Deep learning approach for solving kinetic equations

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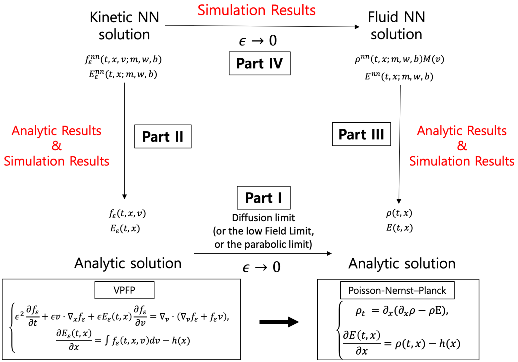
Introduction

Motivation

- The description of physical dynamics in various scales is one of the main questions of interest in the mathematical modeling of complex systems.
- In kinetic theory, the description of the evolution of gases has been explained via the statistical approach on the probabilistic distribution functions on the mesoscopic level, whereas the fluid theory describes the dynamics on the macroscopic level.
- Each of these interpretations and the asymptotic expansions of the mesoscopic equations to the macroscopic equations have been crucial issues.
- We provide a newly-devised numerical method of using a machine learning algorithm for the study of the large-data asymptotic behaviors of the Deep Neural Network (DNN) solutions to the kinetic equation in a bounded domain.

Motivation

- In this work (Lee, Jang, and Hwang, 2021), we establish the commutation of the following diagram of diffusion limit:



The Vlasov-Poisson-Fokker-Planck system

We are interested in the scaling of the system using the change of variables $t' = \varepsilon^2 t$ and $x' = \varepsilon x$ (ε : the ratio of the mean free path of the particles to the typical macroscopic length scale of the particle flow). With these variables, the VPFP system in a bounded interval $\Omega = (-1, 1)$ can be written in the dimensionless form as follows:

$$\begin{aligned} \varepsilon^2 \partial_t f_\varepsilon + \varepsilon v \partial_x f_\varepsilon + \varepsilon E_\varepsilon \partial_v f_\varepsilon &= \partial_v (v f_\varepsilon + \partial_v f_\varepsilon), \quad t \in [0, T],\ x \in \Omega,\ v \in \mathbb{R}, \\ f_\varepsilon(0, x, v) &= f_0(x, v), \\ \partial_x E_\varepsilon &= \int_{\mathbb{R}} f_\varepsilon dv - h(x),\ x \in \Omega, \\ E_\varepsilon(0, -1) &= 0, \\ E_\varepsilon(t, x) &= 0,\ x \in \partial\Omega, \end{aligned} \tag{1}$$

where

- $f_\varepsilon(t, x, v)$: the probabilistic density distribution of particles.
- $E_\varepsilon(t, x)$: the self-consistent electric force.
- $h(x)$: the background charge.

In this work, we consider the VPFP system with the **specular boundary condtion**:

$$f(t, x, v)|_{\gamma_-} = f(t, x, R(x)v), \tag{2}$$

for all $x \in \partial\Omega$, and where $R(x)v \overset{\text{def}}{=} v - 2n_x(n_x \cdot v)$.

The Poisson-Nernst–Planck equation

The PNP system consists of the Nernst-Planck equation that describes the drift and diffusion of ion and the Poisson equation that describes the effect of the self-consistent electric field. In this paper, we consider the following the 1-dimensional Poisson-Nernst-Planck (PNP) system in a bounded interval $\Omega = (-1, 1)$:

$$\begin{aligned} \partial_t \rho &= \partial_x(\partial_x \rho - \rho E), \quad t \in [0, T],\ x \in \Omega, \\ \rho(0, x) &= \rho_0(x), \\ \partial_x E &= \rho(t, x) - h(x),\ x \in \Omega, \\ E(0, -1) &= 0, \\ E(t, x) &= 0,\ x \in \partial\Omega. \end{aligned} \tag{3}$$

where

- $\rho(t, x)$: the density of particles.
- $E_\varepsilon(t, x)$: the self-consistent electric force.
- $h(x)$: the background charge.

