Sparse Identification of Nonlinear Moment Closure Dynamics

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Introduction

Collisional kinetic plasma models (multispecies Vlasov-Maxwell-Landau, etc.) provide high-fidelity simulation of plasma physics, but at great computational cost.
A great variety of model reductions to these systems exist:

- Chapman-Enskog based asymptotic expansions in Kn^{-1} (e.g. Braginskii [1])
- Ansatz-based extensions and regularizations of the Grad 13N Moment scheme [5]
- Dynamical low-rank methods evolve an ansatz for f as a low-rank matrix in x and v. [4]

These methods save computation compared to the full 6 dimensional kinetic equation. Making good use of reduced models requires knowing when they are appropriate to apply.

- **Hybridization**: Split up physical domain into pieces according to predetermined parameter cutoffs
- **Adaptivity**: Dynamically upscale and downscale plasma model according to local conditions

But first: analyze data from full kinetic simulations to discover where fluid-like models provide a good fit.

BGK Shocktube Problem

Neutral fluid BGK model in 1D1V provides a test case for analyzing data-driven moment closure techniques.
Initial-boundary value problem:

$$\begin{cases} \frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} = \left(\frac{\partial f}{\partial t}\right)_{\text{BGK}} = -\frac{f - f_M}{\tau}, & x \in [0, L], t \in [0, \infty) \\ f(0, v, 0) = f(0, v, t) = \mathcal{M}(1, 0, p_L), & x \in [0, L/2) \\ f(L, v, 0) = f(L, v, t) = \mathcal{M}(1, 0, 1), & x \in [L/2, L] \end{cases}$$

with Maxwellian boundary conditions $\mathcal{M}(n, nu, nT)$.

$$\chi(f) = \frac{\int |f - \mathcal{M}(f)|\, dv}{\int |\mathcal{M}(f)|\, dv}$$

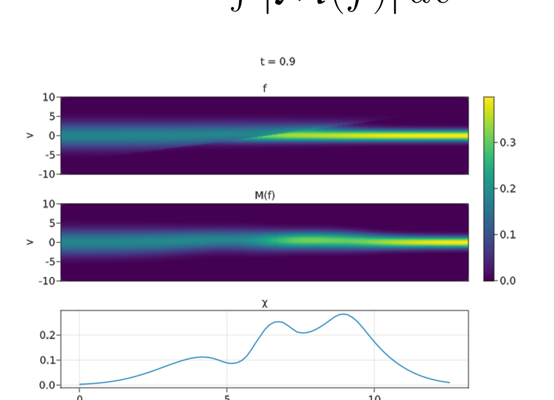

Figure: Representative BGK shocktube solution f and its χ metric

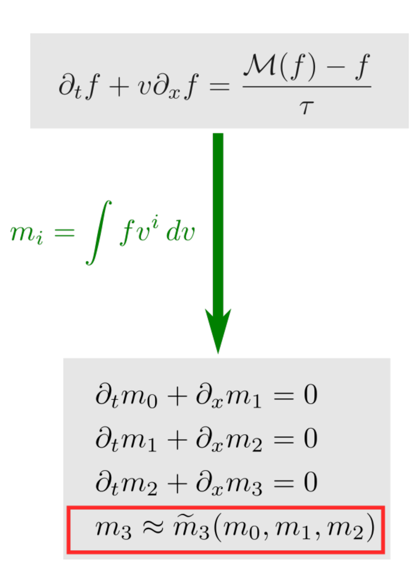

Figure: Schematic of the moment closure problem in 1D1V

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Sparse Regression (SINDy) for BGK m_3

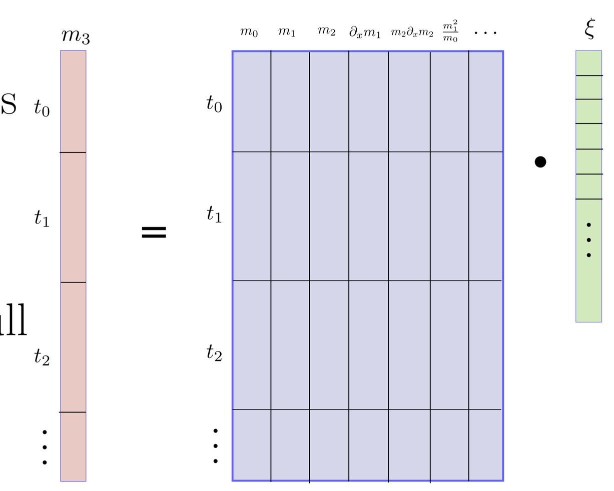
The SINDy technique [2] provides a method for discovering nonlinear dynamics from data.

