An investigation on the structure-preserving deep learning methods for solving the radiative transfer equations

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Joint work with Honyan Li, Song Jiang, Wenjun Sun and Guanyu Zhou

Outline

- Structure-preserving schemes
- Radiative transfer equations(RTEs)
- Asymptotic-preserving neural networks(APNNs)
- Model-data asymptotic-preserving neural networks(MD-APNNs) for gray radiative transfer equations(GRTEs)
- Macroscopic auxiliary asymptotic-preserving neural networks (MA-APNNs) for linear radiative transfer equations(LRTEs)
- Summary and future work

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Structure-preserving schemes

- Conservative hyperbolic PDE

$$\frac{\partial U(\boldsymbol{x})}{\partial t} + \nabla \cdot F(U) = 0,\ \boldsymbol{x} = (t, x_1, x_2, ...) \in \Omega.$$

- Structure-preserving schemes
  - Accuracy, Stability, Conservation
  - Maximal-principle-preserving schemes/Entropy-preserving schemes (Hyperbolic equations)
  - Positivity-preserving schemes (Compressible fulid dynamic equations)
  - Well-balanced schemes (Shallow water wave equations)
  - Divergence-free schemes (MHD, Navier-Stokes equations)
  - Asymptotic-preserving schemes (Kinetic equations, e.g. transport equations, Boltzmann-BGK equations)

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Radiative transfer equations(RTEs)

- Gray radiative transfer equations(GRTEs) are a kind of kinetic model coupled with nonlinear material thermal energy equation. Omitting the scattering terms and the internal source, the scaled form is

$$
\begin{cases}
\dfrac{\epsilon^2}{c}\dfrac{\partial I}{\partial t} + \epsilon\Omega\cdot\nabla_r I = \sigma\left(\dfrac{1}{4\pi}acT^4 - I\right), & (t,r,\Omega)\in\tau\times D\times S^2, \quad (1a)\\
\epsilon^2 C_v \dfrac{\partial T}{\partial t} = \sigma\left(\displaystyle\int_{S^2} I\mathrm{d}\Omega - acT^4\right), & (t,r)\in\tau\times D, \quad (1b)\\
B_{ou}I = I_\Gamma(t,r,\Omega), & (t,r,\Omega)\in\Gamma, \quad (1c)\\
I_{in}I = I_0(r,\Omega), & (t,r,\Omega)\in\{0\}\times D\times S^2, \quad (1d)\\
I_{in}T = T_0(r), & (t,r)\in\{0\}\times D, \quad (1e)
\end{cases}
$$

where $I(t,r,\Omega)$ denotes the radiation intensity, $T(t,r)$ the material temperature, $r=(x,y,z)$ the spatial position variable, t the time variable, $\Omega=(\xi,\eta,\mu)$ the angular direction on the unit sphere S^2 along which the photons propagate , C_v the heat capacity, $\sigma(r,T)$ the opacity, $\epsilon>0$ the scale parameter, a the radiation constant, c the speed of light, B_{ou} the boundary operator, I_{in} the initial operator and I_Γ, I_0, T_0 are given functions.

Radiative transfer equations

- When the material temperature T is the same as the radiation temperature T_r $\left(\int_{S^2} I \mathrm{d}\Omega = acT_r^4\right)$, the gray radiative transfer equation becomes the scaled linear radiative transfer equation

$$\frac{\epsilon^2}{c}\frac{\partial I}{\partial t} + \epsilon\Omega \cdot \nabla_r I = \sigma\left(\frac{1}{4\pi}\int_{S^2} I \mathrm{d}\Omega - I\right). \tag{2}$$

- Application fields: weapon physics, astrophysics, inertial/magnetic confinement fusion, high-temperature flow systems,...
- Challenges of numerical simulation for RTEs
  - High dimensionality
  - Multi-scale characteristics

    $\epsilon = O(1)$: transport regime $\rightarrow \epsilon \ll 1$: diffusion regime
  - Strongly coupled nonlinearity for GRTEs

Radiative transfer equations

- Classical numerical methods for radiative transfer equations
  - Stochastic methods (No ray effect but suffers from statistical noise, deal with high-dimensionality) (e.g. Implicit Monte Carlo(IMC) Method) Fleck Jr et al. 1971, Gentile 2001, McClarren et al. 2009, Densmore 2011, Shi et al. 2018, 2020.
  - Deterministic methods(e.g. FDM/FEM/FVM/DG) with the asymptotic-preserving(AP) technique (deal with multiscale features)

    ▶ Diffusive relaxation schemes for multiscale transport equations Jin et al. 2000, AP schemes for multiscale kinetic and hyperbolic equations Jin et al. 1999, 2012, AP scheme based on micro-macro formulation for linear kinetic equations Lemou et al. 2008, On the diffusive limits of radiative heat transfer system Ghattassi et al. 2022, Diffusive limits of the steady state radiative heat transfer system Ghattassi et al. 2023, ...

    ▶ Asymptotic-preserving(AP) schemes for GRTEs

    AP UGKS for GRTEs Sun et al. 2015, AP angular finite element based UGKS for GRTEs Xu et al. 2020, AP filtered PN method for GRTEs Xu et al. 2021, AP discontinuous Galerkin method for GRTEs Xiong et al. 2022, AP IMEX method for GRTEs Fu et al. 2022.

Radiative transfer equations

- Deep learning methods for radiative transfer equations
  - ▶ PINNs for steady and time-dependent LRTEs Lu et al. 2022, Mishra et al. 2021, Chen et al. 2022, Liu et al. arXiv:2102.12048.
  - ▶ Model-operator-data network(MOD-Net) for RTEs and nonlinear PDEs Zhang et al. 2022, Physics-informed DeepONets(PIDONs) Wang et al. 2021.
  - ▶ Asymptotic-preserving neural networks for multiscale kinetic equations Jin et al. 2023, Jin et al. arXiv:2306.15381, Asymptotic-preserving convolutional deep operator networks(APCONs) for LRTEs Wu et al. arXiv:2306.15891.
  - ▶ Machine learning moment closure models for radiative transfer Huang et al. 2022, 2023.
  - ▶ Element learning to radiative transfer: a systematic approach of accelerating finite element-type methods via machine learning Du et al. arXiv:2308.02467.

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The framework of deep neural networks

- Given an input $\boldsymbol{x} = (t, r, \Omega) \in \tau \times D \times S^2$, the L-layer deep feedforward neural network f_θ is

$$
\begin{aligned}
&f_\theta^{[0]}(\boldsymbol{x}) = \boldsymbol{x}, \\
&f_\theta^{[l]}(\boldsymbol{x}) = \boldsymbol{h} \circ \left(W^{[l-1]} f_\theta^{[l-1]}(\boldsymbol{x}) + b^{[l-1]} \right), \quad 1 \leq l \leq L-1, \\
&f_\theta(\boldsymbol{x}) = f_\theta^{[L]}(\boldsymbol{x}) = W^{[L-1]} f_\theta^{[L-1]}(\boldsymbol{x}) + b^{[L-1]},
\end{aligned}
\tag{3}
$$

$\theta = \left(W^{[l]}, b^{[l]}\right)$, $W^{[l]} \in R^{m_{l+1} \times m_l}$: weight matrix, $b^{[l]} \in R^{m_{l+1}}$: bias term, $''\circ''$: entry-wise operation, $\boldsymbol{h}$: nonlinear activation function of the hidden layers.