In this work, we consider the PNP system with the **no-flux boundary condtion**:

$$(\partial_x \rho - \rho E) \cdot n_x = 0,\ x \in \partial\Omega. \tag{4}$$

Mathematical results on the Fokker-Planck equation

- The existence and the uniqueness of the solutions to the Fokker-Planck equation:
  [Dita, 1985; Protopopescu, 1987; DiPerna and Lions, 1988]
- The existence and the uniqueness of the VPFP system:
  [Victory Jr and O'Dwyer, 1990; Neunzert, Pulvirenti, and Triolo, 1984; Degond, 1986; Jin and Zhu, 2018]
- The asymptotic behavior and the convergence of the solutions to the VPFP system:
  [Carrillo and Toscani, 1998; Carrillo, Soler, and Vázquez, 1996; Carrillo and Soler, 1995]

Part I. On convergence of the VPFP solution to the PNP solution

- Wu, Lin, and Liu (2015) prove that the VPFP system with the Maxwellian reflection boundary condition converges to the PNP system as ε tends to zero for the multi-species model case.
- Using this result, we derive that the solution of our specific VPFP system (1) with the specular boundary condition converge to the solution of the PNP system (3) with the no-flux boundary condition as follows:

$$f_\varepsilon(t,x,v) \to \rho(t,x)M(v) \quad \text{in} \quad L^1(0,T;L^1(\Omega \times \mathbb{R})), \tag{5}$$

where $M(v) = \frac{1}{\sqrt{2\pi}} e^{-\frac{v^2}{2}}$ and

$$E_\varepsilon(t,x) \to E(t,x) \quad \text{in} \quad L^2(0,T;L^p(\Omega)), \quad 1 \leq p < 2 \tag{6}$$

as the Knudsen number ε tends to zero.

An Asymptotic Preserving scheme

- An Asymptotic Preserving (AP) scheme: numerical scheme that preserves the asymptotic limits from the mesoscopic to the macroscopic models [Filbet and Jin, 2010; Jin, 2012]
- In this work, we complete the right diagram of neural network version similar to the left diagram of the numerical analysis version.

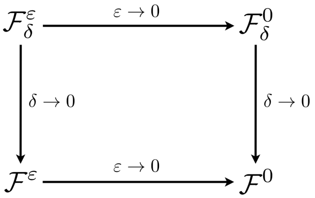


Figure: Illustration of AP schemes (Numerical version)

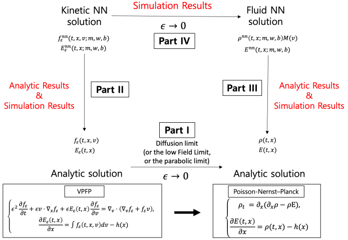


Figure: The diagram of diffusion limit (Neural Network version)

The main results of this work

The main results of this work are as follows.

- (Part II & Part III) We provide the Deep Neural Network solutions to the VPFP system and PNP system using the Deep Learning algorithm.
    - We Provide the theoretical evidence on the convergence of the DNN solutions to the a priori analytic solutions.
    - We analyze our DNN solutions via computing the steady-states for the solutions and via computing the physical quantities of the total mass, the kinetic energy, the entropy, the electric energy and the free energy, and their steady-states.
- (Part IV) We provide the numerical simulation for the trend of the diffusion limit from the DNN solution of the VPFP system to the DNN solution of the PNP system.

Methodology: A Deep Learning Approach

Traditional numerical approaches to the solution of the differential equations.

- Classical finite schemes such as Finite Difference Method, Finite Element Method, and Finite Volume Method can be used to solve the differential equations numerically

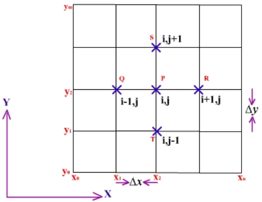


Figure: Finite Difference Method

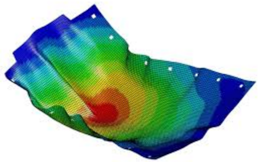
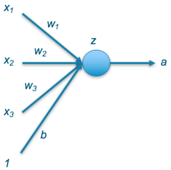


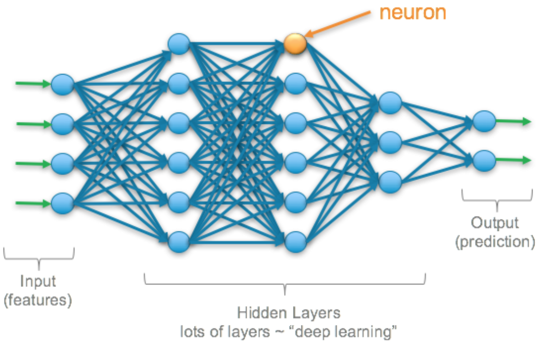
Figure: Finite Element Method

- Difficulties in the numerical methods
  - Construct a specific method to each different problem setups.
  - Need to consider how we split the domains into triangles.

