RUHR-UNIVERSITÄT BOCHUM

Discovering heat flux closures using machine learning methods

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Abstract

In computational plasma physics, kinetic models are used to simulate plasma phenomena where small scale physics is expected to be of importance. These models contain the full information on the particle velocity distribution function but are computationally expensive. Therefore, computationally cheaper models are utilized, which can then be deployed to larger scales e. g. 10-moment fluid models or magnetohydrodynamics (MHD). However, the large scale behavior is critically influenced by small scale behavior [4, 10, 9]. Thus, models are required that can include kinetic processes, in reduced form, into large scale simulations. At the moment, analytical closures are used to close the hierarchy of fluid equations, but these closures, i. e. Landau fluid closures, are strictly valid only in certain regimes [7]. Finding suitable closure equations is an ongoing research topic that gets increasingly more difficult in complex systems. In this study, we try to improve fluid models by learning a suitable symbolic closure for the heat flux by applying the sparse identification of nonlinear dynamics (SINDy) method [3] to data from kinetic simulations of the two stream instability and Landau damping (see poster X5.198 for a direct prediction of the heat flux with ML).

Closure Problem

Vlasov equation (collisionless):

$$\frac{\partial f_s}{\partial t} + v_i \frac{\partial f_s}{\partial x_i} + \frac{q_s}{m_s}\left(E_i + \varepsilon_{abi} v_a B_b\right)\frac{\partial f_s}{\partial v_i} = 0$$

Moments of the distribution function:

$$\mu^{(k)}_{s;\mathrm{l,m,n}\ldots} = \int \mathrm{d}^3 v f_s \underbrace{v_\mathrm{l} v_\mathrm{m} v_\mathrm{n}\ldots}_{\text{k-times}}$$

Moments of the Vlasov equation:

$$\frac{\partial \mu^{(k)}_{s;\mathrm{l,m,n\ldots i}}}{\partial t} = -\frac{\partial \mu^{(k+1)}_{s;\mathrm{l,m,n,\ldots,i,j}}}{\partial x_j} + \frac{q_s}{m_s} \sum_{\substack{\text{cyclic perm.}\\ \text{of free indices}}} \mu^{(k-1)}_{s;\mathrm{l,m,n}\ldots} E_i + \varepsilon_{ipq}\mu^{(k)}_{s;\mathrm{l,m,n,\ldots,p}} B_q$$

Closure equation needed for $k+1$-th moment (red term)!

Methods: Sparse Identification of nonlinear dynamics (SINDy) [5]

- The coefficients $\mathbf{\Xi}$ of candidate terms $\mathbf{\Theta}$ are optimized to match the value of the state variables $\mathbf{X}$ evaluated at different grid points and times.
- Together, the coefficients $\mathbf{\Xi}$ and the candidate terms $\mathbf{\Theta}$ represent a sparse symbolic equation for the divergence of the heat flux.
- The optimization algorithm *sequential thresholded least-squares* (STLSQ) [5] is employed and includes the hyperparameters *threshold* and *sparsity*.

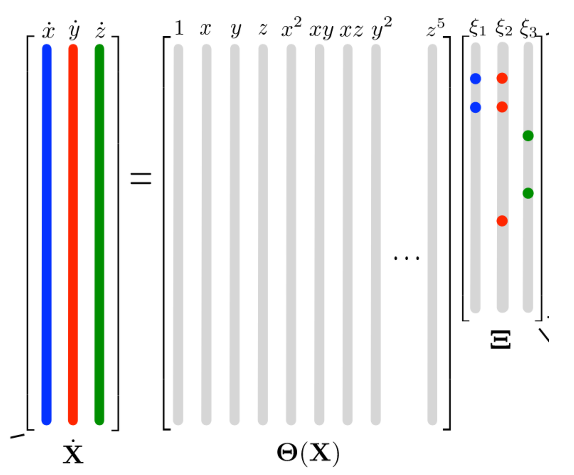

Figure 1: Schematic of the SINDy algorithm [5].