- Solving PDE model with DNN methods
  - Neural network parameterization of solutions(e.g. $f_\theta(\boldsymbol{x}) \rightarrow I(\boldsymbol{x})$)
  - Construction of the loss functions(e.g. $L = \|f_\theta(\boldsymbol{x_i}) - I(\boldsymbol{x}_i)\|_{L^2}^2$)
  - Optimization of the loss functions(e.g. Adam, LBFGS,...)

Asymptotic-preserving neural networks(APNNs)

- Definition of APNNs [Jin et al. 2023]

$$
\begin{tikzcd}
\mathcal{R}(\mathcal{F}^{\varepsilon}) \arrow[rr, "\varepsilon \to 0"] \arrow[d, "\mathcal{R} \to 0"] & & \mathcal{R}(\mathcal{F}^{0}) \arrow[d, "\mathcal{R} \to 0"] \\
\mathcal{F}^{\varepsilon} \arrow[rr, "\varepsilon \to 0"] & & \mathcal{F}^{0}
\end{tikzcd}
$$

Figure 1. Illustration of APNNs.

$\mathcal{F}^{\epsilon}$: the microscopic equation that depends on ϵ

$\mathcal{F}^{0}$: the macroscopic limit as $\epsilon \to 0$ which is independent of ϵ

$\mathcal{R}(\mathcal{F}^{\epsilon})$: the measure(e.g. loss) of $\mathcal{F}^{\epsilon}$ whose solution is approximated by neural network

$\mathcal{R}(\mathcal{F}^{0})$: the asymptotic limit of $\mathcal{R}(\mathcal{F}^{\epsilon})$ as $\epsilon \to 0$

- If $\mathcal{R}(\mathcal{F}^{0})$ is a good measure of $\mathcal{F}^{0}$, the measure(e.g. loss) $\mathcal{R}(\mathcal{F}^{\epsilon})$ is called asymptotic-preserving(AP).

Importance of the AP property in APNNs

- Multiscale one dimensional linear radiative transfer equation($c = 1$)

$$\mathcal{F}^{\epsilon}: \begin{cases} \epsilon^2 \partial_t I + \epsilon \mu \partial_x I = \sigma \left(\frac{1}{2} \int_{-1}^{1} I \mathrm{d}\mu - I \right), (t, x, \mu) \in [0, T] \times [0, 1] \times [-1, 1], \\ I_L(\mu > 0) = 1, \; I_R(\mu < 0) = 0, \; I_0 = 0. \end{cases}$$

- When the scale parameter is tiny($\epsilon \to 0$), the correct limit equation is

$$\mathcal{F}^0 : \partial_t \rho - \frac{1}{3} \partial_x \left(\frac{1}{\sigma} \partial_x \rho \right) = 0, \quad \rho = \frac{1}{2} \int_{-1}^{1} I \mathrm{d}\mu$$

- NNs without AP property(e.g. PINNs) tend to learn the wrong limit

$$\mathcal{R}(\mathcal{F}^0) : \sigma(\rho - I) = 0,$$

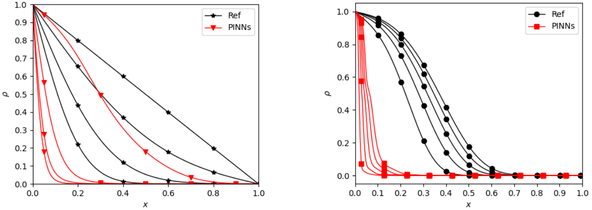

Figure 2. (Left) $T = 2, \sigma = 1, \epsilon = 10^{-8}$. The density ρ at times $t = 0.04, 0.1, 0.3, 2.0$. (Right) $T = 1, \sigma = 1 + (10x)^2, \epsilon = 10^{-3}$. The density ρ at times $t = 0.2, 0.4, 0.6, 0.8, 1.0$.

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Gray radiative transfer equations(GRTEs)

- Consider GRTEs Eq.(1a)(1b),

$$\begin{cases} \frac{\epsilon^2}{c}\frac{\partial I}{\partial t} + \epsilon\Omega \cdot \nabla_r I = \sigma\left(\frac{1}{4\pi}acT^4 - I\right), (t, r, \Omega) \in \tau \times D \times S^2, \\ \epsilon^2 C_v \frac{\partial T}{\partial t} = \sigma\left(\int_{S^2} I \mathrm{d}\Omega - acT^4\right), (t, r) \in \tau \times D. \end{cases}$$

- As the parameter $\epsilon \to 0$, away from boundaries and initial times, the radiation intensity $I(t, r, \Omega)$ approaches to a Planck function at the local temperature, i.e.,

$$I = \frac{1}{4\pi}acT^4,$$

and the local temperature T satisfies the nonlinear diffusion equation

$$\frac{\partial}{\partial t}(C_v T) + a\frac{\partial}{\partial t}(T)^4 = \nabla \cdot \frac{ac}{3\sigma}\nabla (T)^4 . \tag{4}$$

PINNs fail to resolve GRTEs with small scales

- Approximate radiation intensity $I(t, r, \Omega)$ and material temperature $T(t, r)$ by the neural networks $I^{nn}_{\theta_1}(t, r, \Omega)$ and $T^{nn}_{\theta_2}(t, r)$, respectively.
- The PINNs loss function of the original GRTEs Eq.(1) is constructed as the least square of the residuals.

$$
\begin{aligned}
L^{\epsilon}_{\text{PINNs,ge}} = & \left\| \frac{\epsilon^2}{c} \partial_t I^{nn}_{\theta_1} + \epsilon \Omega \cdot \nabla_r I^{nn}_{\theta_1} - \sigma \left(\frac{1}{4\pi} ac (T^{nn}_{\theta_2})^4 - I^{nn}_{\theta_1} \right) \right\|^2_{L^2(K)} \\
& + \left\| \epsilon^2 C_v \partial_t T^{nn}_{\theta_2} - \sigma \left(\int_{S^2} I^{nn}_{\theta_1} \mathrm{d}\Omega - ac (T^{nn}_{\theta_2})^4 \right) \right\|^2_{L^2(\tau \times D)} .
\end{aligned}
$$

Take $\epsilon \to 0$

$$
L^{\epsilon}_{\text{PINNs,ge}} \to \left\| \sigma \left(\frac{1}{4\pi} ac (T^{nn}_{\theta_2})^4 - I^{nn}_{\theta_1} \right) \right\|^2_{L^2(K)} + \left\| \sigma \left(\int_{S^2} I^{nn}_{\theta_1} \mathrm{d}\Omega - ac (T^{nn}_{\theta_2})^4 \right) \right\|^2_{L^2(\tau \times D)} .
$$

The limit is not the loss function of the desired diffusion limit equation (4), PINNs will fail when ϵ is sufficiently small.

