Deep Learning Surrogate Models for Kinetic Landau Fluid Closure

X. Q. Xu[1],

C. H. Ma[2], L.B. Wang[3], B. Zhu[1]

1) Lawrence Livermore National Laboratory, Livermore, CA 94550 USA
2) Princeton Plasma Physics Laboratory, Princeton, NJ 08543-0451, USA
3) Peking University, Beijing, China

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Fluid simulations with kinetic closures can be achieved by Deep Learning, with DL surrogate model closure predicted by the neural networks

Kinetic model:

$$\frac{\partial f}{\partial t} + v\frac{\partial f}{\partial x} + \frac{e}{m}E\frac{\partial f}{\partial v} = 0. \quad (1)$$

Fluid model ($n = \int f dv, mnu = m\int vf dv, p = m\int (v-u)^2 f dv$):

$$\frac{\partial n}{\partial t} + \frac{\partial (un)}{\partial x} = 0, \quad (2)$$

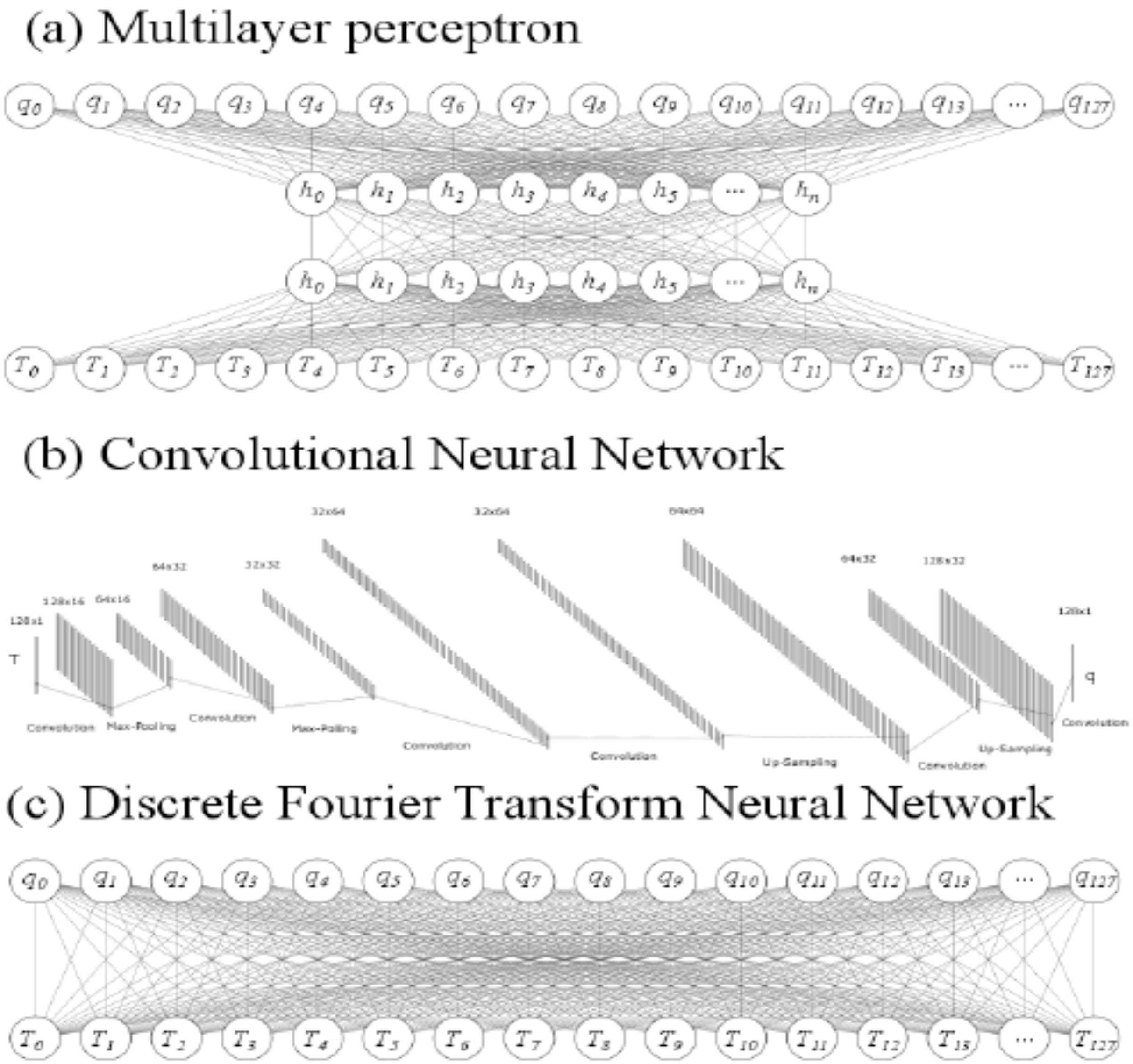
$$\frac{\partial mnu}{\partial t} + \frac{\partial (umnu)}{\partial x} = -\frac{\partial p}{\partial x} + enE, \quad (3)$$