Data

- Simulations of the two stream instability (TS) and Landau damping (LD) are run with the fully kinetic Vlasov module in the muphyII framework [1].
- Physical parameters: weight of the streams $\chi \in \{0.4, 0.5\}$, drift velocity $v_\mathrm{d} \in \{1, 2\} v_\mathrm{th}$ with the thermal velocity v_th, density $n_0 = 1$, initial temperature $T_{\mathrm{e,i0}} = 0.1$ (TS) and $T_{\mathrm{e,i0}} = 1$ (LD)
- TS1: $\chi = 0.5$, $v_\mathrm{d} = 1 v_\mathrm{th}$; TS2: $\chi = 0.4$, $v_\mathrm{d} = 1 v_\mathrm{th}$; TS3: $\chi = 0.4$, $v_\mathrm{d} = 2 v_\mathrm{th}$

Results: Closure Equation for the Divergence of the Electron Heat Flux

- Hyperparameters: STLSQ algorithm with threshold 250 and sparsity constant 10^{-2}
- Candidate terms comprise terms with correct dimensions inspired by works of [6, 8] and analytical closures [11, 2, 12]

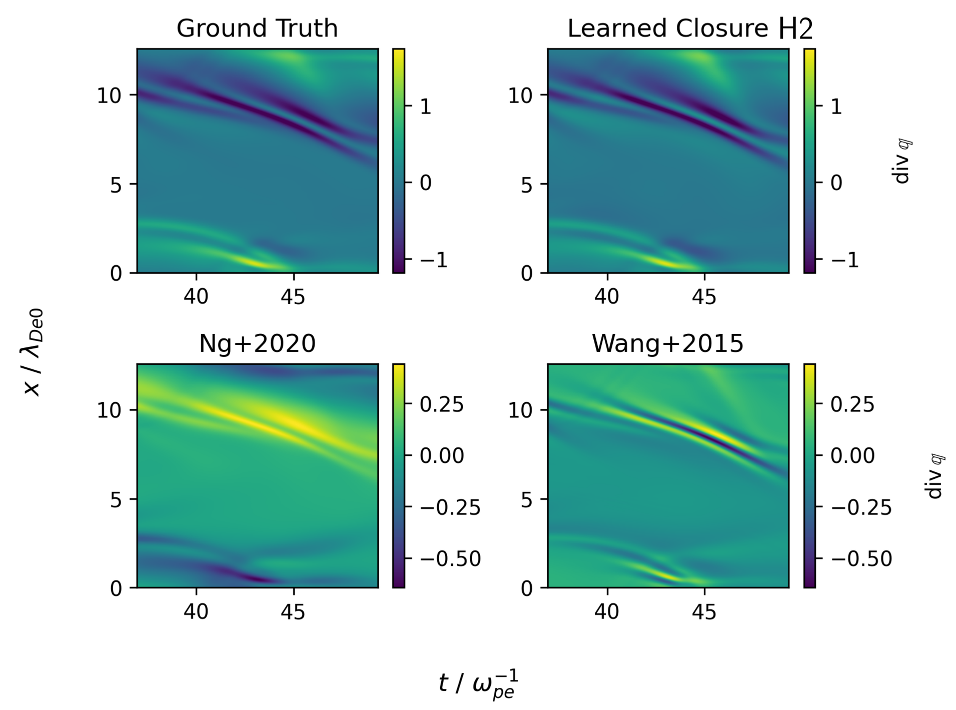

Figure 2: Comparison of the learned closure (H2), analytical closure equations, and the true divergence of the electron heat flux at a given time for the **two stream instability** data (TS2).