Micro-macro decomposition

- Denote by $\langle I \rangle = \frac{1}{4\pi}\int_{S^2} I(t,r,\Omega)\mathrm{d}\Omega$ the integral average of I over the angular variable Ω, and make decomposition of the radiation intensity[Xiong et al. 2022]

$$I(t,r,\Omega) = \rho(t,r) + \frac{\epsilon}{\sqrt{\sigma_0}} g(t,r,\Omega),$$

where the macroscopic quantity $\rho = \langle I \rangle$, the microscopic perturbation g satisfies $\langle g \rangle = 0$ and $\sigma_0 > 0$ is a constant defined as a referred opacity.

- Integrate Eq.(1a) over the angular direction Ω and subtract it from Eq.(1a), together with Eq.(1b), we get the micro-macro coupled system

$$\begin{cases} \frac{1}{c}\partial_t \rho + \frac{1}{\sqrt{\sigma_0}} \langle \Omega \cdot \nabla_r g \rangle = -\frac{1}{4\pi} C_v \partial_t T, & \text{(5a)} \\ \frac{\epsilon^2}{c}\partial_t g + \epsilon \Omega \cdot \nabla_r g - \epsilon \langle \Omega \cdot \nabla_r g \rangle + \sqrt{\sigma_0}\Omega \cdot \nabla_r \rho + \sigma g = 0, & \text{(5b)} \\ \epsilon^2 C_v \partial_t T = \sigma \left(4\pi\rho - acT^4\right). & \text{(5c)} \end{cases}$$

The micro-macro decomposition based APNNs method

- Apply PINNs to solve the micro-macro decomposition system Eq.(5). Perform the neural network approximation

$$g_{\theta_1}^{nn}(t, r, \Omega) \approx g(t, r, \Omega),$$
$$\rho T_{\theta_2}^{nn}(t, r) = (\rho_{\theta_{21}}^{nn}(t, r), T_{\theta_{22}}^{nn}(t, r)) \approx (\rho(t, r), T(t, r))$$

Choose the appropriate activation function $\boldsymbol{h}^o(X)$ at the output layer of $\rho T_{\theta_2}^{nn}$ to guarantee the nonnegativity of ρ and T.

- Design the APNNs loss $L_{\text{APNNs}}^{\epsilon}$

$$L_{\text{APNNs}}^{\epsilon} = L_{\text{APNNs,ge}}^{\epsilon} + L_{\text{APNNs,i}}^{\epsilon} + L_{\text{APNNs,b}}^{\epsilon} + L_{\text{APNNs,c}}^{\epsilon}. \tag{6}$$

The loss for the conservative laws

$$L_{\text{APNNs,c}}^{\epsilon} = \lambda_3 \| \left\langle g_{\theta_1}^{nn} \right\rangle \|_{L^2(\tau \times D)}^2.$$

The micro-macro decomposition based APNNs method

The loss for the micro-macro governing equation

$$
\begin{aligned}
L^{\epsilon}_{\text{APNNs,ge}} = & \left\| \frac{\epsilon^2}{c} \partial_t g^{nn}_{\theta_1} + \epsilon \Omega \cdot \nabla_r g^{nn}_{\theta_1} - \epsilon \left\langle \Omega \cdot \nabla_r g^{nn}_{\theta_1} \right\rangle + \sqrt{\sigma_0} \Omega \cdot \nabla_r \rho^{nn}_{\theta_{21}} + \sigma g^{nn}_{\theta_1} \right\|^2_{L^2(K)} \\
& + \left\| \frac{1}{c} \partial_t \rho^{nn}_{\theta_{21}} + \frac{1}{\sqrt{\sigma_0}} \left\langle \Omega \cdot \nabla_r g^{nn}_{\theta_1} \right\rangle + \frac{1}{4\pi} C_v \partial_t T^{nn}_{\theta_{22}} \right\|^2_{L^2(\tau \times D)} \\
& + \left\| \epsilon^2 C_v \partial_t T^{nn}_{\theta_{22}} - \sigma \left(4\pi \rho^{nn}_{\theta_{21}} - ac (T^{nn}_{\theta_{22}})^4 \right) \right\|^2_{L^2(\tau \times D)} .
\end{aligned}
$$

The loss for the boundary conditions

$$
L^{\epsilon}_{\text{APNNs,b}} = \lambda_1 \left\| B_{ou} \left(\rho^{nn}_{\theta_{21}} + \frac{\epsilon}{\sqrt{\sigma_0}} g^{nn}_{\theta_1} \right) - I_\Gamma \right\|^2_{L^2(\Gamma)} .
$$

The loss for the initial values

$$
L^{\epsilon}_{\text{APNNs,i}} = \lambda_2 \left(\left\| I_{in} \left(\rho^{nn}_{\theta_{21}} + \frac{\epsilon}{\sqrt{\sigma_0}} g^{nn}_{\theta_1} \right) - I_0 \right\|^2_{L^2(D \times S^2)} + \left\| I_{in} T^{nn}_{\theta_{22}} - T_0 \right\|^2_{L^2(D)} \right) .
$$

Analyse the asymptotic-preserving(AP) property

As $\epsilon \to 0$,

$$
\begin{aligned}
L^{\epsilon}_{\text{APNNs,ge}} \to & \left\| \sqrt{\sigma_0}\Omega \cdot \nabla_r \rho^{nn}_{\theta_{21}} + \sigma g^{nn}_{\theta_1} \right\|^2_{L^2(K)} \\
& + \left\| \frac{1}{c}\partial_t \rho^{nn}_{\theta_{21}} + \frac{1}{\sqrt{\sigma_0}} \langle \Omega \cdot \nabla_r g^{nn}_{\theta_1} \rangle + \frac{1}{4\pi} C_v \partial_t T^{nn}_{\theta_{22}} \right\|^2_{L^2(\tau \times D)} \\
& + \left\| \sigma \left(4\pi \rho^{nn}_{\theta_{21}} - ac (T^{nn}_{\theta_{22}})^4 \right) \right\|^2_{L^2(\tau \times D)} \equiv L_{\text{APNNs,ge}},
\end{aligned}
$$

which can be regarded as the PINN loss of the following system

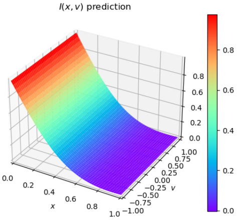
$$
\begin{cases}
\sqrt{\sigma_0}\Omega \cdot \nabla_r \rho + \sigma g = 0, & \text{(7a)} \\
\frac{1}{c}\partial_t \rho + \frac{1}{\sqrt{\sigma_0}} \langle \Omega \cdot \nabla_r g \rangle + \frac{1}{4\pi} C_v \partial_t T = 0, & \text{(7b)} \\
\sigma \left(4\pi \rho - ac T^4 \right) = 0. & \text{(7c)}
\end{cases}
$$

Applying Eqs.(7a) and (7c) into Eq.(7b), the desired diffusion limit equation Eq.(4) is obtained. That means the loss function $L^{\epsilon}_{\text{APNNs}}$ is asymptotic-preserving.

