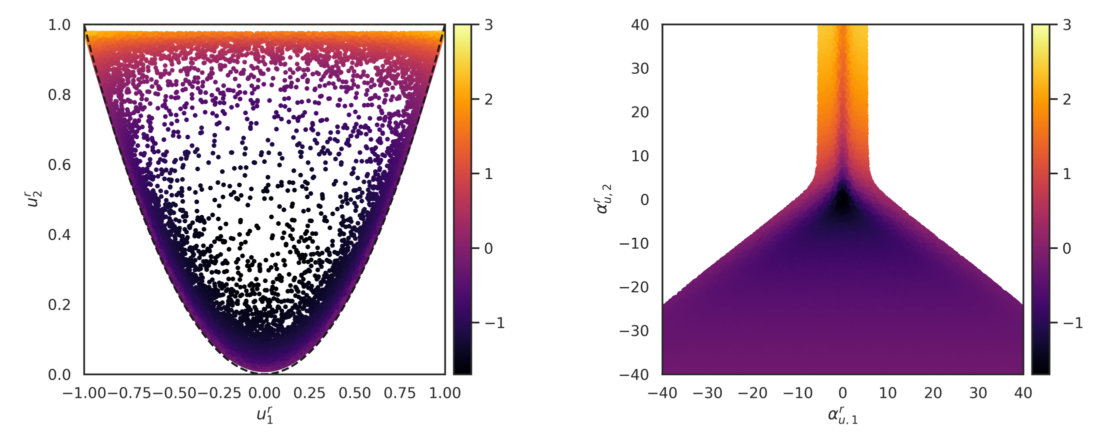

Figure 3:Entropy over the moment space (left) and Lagrange multiplier space (right).

Use convexity of the network and the data-space, as well as normalization to construct an interpolation error bound depending on the training data U_T

$$\|\alpha_u - \partial_u \mathcal{N}_\theta(u)\| \le \epsilon(U_T). \tag{8}$$

Important Result

Convex neural networks yield a structure preserving and efficient closure for complex moment systems. Simulation time can be reduced by over 87%, while accuracy is maintained. Convexity of the neural network and the data-space is leveraged to create an error-bound obeying sampling strategy.

The Challenge

Equation (3) is a convex, ill-conditioned non-linear optimization problem and has to be solved in each grid cell at each time step of a simulation.
Over 90% of the computational expense of the solver is spent on the entropy closure.

Timings

Table 1:Timings of the Newton based benchmark and the neural network entropy based solver.

compute cores	Newton [s]	$\mathcal{N}_\theta$ [s]	Ratio [%]
4	757.88	80.81	89.33
12	258.64	33.60	87.01

References

[1] C. David Levermore.
Entropy-based moment closures for kinetic equations.

[2] Brandon Amos, Lei Xu, and J. Zico Kolter.
Input convex neural networks.

Code: https://github.com/ScSteffen/neuralEntropyClosures
Code: https://github.com/CSMMLab/KiT-RT

Contact

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