Minimization formulation:

$$\min_{\xi} \left(\|\mathbf{A}\xi - m_3\|^2 + \lambda \|\xi\|_1 \right) \implies \tilde{m}_3 = \mathbf{A}\xi$$

A large nonlinear predictor library $\mathbf{A}$ consists of products of lower moments and their spatial derivatives.

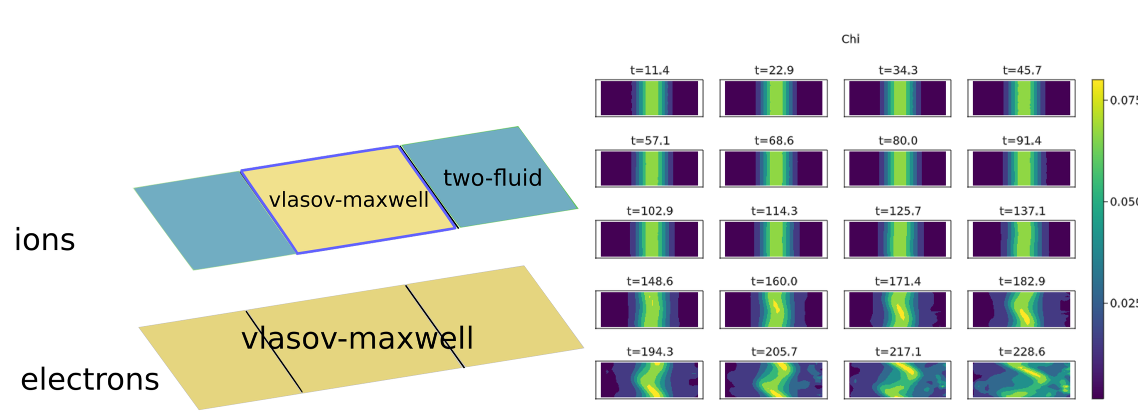
Dataset consists of 3 BGK full kinetic simulations with varying collision time τ and shock strength.



Vlasov-Maxwell Simulation of Kelvin-Helmholtz Instability

$$\partial_t f_\alpha + \mathbf{v} \cdot \nabla_{\mathbf{x}} f_\alpha + \frac{q_\alpha}{m_\alpha}(\mathbf{E} + \mathbf{v} \times \mathbf{B}) \cdot \nabla_{\mathbf{v}} f_\alpha = 0, \quad (1)$$

where α ranges over the particle species $\{e, i\}$, and the fields $\mathbf{E}, \mathbf{B}$ are evolved with Maxwell's equations.
[3] and [6] simulate the KH instability. Here we use data from [3] on a hybridized domain:



(a) Schematic of the domain hybridization (b) Maxwellian deviation χ

Figure: The KH instability evolution sees χ grow in the highlighted region, where the ion species is treated kinetically.

Braginskii-like Heat Flux Closures

A Chapman-Enskog expansion of the *collisional* version of (1) gives a perturbative closure relationship for the ion heat flux in terms of the temperature:

$$\mathbf{q}^i = \int f_i |\mathbf{v} - \mathbf{u}|^2 \mathbf{v}\, d\mathbf{v}$$

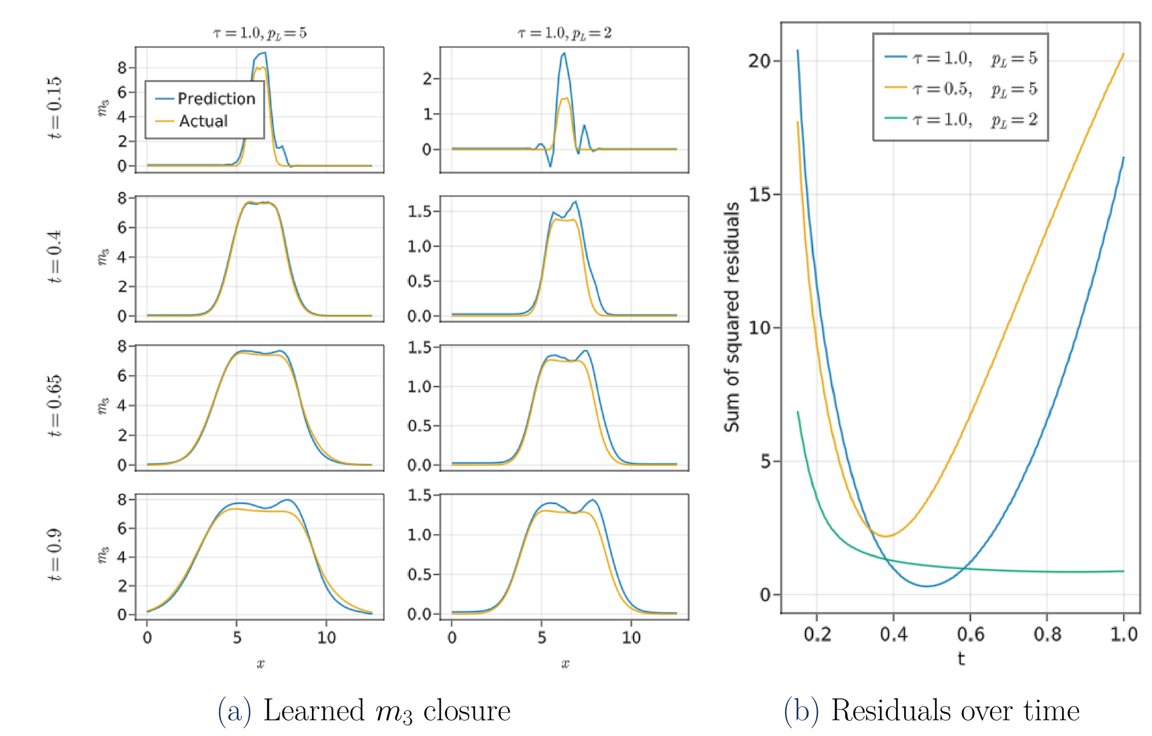
$$\underset{\text{Braginskii}}{\approx} -\kappa_\parallel \nabla_\parallel T_i - \kappa_\perp \nabla_\perp T_i + \kappa_\wedge (\hat{b} \times \nabla T_i) + O(\epsilon^2). \quad (2)$$

Note

A Chapman-Enskog expansion of (1) cannot be justified without a collision term; however the form of (2) suggests a function library to learn a moment closure for $\mathbf{q}$

SINDy results

Learned solution is not actually sparse: 89(!) out of 116 coefficients are nonzero, even with L^1 regularization.



(a) Learned m_3 closure (b) Residuals over time

Figure: SINDy results. Fit captures shock speeds reasonably well, but residuals suggest poor generalization.

The magnetic field $\mathbf{B}$ is almost exactly constant, so we fit heat flux closures of the form

$$q_x \approx -\kappa_\perp \partial_x T_i - \kappa_\wedge \partial_y T_i$$
$$q_y \approx -\kappa_\perp \partial_y T_i + \kappa_\wedge \partial_x T_i,$$

using a least-squares approach,

$$\min_{\boldsymbol{\xi}_x} \left\| \left[n_i T_i \partial_x T_i \;\; n_i T_i \partial_y T_i \right] \cdot \boldsymbol{\xi}_x - q_x \right\|^2,$$
$$\min_{\boldsymbol{\xi}_y} \left\| \left[n_i T_i \partial_y T_i \;\; n_i T_i \partial_x T_i \right] \cdot \boldsymbol{\xi}_y - q_y \right\|^2.$$