What is a Deep Learning?

- There have been many studies to utilize an Neural Network (NN) to solve Differential Equations from the past.
- A Deep Learning algorithm is a non-linear function approximation method using a Deep Neural Network(DNN) structure.





Deep Neural Network method

Physics informed neural network (PINN) is proposed by Raissi, Perdikaris, and Karniadakis (2019).

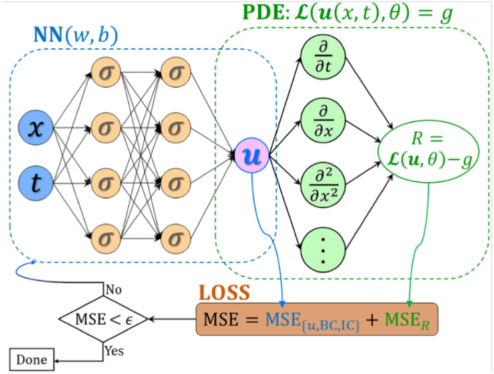


Figure: Physics informed neural network framework (Lu et al., 2019)

Deep Neural Network method

We take two different neural network structures which share the same inputs to approximate the coupled nonlinear VPFP system.

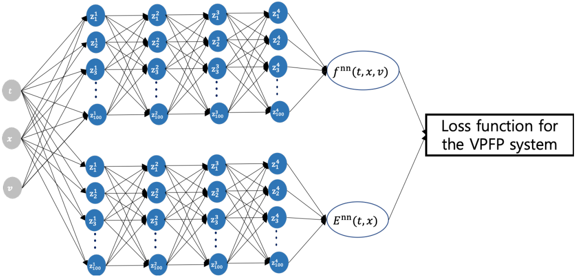


Figure: The DNN structure for the VPFP system

- Activation function $\bar{\sigma}$: hyper-tangent activation function ($\bar{\sigma}(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$)
- Optimizer: Adam (Adaptive Moment Estimation) optimizer)

Grid points

To approximate the kinetic solution $f(t, x, v)$ via the Deep Learning algorithm, we make the data of grid points for each variable domain.

- Grid points for training $f_\varepsilon^{nn}(t, x, v; m, w, b)$ are chosen randomly as follows:

$$\{(t_i, x_j, v_k)\}_{i,j,k} \in [0, T] \times \Omega \times V \tag{7}$$

for the governing equation,

$$\{(t = 0, x_j, v_k)\}_{j,k} \in \Omega \times V \tag{8}$$

for the initial condition and

$$\{(t_i, x = -1 \text{ or } 1, v_k)\}_{i,k} \in [0, T] \times V \tag{9}$$

for the boundary condition with $T = 1$ or $T = 5$, $\Omega = [-1, 1]$ and $V = [-10, 10]$ (truncation the velocity domain).

Loss functions for the VPFP system

- Loss function for the governing eqautions:

$$Loss^{fp}_{GE(1)}(f^{nn}) \stackrel{\text{def}}{=} \int_{(0,T)} dt \int_{(-1,1)} dx \int_V dv |\partial_t f^{nn}(t,x,v;m,w,b) + v\partial_x f^{nn}(t,x,v;m,w,b) + E^{nn}\partial_v f^{nn} - (\partial_{vv} f^{nn}(t,x,v;m,w,b) + \partial_v(vf^{nn})(t,x,v;m,w,b))|^2, \quad (10)$$

and

$$Loss^{fp}_{GE(2)}(f^{nn}) \stackrel{\text{def}}{=} \int_{(0,T)} dt \int_{(-1,1)} dx |\partial_x E^{nn}(t,x;m,w,b) - \int_V dv\ f^{nn}(t,x,v;m,w,b)|^2, \quad (11)$$