The stationary nonlinear GRTEs

- We compare the performance between PINNs and APNNs for the 1D steady nonlinear radiative transfer equation with $a = c = \sigma = 1$.

$$\begin{cases} \epsilon v \partial_x I(x,v) = \sigma \left(acT^4(x) - I(x,v) \right) & x \in [0,1],\ v \in [-1,1], \\ \epsilon^2 \partial_{xx} T(x) = \sigma \left(acT^4(x) - \langle I(x,v) \rangle \right) & x \in [0,1],\ v \in [-1,1], \\ I(0, v>0) = 1, \qquad I(1, v<0) = 0, \\ T(0) = 1, \qquad T(1) = 0. \end{cases}$$



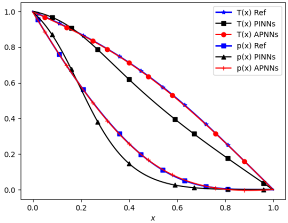


Figure 3. Diffusion regime with $\epsilon = 10^{-3}$. (Left) I of APNNs. (Right) T and ρ: Ref v.s. PINNs v.s. APNNs. PINNs do badly while APNNs perform well.

Time-dependent linear transport equations

- Diffusion regime with a variable scattering frequency
  $x \in [0,1], \quad t \in [0,1], \quad \mu \in [-1,1], \quad \sigma = 1 + (10x)^2, \quad c = 1,$
  $\epsilon = 10^{-3}, \quad I_L(\mu > 0) = 1, \quad I_R(\mu < 0) = 0, \quad I_0 = 0.$

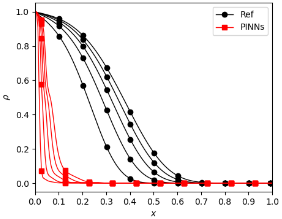


Figure 4. Diffusion regime with $\epsilon = 10^{-3}$. The density ρ at times $t = 0.2, 0.4, 0.6, 0.8, 1.0$. (Left) Ref v.s. PINNs. (Right) Ref v.s. APNNs.

$L^2_{\text{error}}(\rho)$	$t = 0.2$	$t = 0.4$	$t = 0.6$	$t = 0.8$	$t = 1.0$
PINNs	9.25e-01	8.99e-01	8.75e-01	8.51e-01	8.27e-01
APNNs	3.44e-02	2.76e-02	2.59e-02	2.56e-02	2.33e-02

Table 1. Diffusion regime with $\epsilon = 10^{-3}$. The errors of PINNs and APNNs.

The time-dependent nonlinear GRTEs

- Problem I

  Consider the 1D time-dependent GRTEs with temperature-independent opacity $\sigma = 10\text{cm}^{-1}$ and heat capacity $C_v = 0.01\text{GJ}/\text{cm}^3$KeV on a slab of length 0.25cm which is initially at equilibrium at 1keV, that means initial conditions are given by

  $$T(0,x) = 1, \quad I(0,x,\mu) = \frac{1}{2}acT(0,x)^4,$$

  and the reflection condition and incident Planckian source condition on the left and right boundaries are

  $$I(t,0,\mu > 0) = I(t,0,-\mu), \quad I(t,0.25,\mu < 0) = \frac{1}{2}ac(0.1)^4,$$

  where the light speed $c = 29.98$cm/ns and the radiation constant $a = 0.01372$ GJ/cm^3 $-$ KeV^4.

The time-dependent nonlinear GRTEs

- Results of APNNs

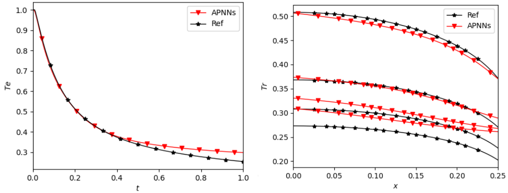


Figure 5. $\epsilon = 1$. (Left) Ref v.s. APNNs of the material temperature T(denote T as Te in all pictures) at $x = 0.0025$. (Right) Ref v.s. APNNs of the radiation temperature T_r at times $t = 0.2, 0.4, 0.6, 0.8$.

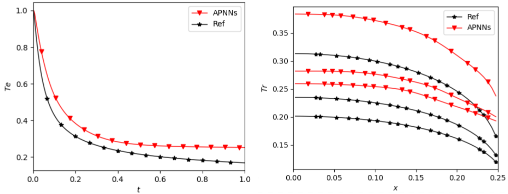


Figure 6. $\epsilon = 10^{-6}$. (Left) Ref v.s. APNNs of the material temperature T at $x = 0.0025$. (Right) Ref v.s. APNNs of the radiation temperature T_r at times $t = 0.2, 0.4, 0.6$.

Model-data asymptotic-preserving neural networks(MD-APNNs)

- Add a data regularization term [1] to the APNN loss function for solving the strongly coupled nonlinearity

$$L^{\epsilon,nn}_{\text{MD-APNNs,l}} = \lambda_0 \frac{1}{N_0} \sum_{i=1}^{N_0} \left(\left| T^{nn}_{\theta_{22}}(t_i, r_i) - T^*(t_i, r_i) \right|^2 \right).$$

where $\{T^*(t_i, r_i)\}_{i=1}^{N_0}$ are some label data via UGKS on coarse grids and (t_i, r_i) are low-discrepancy Sobol sequence points [Mishra et al. 2021].

[1] L. Zhang, T. Lou, Y. zhang, W.E, Z.-Q.J. Xu, Z. Ma, Mod-Net: A machine learning approach via model-operato-data network for solving pdes, Communications in Computational Physics, 32(2)(2022) 299-335.

- Results of MD-APNNs

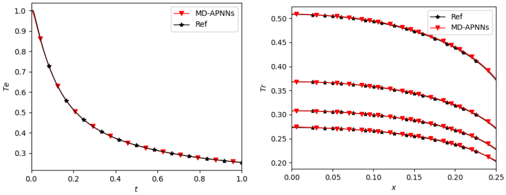


Figure 7. $\epsilon = 1$. (Left) Ref v.s. MD-APNNs of the material temperature T at $x = 0.0025$. (Right) Ref v.s. MD-APNNs of the radiation temperature T_r at times $t = 0.2, 0.4, 0.6, 0.8$.

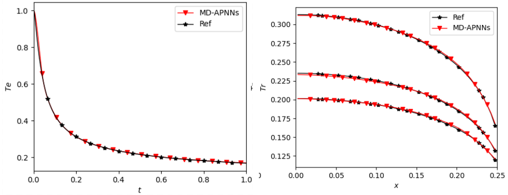


Figure 8. $\epsilon = 10^{-6}$. (Left) Ref v.s. MD-APNNs of the material temperature T at $x = 0.0025$. (Right) Ref v.s. MD-APNNs of the radiation temperature T_r at times $t = 0.2, 0.4, 0.6$.

The time-dependent nonlinear GRTEs

L^2 error	T	$T_r(t=0.2)$	$T_r(t=0.4)$	$T_r(t=0.6)$	$T_r(t=0.8)$
APNNs	5.05e-02	1.94e-02	1.30e-02	5.75e-02	1.21e-01
MD-APNNs	4.95e-03	3.21e-03	2.84e-03	2.48e-03	3.80e-03

Table 2. Kinetic regime with $\epsilon = 1$: the errors of T and T_r (at $t = 0.2, 0.4, 0.6, 0.8$) for APNNs and MD-APNNs.