Heat Flux Regression Results

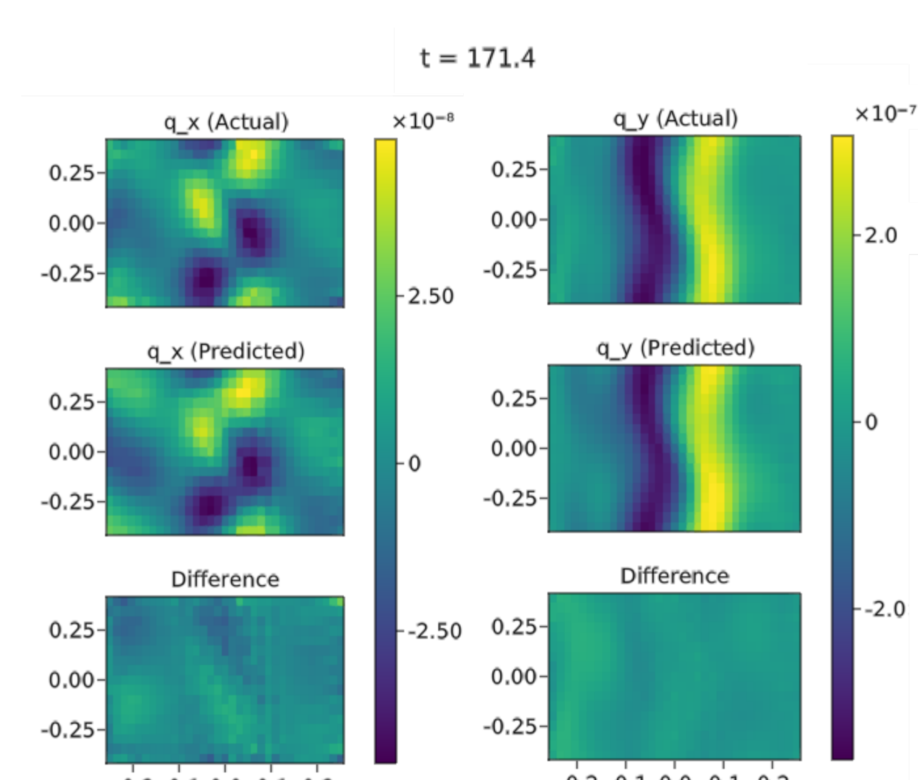


Figure: The simple linear regression described above predicts the shape of the heat flux in both x and y

The time-integrated L^1 error is 43% in q_x and only 18% in q_y.

Conclusion

Sparse Identification of Nonlinear Dynamics is likely not a suitable tool for moment closure problems, as evidenced by the failure of sparsity on even a simple moment closure problem. Asymptotic analysis such as the Chapman-Enskog expansion is a more promising route for the discovery of relationships between lower and higher moments. Even in a fully noncollisional plasma simulation, the Chapman-Enskog derived Braginskii closure accounts for 60-80% of the ion heat flux.

Future Work and Open Questions

Open Questions:

- Is there a different SINDy library of nonlinear functions that will give better results?
- Do the learned moment closures lead to a stable system? Can a SINDy type framework be designed which will ensure hyperbolicity of the resulting moment system?
- Can the observed moderate quality of fit to a Braginskii-like moment closure be predicted by some other asymptotic expansion of Equation (1)?

Future Work:

- Repeat Kelvin-Helmholtz instability simulations with a range of collisionalities.
- Develop a generic moment closure evaluation tool to determine whether proposed moment closures can stably and accurately reproduce kinetic results.

References

[1] S.I. Braginskii. Transport Processes in a Plasma. In *Reviews of Plasma Physics*, volume 1. 1965.

[2] Steven L. Brunton, Joshua L. Proctor, and J. Nathan Kutz. Discovering governing equations from data by sparse identification of nonlinear dynamical systems. *Proceedings of the National Academy of Sciences*, 113(15):3932–3937, April 2016.

[3] I A M Datta and U Shumlak. Computationally efficient high-fidelity plasma simulations by coupling multi-species kinetic and multi-fluid models on decomposed domains.

[4] Lukas Einkemmer and Christian Lubich. A low-rank projector-splitting integrator for the Vlasov–Poisson equation. *arXiv:1801.01103 [physics]*, June 2018.

[5] Harold Grad. On the kinetic theory of rarefied gases. *Communications on Pure and Applied Mathematics*, 2(4):331–407, December 1949.

[6] G. V. Vogman, J. H. Hammer, U. Shumlak, and W. A. Farmer. Two-fluid and kinetic transport physics of Kelvin–Helmholtz instabilities in nonuniform low-beta plasmas. *Physics of Plasmas*, 27(10):102109, October 2020.

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