- Loss function for the initial condtions:

$$Loss^{fp}_{IC(1)}(f^{nn}) \stackrel{\text{def}}{=} \int_{(-1,1)} dx \int_V dv \left| f^{nn}(0,x,v) - f_0(x,v) \right|^2, \quad (12)$$

and

$$Loss^{fp}_{IC(2)}(f^{nn}) \stackrel{\text{def}}{=} \int_{(-1,1)} dx \left| E^{nn}(0,x;m,w,b) - \left(\int_{-1}^{x} dy \int_{\mathbb{R}} dv f_0(y,v) - (x+1) \right) \right|^2. \quad (13)$$

Loss functions for the VPFP system

- Loss function for the *specular* boundary condition for f and the Dirichlet boundary condition for E:

$$Loss^{fp}_{BC(1)}(f^{nn}) \stackrel{\text{def}}{=} \int_{(0,T)} dt \int_{\gamma_-} dxdv \left| f^{nn}(t,x,v;m,w,b) - f^{nn}(t,x,-v;m,w,b) \right|^2, \quad (14)$$

and

$$Loss^{fp}_{BC(2)}(f^{nn}) \stackrel{\text{def}}{=} \int_{(0,T)} dt \sum_{x\in\{-1,1\}} \left| E^{nn}(t,x;m,w,b) \right|^2. \quad (15)$$

- Finally, we define the total loss as

$$Loss^{fp}_{Total}(f^{nn}) \stackrel{\text{def}}{=} Loss^{fp}_{GE} + Loss^{fp}_{IC} + Loss^{fp}_{BC}. \quad (16)$$

* We compute these loss functions via the approximation of the integration by the Riemann sum on the grid points.
* We define the loss functions for the PNP system similarly.

Deep Learning algorithm for the VPFP system

Finally, we summarize our Deep Learning algorithm for the VPFP system as follows:

Algorithm 1 Deep Learning algorithm for the VPFP system

```
for number of epochs do
    Sampling data:
        Sample m samples t_1, t_2, ..., t_m from [0,1] (or [0,5]).
        Sample n samples x_1, x_2, ..., x_n from [-1,1].
        Sample p samples v_1, v_2, ..., v_p from [-10,10].
        Make a pair the samples to set the training data as (7), (8) and (9).
        Add new top-k training data paired with the velocity samples.
    Evaluate the loss function:
        Approximate the derivative of the DNN output (Autograd).
        Approximate the integration of the DNN output (Trapezoidal rule).
        Evaluate the loss function for the VPFP system (16).
    Updating parameters:
        Update neural network parameters using the Adam optimizer:

            w ← w^new,
            b ← b^new,

        in the direction of minimizing the pre-defined loss function.
end for
```

Theoretical results and neural network simulations

Theoretical results

- We first prove that there exists a sequence of neural network parameters (neuron numbers m, weights w and biases b) such that the total loss function $Loss_{Total}^{fp}$ converges to 0.

Theorem (Theorem 3.4 of Hwang et al., 2020)

Assume that the number of layers $L = 2$ and that the solution f to (1) with (2) which belongs to $\widehat{C}^{(1,1,2)}([0,T] \times [-1,1] \times V)$, and the activation function $\bar{\sigma}(x) \in C^{(2,2,3)}([0,T] \times [-1,1] \times V)$ is non-polynomial. Then, there exists $\{m_{[j]}, w_{[j]}, b_{[j]}\}_{j=1}^{\infty}$ such that a sequence of the DNN solutions f^{nn} with $m_{[j]}$ nodes, denoted by

$$\{f_j(t,x,v) = f^{nn}(t,x,v; m_{[j]}, w_{[j]}, b_{[j]})\}_{j=1}^{\infty}$$

satisfies

$$Loss_{Total}^{fp}(f_j) \to 0 \text{ as } j \to \infty. \tag{17}$$

Theoretical results

- Second, we also prove that if we minimize the total loss function $Loss^{fp}_{Total}$, it implies that the Deep Neural Network solution converges to an analytic solution.
- We assume that our compact domain $V = [-10, 10]$ of the v-variable is chosen sufficiently large so that we can have

$$||f||_{L^1_x([-1,1];L^1_v(\mathbb{R}\setminus V))} \leq \epsilon \text{ and } \left|\partial^k_v f(t,x,v) - \partial^k_v f^{nn}(t,x,v)\right|_{v\in\partial V} \leq \epsilon, \qquad (18)$$

for some sufficiently small $\epsilon > 0$ and $k = 0, 1$.