L^2 error	T	$T_r(t=0.2)$	$T_r(t=0.4)$	$T_r(t=0.6)$
APNNs	2.38e-01	2.51e-01	2.40e-01	3.31e-01
MD-APNNs	2.62e-02	3.80e-03	7.35e-03	4.87e-03

Table 3. Diffusion regime with $\epsilon = 10^{-6}$: the errors of T and T_r (at $t = 0.2, 0.4, 0.6$) for APNNs and MD-APNNs.

The time-dependent nonlinear GRTEs

- Problem II

  We solve the 1D example with smooth initial data at the equilibrium

$$T(0,x)=\frac{3+\sin(\pi x)}{4}, \quad I(0,x,\mu)=\frac{1}{2}acT(0,x)^4,$$

  and periodic boundary condition. The spatial domian is $[0,2]$, time interval is $[0,0.5]$, angular direction is $[-1,1]$ and the parameters are set as $a=c=1$, $C_v=0.1, \sigma=10$.

- Results under diffusion regime

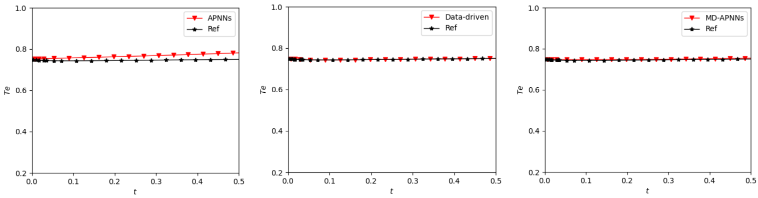


Figure 9. Diffusion regime with $\epsilon=10^{-3}$. From left to right, Ref v.s. APNNs, Ref v.s. Data-driven and Ref v.s. MD-APNNs of T at $x=0.0025$.

The time-dependent nonlinear GRTEs

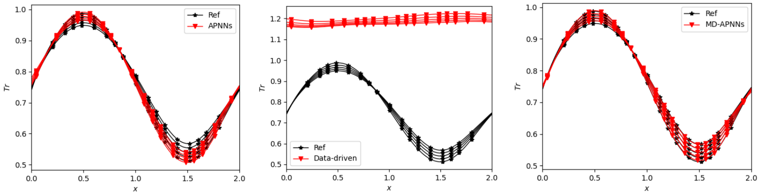


Figure 10. Diffusion regime with $\epsilon = 10^{-3}$. From left to right, Ref v.s. APNNs, Ref v.s. Data-driven and Ref v.s. MD-APNNs of T_r at times $t = 0.2,\ 0.4,\ 0.6,\ 0.8,\ 1.0$.

L^2 error	T	$T_r(t=0.2)$	$T_r(t=0.4)$	$T_r(t=0.6)$	$T_r(t=0.8)$	$T_r(t=1.0)$
Data-driven	6.37e-04	6.28e-01	6.02e-01	5.81e-01	5.64e-01	5.50e-01
APNNs	2.82e-02	7.10e-03	1.16e-02	1.54e-02	1.89e-02	2.23e-02
MD-APNNs	4.18e-03	3.37e-03	3.12e-03	3.11e-03	3.97e-03	5.67e-03

Table 4. Diffusion regime with $\epsilon = 10^{-3}$: the errors of T and T_r (at $t = 0.2, 0.4, 0.6, 0.8, 1.0$) for APNNs, Data-driven and MD-APNNs.

The time-dependent nonlinear GRTEs

- 2D time-dependent nonlinear radiative transfer equation

  We consider smooth initial conditions at the equilibrium

$$
\begin{aligned}
\rho(0,x,y) &= \frac{ac}{4\pi}\left((a_1+b_1\sin x)(a_2+b_2\sin y)\right)^4,\\
g(0,x,y) &= -\frac{\Omega\cdot\nabla\rho(0,x,y)}{\sigma},\\
T(0,x,y) &= (a_1+b_1\sin x)(a_2+b_2\sin y).
\end{aligned}
$$

  Here, $\sigma=1, a=c=C_v=1, a_1=a_2=0.8$, $b_1=b_2=0.1$.
  The periodic boundary conditions are used in both space directions.

- Results under transport regime

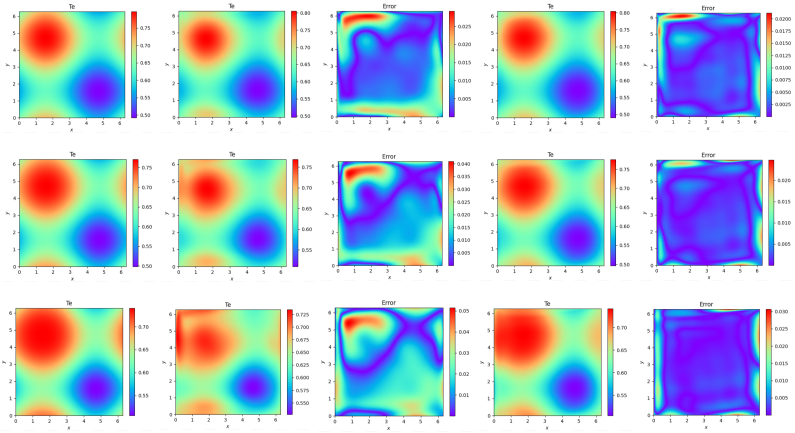


Figure 11. Transport regime with $\epsilon = 1$. Contour plots of the material temperature T at times $t = 0.2, 0.4, 0.6$. From left to right in each line, Ref, APNNs, Absolute errors between Ref and APNNs, MD-APNNs and Absolute errors between Ref and MD-APNNs.

The time-dependent nonlinear GRTEs

- Results under diffusion regime

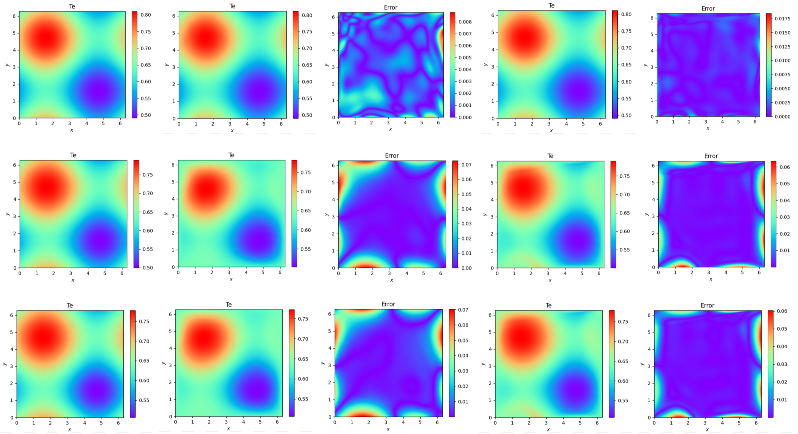


Figure 12. Diffusion regime with $\epsilon = 10^{-6}$. Contuor plots of the material temperature T at times $t = 0.0, 0.6, 1.0$. From left to right in each line, Ref, APNNs, Absolute errors between Ref and APNNs, MD-APNNs and Absolute errors between Ref and MD-APNNs.