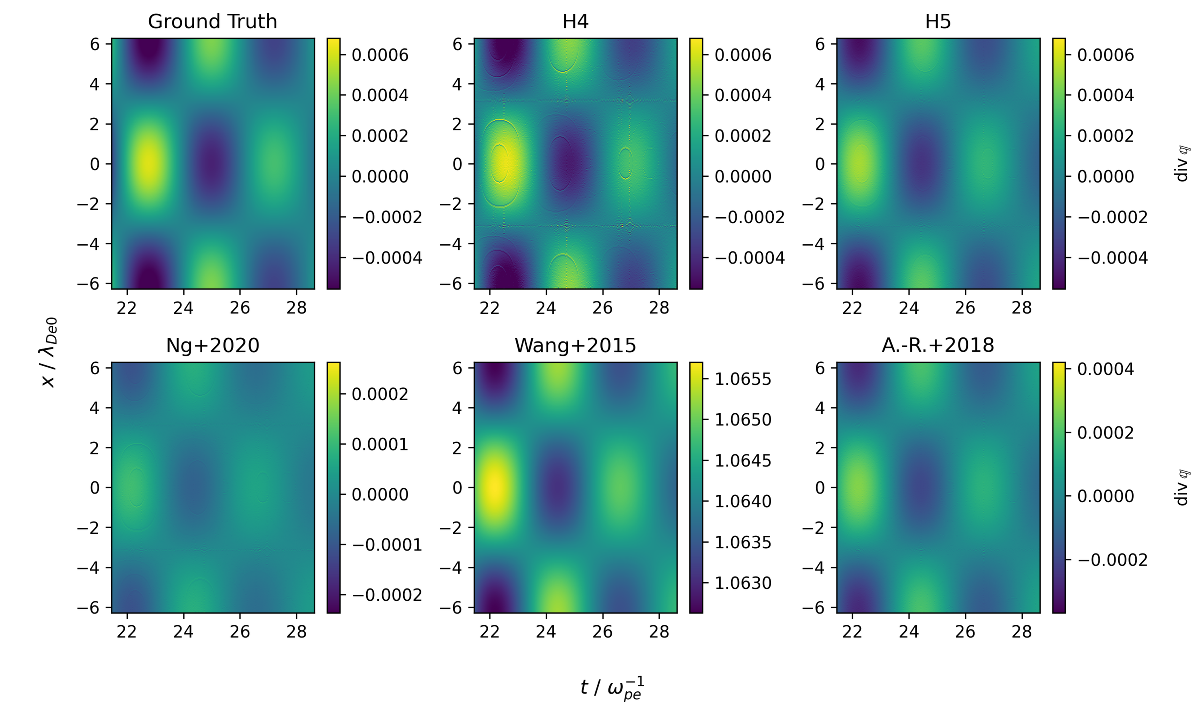

Figure 3: Comparison of learned (H4, H5) and analytical closure equations as well as the true divergence of the electron heat flux at a given time for the **Landau damping** data (LD).

Table 1: Best results learning a closure equation for the divergence of the heat flux in case of Landau damping (LD) and the two-stream instability (TS) with SINDy. k_0/d_{e0} was set to 1 for the training and can be computed from the learned coefficients.

No.	sim.	Learned Closure Equation (SINDy)
H1	TS1	$-3.0648 p_{xx}\partial_x u_x$
H2	TS2	$-3.2144 p_{xx}\partial_x u_x$
H3	TS3	$-3.8028 p_{xx}\partial_x u_x$
H4	LD	$-12.9737 n \frac{2v_\mathrm{th}}{3\sqrt{\pi}\lvert k_0\rvert}\partial_x^2 T_{xx} + 2.3590 \frac{2v_\mathrm{th}}{\sqrt{\pi}\lvert k_0\rvert}\frac{2}{3}\partial_x^2 p_{xx} + 1.6201 p_{xx}\partial_x u_x$
H5	LD	$1.7320 n \frac{2v_\mathrm{th}}{3\sqrt{\pi}\lvert k_0\rvert}\partial_x^2 T_{xx} - 2.5608 \frac{2v_\mathrm{th}}{\sqrt{\pi}\lvert k_0\rvert}\frac{2}{3}\partial_x^2 p_{xx}$

Coefficients were rounded to the fourth digit. The indices denote the components of the quantities.

Analytical Closures

- Ng+2020 [11]:
  $(\mathrm{div}\, q)_{xx} = -n \frac{2v_\mathrm{th}}{3\sqrt{\pi}|k_0|}\partial_x^2 T_{xx}$
- Wang+2015 [12]:
  $(\mathrm{div}\, q)_{xx} = \frac{2v_\mathrm{th}}{\sqrt{\pi}}|k_0|\frac{2}{3}p_{xx}$
- A.-R.+2018 [2]:
  $(\mathrm{div}\, q)_{xx} = -\frac{2v_\mathrm{th}}{\sqrt{\pi}|k_0|}\frac{2}{3}\partial_x^2 p_{xx}$

Summary and Outlook

- Learned closure equation fits the ground truth better (TS) or similarly (LD) than typical analytical closure equations.
- However, both the identified candidate terms (see H4 and H5) and the learned coefficients (H1, H2 and H3) depend not only on the physical problem, but also with the initial conditions of this simulation. This may hinder applicability of the learned closures to fluid simulations.
- The validation of the learned closures in 10-moment simulations compared to the analytical closures and fully kinetic simulations requires further investigation.

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