Theorem

Assume that f is a solution to (1) with (2) which belongs to $\widehat{C}^{(1,1,2)}([0,T]\times[-1,1]\times V)$. If the solution f and the Deep Neural Network solution $f^{nn}(t,x,v;m,w,b)$ satisfy (18), then it implies that

$$\|f^{nn}(\cdot,\cdot,\cdot;m,w,b) - f\|_{L^\infty_t([0,T];L^2_{x,v}([-1,1]\times V))} \leq C(Loss^{fp}_{Total}(f^{nn}) + \epsilon), \qquad (19)$$

where C is a positive constant depending only on T.

Neural network simulations for the VPFP system

The entropy of the system "Ent", the total kinetic energy "KE", and the electric potential energy "EE" of the system are defined as

$$\mathrm{Ent}(t) \stackrel{\mathrm{def}}{=} -\int_{\Omega\times\mathbb{R}} f_\varepsilon \log f_\varepsilon \, dxdv, \tag{20}$$

$$\mathrm{KE}(t) \stackrel{\mathrm{def}}{=} \frac{1}{2}\int_{\Omega\times\mathbb{R}} |v|^2 f_\varepsilon \, dxdv, \tag{21}$$

and

$$\mathrm{EE}(t) \stackrel{\mathrm{def}}{=} \frac{1}{2}\int_{\Omega} |E_\varepsilon|^2 dx. \tag{22}$$

The Lyapunov functional is also called the free energy defined as

$$\mathrm{FE}(t) \stackrel{\mathrm{def}}{=} -\mathrm{Ent}(t) + \mathrm{KE}(t) + \mathrm{EE}(t). \tag{23}$$

We expect that the free energy (23) is a non-increasing function.

Neural network simulations for the VPFP system

It is well-known that the the VPFP system (1) with the specular boundary condition has the global equilibrium state $(f_{\varepsilon,\infty}, E_{\varepsilon,\infty})$ as

$$f_{\varepsilon,\infty}(x,v) = \frac{\|f_0(\cdot,\cdot)\|_{L^1_{x,v}}}{|\Omega|} M(v), \quad E_{\varepsilon,\infty}(x) = -\partial_x \Phi_\infty(x) = 0, \tag{24}$$

where $M(v) \overset{\text{def}}{=} \frac{1}{\sqrt{2\pi}} e^{-\frac{v^2}{2}}$ is the normalized Maxwellian and $|\Omega| = 2$ in our case. We consider the following initial condition :

$$f(0,x,v) = f_0(x,v) = \begin{cases} e^{x-1}\left(1 - \cos(\frac{\pi}{2} v)\right), & \text{if } v \in (-4,4), \\ 0, & \text{otherwise,} \end{cases} \tag{25}$$

We expect that the neural network solutions of the VPFP system reach the steady-state.

Neural network simulations for the VPFP system

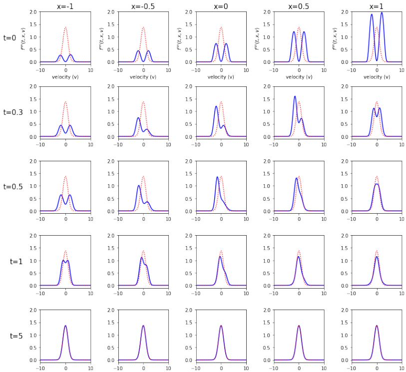


Figure: The pointwise values of $f^{nn}(t,x,v;m,w,b)$ as time t varies at each position x's. $x=-1,-0.5,0,0.5,1$ are the points to explain the convergence to the global Maxwellian $\frac{\|f_0(\cdot,\cdot)\|_{L^1_{x,v}}}{|\Omega|}M(v)$. The steady-state (global Maxwellian) is given via the red-dotted lines.