Outline

- Structure-preserving schemes
- Radiative transfer equations(RTEs)
- Asymptotic-preserving neural networks(APNNs)
- Model-data asymptotic-preserving neural networks(MD-APNNs) for gray radiative transfer equations(GRTEs)
- Macroscopic auxiliary asymptotic-preserving neural networks (MA-APNNs) for linear radiative transfer equations(LRTEs)
- Summary and future work

Linear radiative transfer equations

- Consider the LRTEs Eq.(2) over the bounded domain with additional absorption and source term and let $c = 1$.

$$
\begin{cases}
\epsilon^2 \dfrac{\partial I}{\partial t} + \epsilon \Omega \cdot \nabla_r I = \sigma \left(\dfrac{1}{4\pi} \displaystyle\int_{S^2} I \mathrm{d}\Omega - I \right) - \epsilon^2 \alpha I + \epsilon^2 G, & \text{(8a)} \\
\qquad\qquad\qquad\qquad (t, r, \Omega) \in \tau \times D \times S^2, & \\
B_{ou} I = I_\Gamma, \qquad (t, r, \Omega) \in \Gamma, & \text{(8b)} \\
I_{in} I = I_0, \qquad (t, r, \Omega) \in \{0\} \times D \times S^2. & \text{(8c)}
\end{cases}
$$

$I(t, r, \Omega)$: radiation intensity, $r = (x, y, z) \in R^3$: spatial variable, t: time variable, $\Omega = (\xi, \eta, \mu) \in S^2 (i.e. \xi^2 + \eta^2 + \mu^2 = 1)$: angular variable, $\sigma(r)$: scattering coefficient, $\alpha(r)$: absorption coefficient, $G(r)$: internal source.

Linear radiative transfer equations

- Diffusion limit equation
  As the parameter $\epsilon \to 0$, the radiation intensity $I(t, r, \Omega)$ tends to its own average density $\rho := \langle I \rangle = \frac{1}{4\pi} \int_{S^2} I \mathrm{d}\Omega$, which is a solution of the asymptotic diffusion limit

$$\partial_t \rho - \left\langle \Omega^2 \right\rangle \nabla_r \left(\frac{1}{\sigma} \nabla_r \rho \right) + \alpha \rho - G = 0. \tag{9}$$

  When the angle is one-dimensional, $\left\langle \Omega^2 \right\rangle = 1/3$ and the angles are distributed on the unit circle, $\left\langle \Omega^2 \right\rangle = 1/2$.

- For the LRTEs Eq.(8a), perform angle integration on both sides of it, the macroscopic auxiliary equation is obtained,

$$\epsilon^2 \partial_t \rho + \epsilon \langle \Omega \cdot \nabla_r I \rangle = \sigma \left(\frac{1}{4\pi} \int_{S^2} I \mathrm{d}\Omega - \rho \right) - \epsilon^2 \alpha \rho + \epsilon^2 G.$$

  which is usually used in UGKS to combine with the original radiative transfer equation.

The MA-APNN method for LRTEs

- Macroscopic Auxiliary Asymptotic-Preserving Neural Networks

  Rewriting the linear radiative transfer equation Eq.(8a) [2]

$$I = \langle I \rangle - \frac{\epsilon^2}{\sigma}\partial_t I - \frac{\epsilon}{\sigma}\Omega \cdot \nabla_r I - \frac{\epsilon^2}{\sigma}\alpha I + \frac{\epsilon^2}{\sigma}G. \tag{10}$$

  Replacing I with the right handside of Eq.(10)

$$\begin{aligned}
I = \langle I \rangle - \epsilon\frac{1}{\sigma}\Omega \cdot \nabla_r \langle I \rangle - \epsilon^2 \left(\frac{1}{\sigma}\partial_t \langle I \rangle - \frac{1}{\sigma}\Omega \cdot \nabla_r (\frac{1}{\sigma}\Omega \cdot \nabla_r I) + \frac{1}{\sigma}\alpha I - \frac{1}{\sigma}G\right) \\
+ \epsilon^3 \left(\frac{1}{\sigma}\partial_t (\frac{1}{\sigma}\Omega \cdot \nabla_r I) + \frac{1}{\sigma}\Omega \cdot \nabla_r \big(\frac{1}{\sigma}\partial_t I + \frac{1}{\sigma}\alpha I - \frac{1}{\sigma}G)\right) \\
+ \epsilon^4 \left(\frac{1}{\sigma}\partial_t \big(\frac{1}{\sigma}\partial_t I + \frac{1}{\sigma}\alpha I - \frac{1}{\sigma}G)\right).
\end{aligned}$$

[2] M. Ghattassi, X. Huo, N. Masmoudi, On the diffusive limits of radiative heat transfer system i: well-prepared initial and boundary conditions, SIAM Journal on Mathematical Analysis 54 (5) (2022) 5335–5387.

The MA-APNN method for LRTEs

Replacing I with the right handside of Eq.(10)

$$I = \langle I \rangle - \frac{\epsilon}{\sigma}\Omega \cdot \nabla_r \langle I \rangle - \frac{\epsilon^2}{\sigma}\left(\partial_t \langle I \rangle - \Omega \cdot \nabla_r (\frac{1}{\sigma}\Omega \cdot \nabla_r \langle I \rangle) + \alpha I - G\right) \\ + \epsilon^3 \mathcal{A}(I,G) + \epsilon^4 \mathcal{B}(I,G), \tag{11}$$

where

$$\mathcal{A}(I,G) = \frac{1}{\sigma}\partial_t (\frac{1}{\sigma}\Omega \cdot \nabla_r I) + \frac{1}{\sigma}\Omega \cdot \nabla_r \left(\frac{1}{\sigma}\left(\partial_t I + \alpha I - G - \Omega \cdot \nabla_r (\frac{1}{\sigma}\Omega \cdot \nabla_r I)\right)\right),$$

$$\mathcal{B}(I,G) = \frac{1}{\sigma^2}\partial_t \left(\partial_t I + \alpha I - G\right) - \frac{1}{\sigma}\Omega \cdot \nabla_r \left(\frac{1}{\sigma}\Omega \cdot \nabla_r \left(\frac{1}{\sigma}\left(\partial_t I + \alpha I - G\right)\right)\right).$$

Performing angle integration on both sides of Eq.(11)

$$\partial_t \rho - \langle \Omega^2 \rangle \nabla_r \left(\frac{1}{\sigma}\nabla_r \rho\right) + \alpha\rho - G - \epsilon \langle \sigma \mathcal{A}(I,G) \rangle - \epsilon^2 \langle \sigma \mathcal{B}(I,G) \rangle = 0. \tag{12}$$

- Remark

  (1) Eq.(12) is the equivalent macroscopic auxiliary equation obtained by continuous substitution. It contains diffusion limit equation explicitly. Add it to the model as additional constraint information.

  (2) MA-APNNs need a high requirement for the smoothness of the solutions of LRTEs.