$$\frac{\partial p}{\partial t} + \frac{\partial (up)}{\partial x} = -2p\frac{\partial u}{\partial x} - \frac{\partial q}{\partial x}. \quad (4)$$

Kinetic closure

$$q = \sqrt{2} n_0 v_t \frac{(2\zeta^3 - 3\zeta)\, Z(\zeta) + 2\zeta^2 - 2}{(2\zeta^2 - 1)\, Z(\zeta) + 2\zeta} \hat{k} T \qquad \zeta = \frac{\omega + i\nu}{\sqrt{2}|k| v_t} \quad (5)$$

With such a complicated spatiotemporal closure, how can one implement it into a fluid simulation in configuration space?



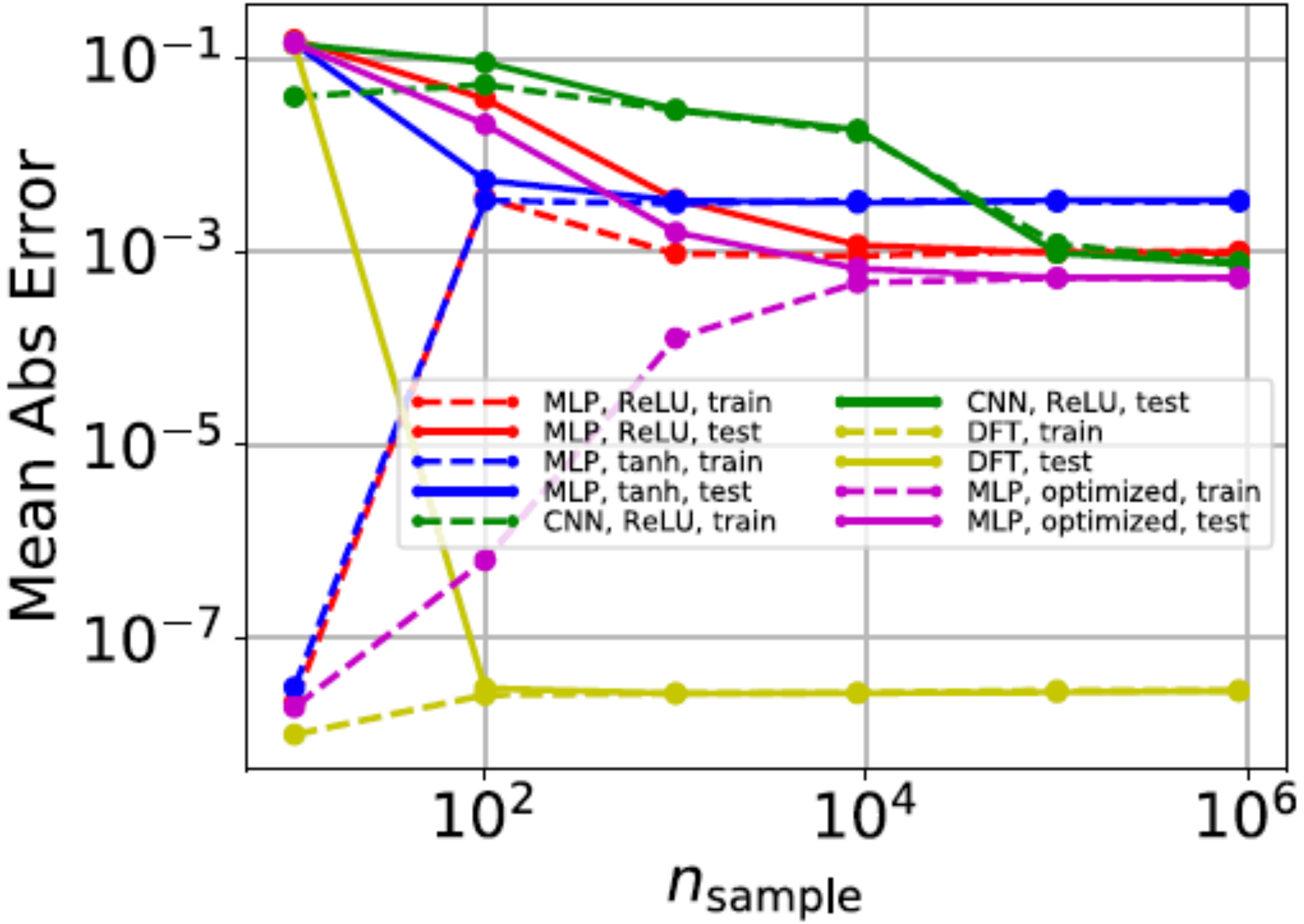
Neural networks:

- MLP: two hidden layers, fully connected
- CNN: Deep partially connected convolutional layers
- DFT: No hidden layers, fully connected

hyperparameters:

- Constructed with Tensorflow and Keras
- Optimizer: Adam
- Loss function: mean-squared-error(MSE)

Mean-Absolute-Error vs the number of training samples for different types of neural networks with different activation functions

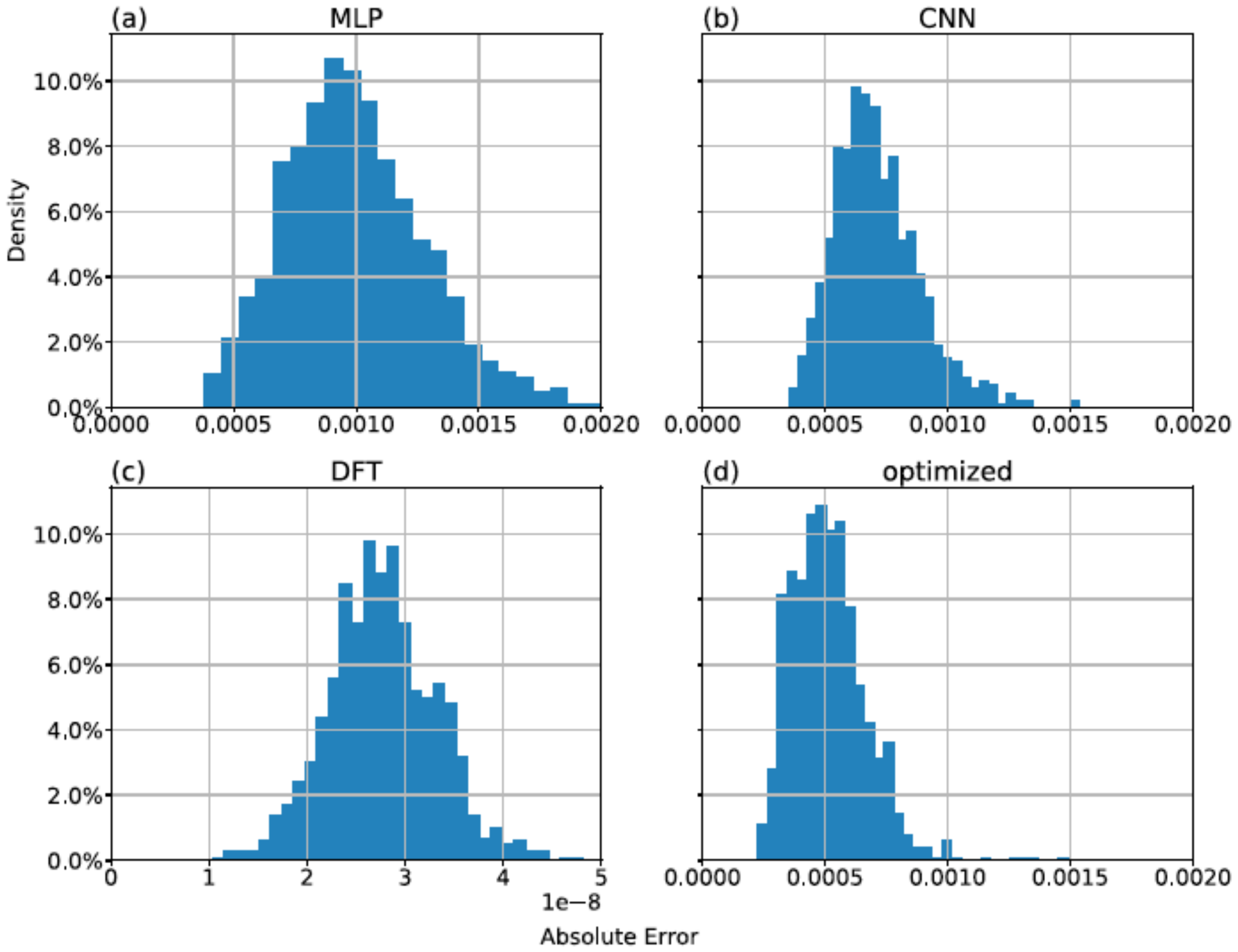


HP Landau closure
Hammett and Perkins PRL 1990

$$q_k = -n_0\sqrt{\frac{8}{\pi}}v_t\frac{ikT_k}{|k|}$$

$$q(x) = -n_0\sqrt{\frac{8}{\pi^3}}v_t\int_0^\infty dx'\left[T(x+x') - T(x-x')\right]/x'.$$

Probability distribution function (PDF) of absolute error for different neural network models when $n_{sample} = 10^6$



The Mean absolute errors for different NN

$\varepsilon_{MLP} = 9.72 \times 10^{-4}$

$\varepsilon_{CNN} = 7.45 \times 10^{-4}$

$\varepsilon_{optimized} = 5.49 \times 10^{-4}$ for MLP

$\varepsilon_{DFT} = 2.69 \times 10^{-8}$

Relative error (MRE) comparison of HP closure between DL surrogate model & non-Fourier (NF)