Neural network simulations for the VPFP system

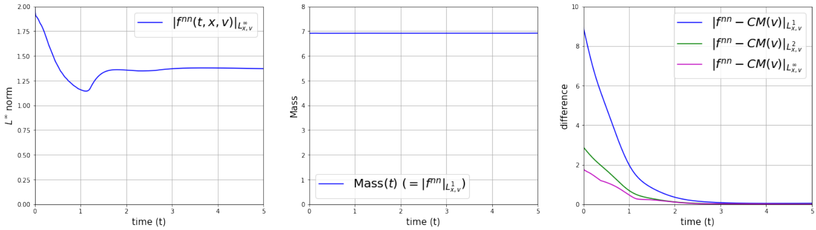


Figure: The time-asymptotic behaviors of the L^∞ norm, L^1 norm of $f^{nn}(t,x,v;m,w,b)$ (the first and the second plot) and the L^1 norm, L^2 norm, and L^∞ norm of the difference between $f^{nn}(t,x,v;m,w,b)$ and the global Maxwellian $\frac{\|f_0(\cdot,\cdot)\|_{L^1_{x,v}}}{|\Omega|}M(v)$.

- It is notable that the total mass $Mass(t)$ of the distribution $f^{nn}(t,x,v;m,w,b)$ is conserved over time in the second plot.
- Also, note that the third plot shows that the distribution $f^{nn}(t,x,v;m,w,b)$ converges to the global Maxwellian.

Neural network simulations for the VPFP system

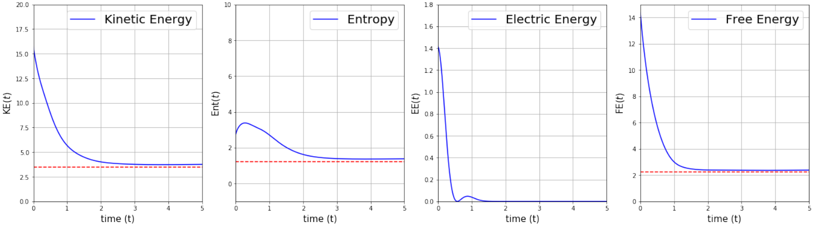


Figure: The time-asymptotic behaviors of the macroscopic quantities of $f^{nn}(t, x, v; m, w, b)$ and $E^{nn}(t, x; m, w, b)$. The steady-state values of the kinetic energy, the entropy, the free energy are indicated in the red-dotted lines.

- Note that the free energy is monotonically decreasing.

Neural network simulations for the diffusion limit

- We consider the convergence of the VPFP solutions to the PNP solution.
- We expect that the neural network solutions of the VPFP system and the PNP system have the trend of diffusion limit as explained in the equations (5) and (6).
- To observe the trend of the convergence, we compare the neural network solutions to the VPFP system with the Knudsen numbers $\varepsilon = 1, 0.5, 0.2, 0.1, 0.05$ and the corresponding neural network solutions to the PNP system.

It is worth noting that we do not change the number of the grid points for the VPFP system with any Knudsen numbers, i.e., we analyze the diffusion limit in the sense of the Asymptotic-Preserving (AP) scheme.

Neural network simulations for the diffusion limit

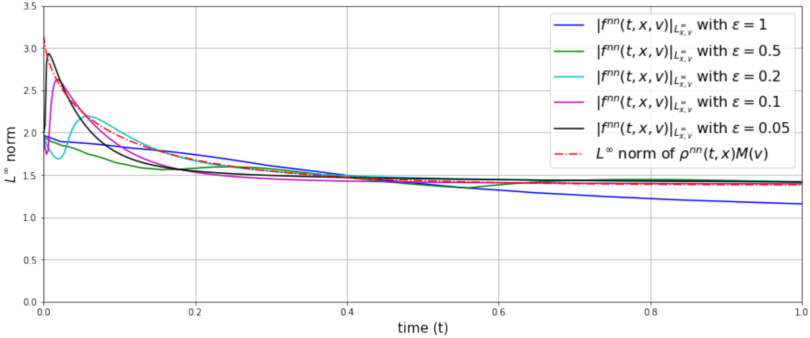


Figure: The time-asymptotic behavior of the $L^\infty_{x,v}$ norm of $f^{nn}_\varepsilon(t,x,v;m,w,b)$ and $\rho^{nn}(t,x;m,w,b)M(v)$ over time t as the Knudsen number ε varies. Each value is drawn in different colors as shown in the legend.

- We can observe that the L^∞ norm of the solution $f^{nn}_\varepsilon(t,x,v;m,w,b)$ converges pointwisely to the L^∞ norm of the $\rho^{nn}(t,x;m,w,b)M(v)$ as the Knudsen number ε becomes close to zero.