The MA-APNN method for LRTEs

Eq.(8a) and Eq.(12) constitute the multiscale coupled formulation

$$\begin{cases} \epsilon^2 \partial_t I + \epsilon \Omega \cdot \nabla_r I = \sigma \left(\frac{1}{4\pi} \int_{S^2} I \mathrm{d}\Omega - I \right) - \epsilon^2 \alpha I + \epsilon^2 G, \\ \partial_t \rho - \left\langle \Omega^2 \right\rangle \nabla_r \left(\frac{1}{\sigma} \nabla_r \rho \right) + \alpha \rho - G - \epsilon \left\langle \sigma \mathcal{A}(I, G) \right\rangle - \epsilon^2 \left\langle \sigma \mathcal{B}(I, G) \right\rangle = 0. \end{cases} \tag{13}$$

When $\epsilon \to 0$, the above system Eq.(13) is simplified as

$$\begin{cases} \sigma \left(\rho - I \right) = 0, \\ \partial_t \rho - \left\langle \Omega^2 \right\rangle \nabla_r \left(\frac{1}{\sigma} \nabla_r \rho \right) + \alpha \rho - G = 0, \end{cases} \tag{14}$$

which is the expected diffusion limit equation.

The exponentially weighted MA-APNN loss function

Using a nonnegative I_θ^{nn} to approximate I

$$I_\theta^{nn}(t,r,\Omega) := \exp(-\tilde{I}_\theta^{nn}(t,r,\Omega)) \approx I(t,r,\Omega), \quad \langle I_\theta^{nn}(t,r,\Omega)\rangle \approx \rho(t,r).$$

The asymptotic-preserving MA-APNN loss function for the governing equations

$$\begin{aligned} L^{\epsilon}_{\text{MA-APNNs,ge}} = & \left\| \lambda_{\nu,\beta}^{\frac{1}{2}} \left(\epsilon^2 \partial_t I_\theta^{nn} + \epsilon \Omega \cdot \nabla_r I_\theta^{nn} - \sigma\left(\langle I_\theta^{nn}\rangle - I_\theta^{nn}\right) + \epsilon^2 \alpha I_\theta^{nn} - \epsilon^2 G\right)\right\|^2_{L^2(\tau\times D\times S^2)} \\ & + \left\| (1-\lambda_{\nu,\beta})^{\frac{1}{2}} \Big(\partial_t \langle I_\theta^{nn}\rangle - \langle \Omega^2\rangle \nabla_r \big(\frac{1}{\sigma}\nabla_r \langle I_\theta^{nn}\rangle\big) + \alpha \langle I_\theta^{nn}\rangle - G \right. \\ & \left. - \epsilon \langle \sigma \mathcal{A}(I_\theta^{nn}, G)\rangle - \epsilon^2 \langle \sigma \mathcal{B}(I_\theta^{nn}, G)\rangle \Big) \right\|^2_{L^2(\tau\times D)}, \end{aligned}$$

where $\lambda_{\nu,\beta}(r) := e^{-\nu(r)\beta_1} + \beta_2$ with $\nu(r) = \frac{\sigma(r)}{\epsilon^2} + \alpha(r)$. Here, $\beta = (\beta_1, \beta_2) > 0$ is the tunable parameter satisfying $1 - \max_r \lambda_{\nu,\beta}(r) > 0$.

Feature: with the designed exponential weight, the loss function adaptively learns the state of photon evolution according to the change of model parameters.

The exponentially weighted MA-APNN loss function

The loss for boundary conditions

$$L^{\epsilon}_{\text{MA-APNNs,b}} = \lambda_b \left(\| B_{ou} I^{nn}_{\theta} - I_{\Gamma} \|^2_{L^2(\tau \times \partial D \times S^2)} + \| B_{ou} \langle I^{nn}_{\theta} \rangle - \langle I_{\Gamma} \rangle \|^2_{L^2(\tau \times \partial D)} \right).$$

The loss for initial conditions

$$L^{\epsilon}_{\text{MA-APNNs,i}} = \lambda_i \left(\| I_{in} I^{nn}_{\theta} - I_0 \|^2_{L^2(D \times S^2)} + \| I_{in} \langle I^{nn}_{\theta} \rangle - \langle I_0 \rangle \|^2_{L^2(D)} \right).$$

Under specific conditions (e.g. periodic boundary), the loss for the mass conservation laws

$$L^{\epsilon}_{\text{MA-APNNs,c}} = \lambda_c \left\| \epsilon \partial_t \int_D \langle I^{nn}_{\theta} \rangle \, \mathrm{d}r + \int_{\partial D} \langle \Omega \cdot n_r I^{nn}_{\theta} \rangle \mathrm{d}r + \epsilon \int_D \alpha \langle I^{nn}_{\theta} \rangle \, \mathrm{d}r - \epsilon \int_D G \mathrm{d}r \right\|^2_{L^2(\tau)}$$

The exponentially weighted MA-APNN loss function

- Analyze the AP property

As $\sigma(r),\ \beta_1,\ \beta_2 > 0,\ \epsilon \to 0,$

$$
\begin{aligned}
&\lambda_{\nu,\beta}(r) \to \beta_2, \\
&L^{\epsilon}_{\text{MA-APNNs,ge}} \to \beta_2 \left\| -\sigma \left(\langle I_\theta^{nn} \rangle - I_\theta^{nn} \right) \right\|^2_{L^2(\tau \times D \times S^2)} \\
&+ (1-\beta_2) \left\| \partial_t \langle I_\theta^{nn} \rangle - \left\langle \Omega^2 \right\rangle \nabla_r \left(\frac{1}{\sigma} \nabla_r \langle I_\theta^{nn} \rangle \right) + \alpha \langle I_\theta^{nn} \rangle - G \right\|^2_{L^2(\tau \times D)},
\end{aligned} \tag{15}
$$

which is the PINN loss of the diffusion limit system (14).

Diffusion regime with a constant scattering frequency

$$x \in [0,1], \quad t \in [0,2], \quad \mu \in [-1,1], \quad I_L(\mu > 0) = 1, \quad I_R(\mu < 0) = 0,$$
$$I_0 = 0, \quad \sigma = 1, \quad \alpha = 0, \quad G = 0, \quad \epsilon = 10^{-8}.$$

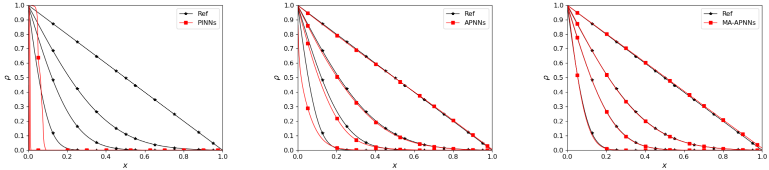


Figure 13. Diffusion regime with $\epsilon = 10^{-8}$. The density ρ at times $t = 0.01, 0.05, 0.15, 2.00$. (Left) Ref v.s. PINNs. (Middle) Ref v.s. APNNs. (Right) Ref v.s. MA-APNNs.

$L^2_{\text{error}}(\rho)$	$t = 0.01$	$t = 0.05$	$t = 0.15$	$t = 2.00$	Training time
PINNs	9.75e-01	9.71e-01	9.65e-01	8.96e-01	17min 34s
APNNs	3.81e-01	8.18e-02	2.37e-02	8.95e-03	2h 45min
MA-APNNs	3.16e-02	5.79e-03	5.30e-03	1.35e-02	1h 24min

Table 5. Diffusion regime with $\epsilon = 10^{-8}$. The errors and training time of PINNs, APNNs and MA-APNNs.