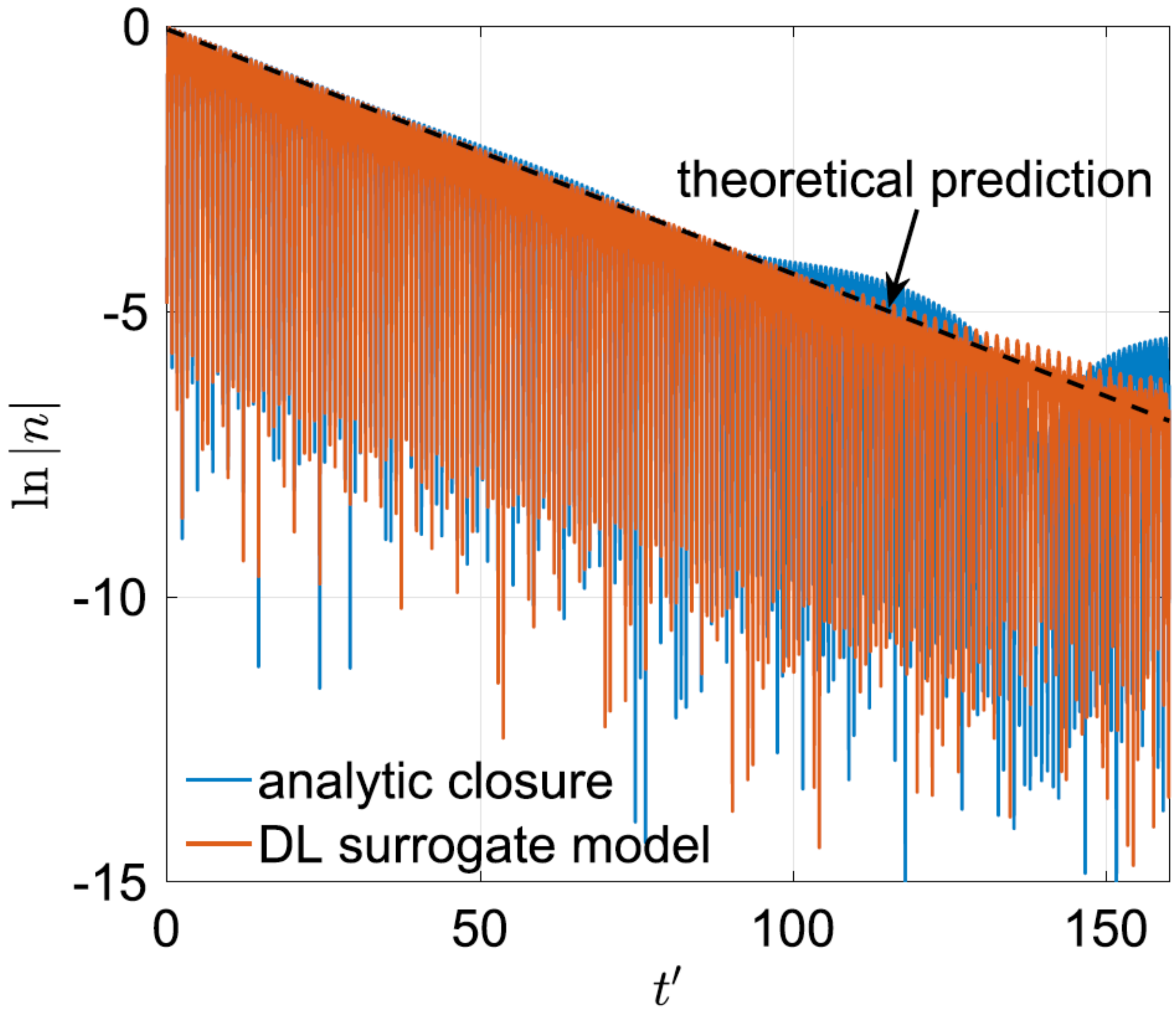
$$\mathrm{MRE} = \frac{1}{n_s N_z} \sum_{i=0}^{n_s-1} \frac{\sum_{j=0}^{N_z-1} |q_{\{\}}[i;j] - q_{kinetic}[i;j]|}{\max(q_{kinetic}[i;:])}$$

N_s=10000, N_z=128, N_{layers}=3, $N_{neuron}=2^{10}$, N_k=7

$k_{\max}$	ν	N_s	MRE for DL	MRE for NF	MRE for NF estimates
4	(0,100)	10^6	0.038%	0.12%	$<$ 0.17%
4	(0,10)	10^6	0.012%	0.12%	$<$ 0.17%
8	(0,100)	10^6	0.062%	0.1%	$<$ 0.15%
8	(0,10)	10^6	0.025%	0.1%	$<$ 0.15%
16	(0,100)	10^6	0.07%	0.13%	$<$ 0.22%
16	(0,10)	10^6	0.025%	0.13%	$<$ 0.22%
8	(0,100)	10^7	0.025%	0.1%	$<$ 0.15%
8	(0,100)	10^7	0.02%(5L)	0.1%	$<$ 0.15%
8	(0,10)	10^7	0.015%	0.1%	$<$ 0.15%
8	(-1,100)	10^7	0.023%	0.1%	$<$ 0.15%
8	(-1,10)	10^7	0.013%	0.1%	$<$ 0.15%

Comparison of fluid simulations between analytical and DL surrogate model closures for collisionless kinetic Langmuir waves

N_s=10000, N_z=128, N_{layers}=3, N_{neuron}=2^{10}, N_k=7



- **For the DL model, there is a concern about the error accumulation problem**
- **Our results show that simulations with the deep learning surrogate model are as good as, if not better than, simulations with the analytic closure in terms of long-term numerical stability in the linear Landau damping test.**

Summary & Discussion

- Appropriate neural networks are capable to calculate Landau fluid closure;

- NN can be implemented in global fluid legacy codes, such as BOUT++ for the LF closure in configuration space

- Training neural network closure with kinetic simulation data:

  Kinetic codes —train→ NN —closure→ BOUT++

- Training more neural network closures for macroscopic fluid simulation codes to capture microdetails, such as
  - turbulence fluxes,
  - Trapped particles
  - …