Neural network simulations for the diffusion limit

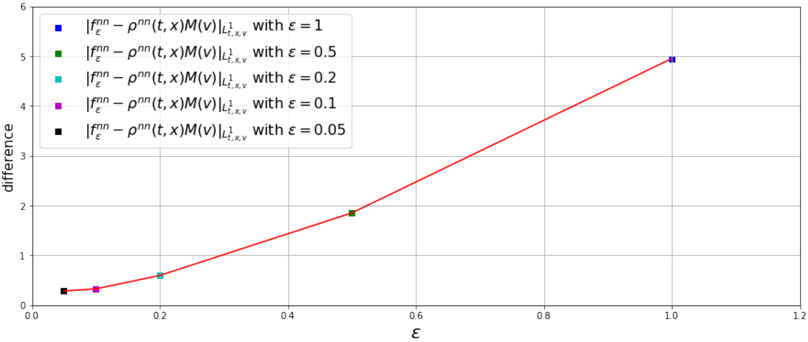


Figure: The values of $L^1_{t,x,v}$ norm of the difference between $f_\varepsilon^{nn}(t,x,v;m,w,b)$ and $\rho^{nn}(t,x;m,w,b)M(v)$ as ε varies.

- The graph shows that the $L^1_{t,x,v}$ norm of the difference between f_ε^{nn} and $\rho^{nn}M$ becomes smaller as the Knudsen number ε tends to zero.

Extend to FPL equation

Extend to Fokker-Planck-Landau equation (Lee, Jang, and Hwang, 2022)

Using the additional operator learning method to approximate the homogeneous Fokker-Planck-Landau (FPL) equation

$$\partial_t f(t,v) = \nabla_v \cdot (D(f)\nabla f - F(f)f)$$

with the complex integral terms $D(f)$ and $F(f)$.

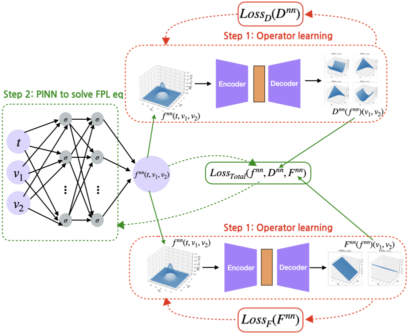


Figure: Overview of the proposed framework to approximate the solution to the FPL equation.

Extend to Fokker-Planck-Landau equation (Lee, Jang, and Hwang, 2022)

Using the additional operator learning method to approximate the homogeneous Fokker-Planck-Landau (FPL) equation

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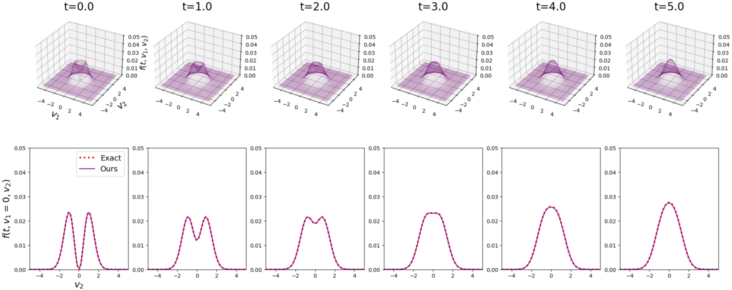

Figure: The pointwise values of $f^{nn}(t, v_1, v_2; m, w, b)$ as t varies for BKW initial condition. Note that the upper row shows the 3-d plots of the distribution $f(t, v_1, v_2)$ and the lower row shows its cross section with $v_1 = 0$ for visualization purposes. The exact values of the BKW solution are given via the red-dotted lines.

Conclusion

Conclusion

- We establish the commutation of the neural network version diagram of diffusion limit.
- To this end, we have introduced the Deep Neural Network (DNN) solutions to the VPFP system and the PNP system using the Deep Learning algorithm.
- We also provide the theoretical supports on which the approximated DNN solutions converge to analytic solutions of each system as the proposed total loss function tends to zero.
- We compare the neural network simulation results to existing analytic results and predict the long-time behavior of the solutions.
- We extend the Deep learning method to the FPL equation using the operator learning method.

Future direction

- Approximate the solutions of more general ordinary and partial differential equations (Full Boltzmann equation).
- Extend to special domains of high dimensional equations using randomly sampled points.
- Use more complicated neural network architectures such as CNN, RNN.

Thank You

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