Intermediate regime with a variable scattering frequency and source term

$$x \in [0,1], \quad t \in [0,1], \quad \mu \in [-1,1], \quad I_L(\mu > 0) = 0, \quad I_R(\mu < 0) = 0,$$
$$I_0 = 0, \quad \sigma = 1 + (10x)^2, \quad \alpha = 0, \quad G = 1, \quad \epsilon = 10^{-2}.$$

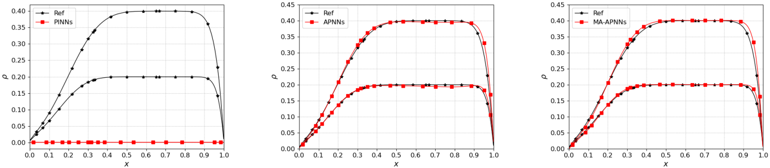
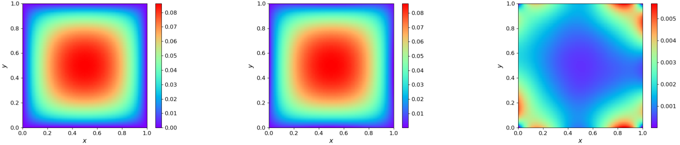


Figure 14. Intermediate regime with $\epsilon = 10^{-2}$. The density ρ at times $t = 0.2, 0.4$. (Left) Ref v.s. PINNs. (Middle) Ref v.s. APNNs. (Right) Ref v.s. MA-APNNs.

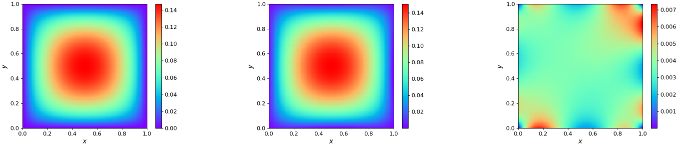
$L^2_{\text{error}}(\rho)$	$t = 0.2$	$t = 0.4$	Training time
PINNs	9.98e-01	9.99e-01	30min 9s
APNNs	2.87e-02	3.24e-02	4h 37min
MA-APNNs	2.70e-02	3.44e-02	2h 25min

Table 6. Intermediate regime with $\epsilon = 10^{-2}$. The errors and training time of PINNs, APNNs and MA-APNNs.

$$D \in [0,1]\times[0,1], \quad t \in [0,1], \quad I_B(t,\boldsymbol{x},\boldsymbol{v}) = 0,\ n_{\boldsymbol{x}}\cdot\boldsymbol{v} < 0,\ \boldsymbol{x}\in\partial D,$$
$$I_0(\boldsymbol{x},\boldsymbol{v}) = 0, \quad \sigma = 1, \quad \alpha = 0, \quad G = 1, \quad \epsilon = 10^{-8}.$$



(a) $\rho^{\text{Ref}}, t = 0.1$ (b) $\rho_\theta^{nn}, t = 0.1$ (c) $|\rho^{\text{Ref}} - \rho_\theta^{nn}|, t = 0.1$



(d) $\rho^{\text{Ref}}, t = 0.8$ (e) $\rho_\theta^{nn}, t = 0.8$ (f) $|\rho^{\text{Ref}} - \rho_\theta^{nn}|, t = 0.8$

Figure 15. The 2D LRTEs in the diffusion regime ($\epsilon = 10^{-8}$). The L^2 relative errors at times $t = 0.1, 0.8$ are $3.98e-02$ and $4.79e-02$, respectively.

Uncertainty quantification (UQ) problems

- Considering the linear transport equation with cosine scattering coefficient $\sigma(z)$.

$x \in [0,1], \quad t \in [0,1], \quad \mu \in [-1,1], \quad I(t,0,\mu,\boldsymbol{z}) = 0, \quad I(t,1,\mu,\boldsymbol{z}) = 0,$

$I(0,x,\mu,\boldsymbol{z}) = 0, \quad \sigma(\boldsymbol{z}) = 1 + 0.1\sum_{i=1}^{10}\cos(\pi z_i), \quad \alpha = 0, \quad \epsilon = 1,$

$G = \frac{x(1-x)}{22}\left(\mu + 11 + \sum_{i=1}^{10} z_i\right) + \frac{\mu t}{22\epsilon}(1-2x)\left(\mu + 11 + \sum_{i=1}^{10} z_i\right) + \frac{1}{\epsilon^2}\sigma(\boldsymbol{z})tx(1-x)\mu,$

$\boldsymbol{z} = (z_1, z_2, z_3, z_4, z_5, z_6, z_7, z_8, z_9, z_{10}) \sim U([-1,1]^{10}).$

At this time, the exact solution is

$$I(t,x,\mu,\boldsymbol{z}) = \frac{tx(1-x)}{22}\left(\mu + 11 + \sum_{i=1}^{10} z_i\right), \quad \rho(t,x,\boldsymbol{z}) = \frac{tx(1-x)}{22}\left(11 + \sum_{i=1}^{10} z_i\right),$$

and the expectation of ρ with respect to random variable $\boldsymbol{z}$ is $E(\rho) = \frac{1}{2}tx(1-x)$.

Uncertainty quantification (UQ) problems

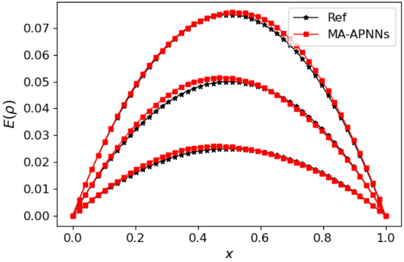


Figure 16. The expectation $\boldsymbol{E}(\rho)$ at $t = 0.2, 0.4, 0.6$.

L^2_{error}	$t = 0.2$	$t = 0.4$	$t = 0.6$
MA-APNNs	4.49e-02	3.63e-02	2.12e-02

Table 7. High dimensional transport regime. The errors of MA-APNNs.

Outline

- Structure-preserving schemes
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- Summary and future work

Summary and future work

- Summary
  - Design a MD-APNNs method based on micro-macro decomposition to solve multiscale nonlinear gray transfer radiative model. [3]
  - Design a exponentially weighted MA-APNN method to solve multiscale linear radiative transfer model. [4]
- Feature
  - MD-APNNs and MA-APNNs mainly establish the AP loss through the direct transformation construction of the original model, which is the pre-processing part in the whole learning optimization process of the neural network.
- Future work
  - Develop asymptotic-preserving neural operator methods to solve a class of GRTEs.
  - Develop MA-APNNs to solve the Boltzmann-BGK equations.

[3] H. Li, S. Jiang, W. Sun, L. Xu, G. Zhou, A model-data asymptotic-preserving neural network method based on micro-macro decomposition for gray radiative transfer equations, Communications in Computational Phisics (2023) (Accepted).

[4] H. Li, S. Jiang, W. Sun, L. Xu, G. Zhou, Macroscopic auxiliary asymptotic-preserving neural networks for the linear radiative transfer equations, arXiv preprint arXiv:2403.01820 (2024).

Thanks for your attention!