Scientific Machine Learning of Radiative Transfer Equations

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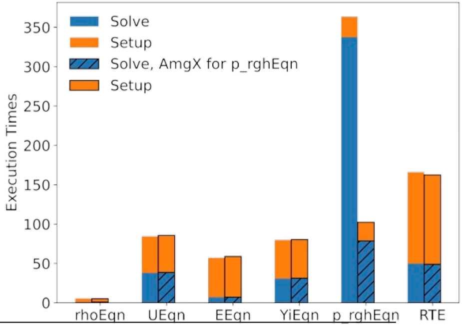
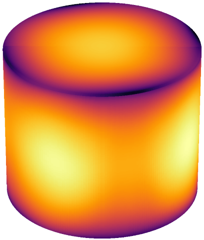
Problem

Simulation of fires is computationally expensive

- `FireFOAM`[1,2] simulations can take weeks or even months
- Solving *Radiative Transfer Equations (RTEs)* is the most costly sub-routine
- *Finite Volume Discrete Ordinates Method (FVDOM)* suffers from the ray effect



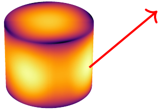


[1] Yi Wang, Prateep Chatterjee, and John L de Ris. "Large eddy simulation of fire plumes". In: *Proceedings of the Combustion Institute* 33.2 (2011), pp. 2473–2480.

[2] Yi Wang et al. "Numerical simulation of sprinkler suppression of rack storage fires". In: *Fire Safety Science* 11 (2014), pp. 1170–1183.

Challenge

Speeding up fire simulation requires replacing a complex RTE solver



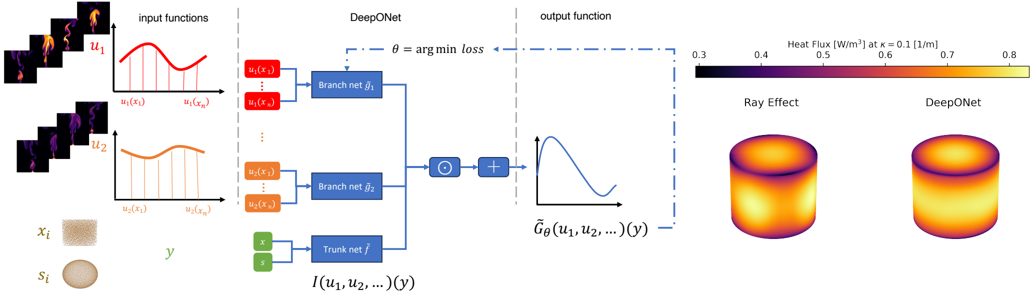
- The RTE is a high dimensional integro-differential equation e.g. 3 spatial coordinates $+$ 2 propagation directions
- The RTE must be solved for many different random coefficients
  - Coefficients appear in both the governing equation and boundary condition
  - Different coefficients appear when resolving the spectral dependence
  - Different coefficients appear across time steps in a `FireFOAM` simulation

coefficient	absorption	black-body emissive power	surface emissivity	diffusive reflection	spectular reflection
RTE notation	κ	$aT^4\sigma/\pi$	ϵ	ρ^d	ρ^s
SciML notation	u^1	u^2	u^3	u^4	u^5

Solution

Accelerate fire simulation with *Scientific Machine Learning (SciML)* of RTEs

- Principal Component Analysis (PCA) - Deep Operator Networks (DeepONets)[3]
- Trained SciML models enable rapid inference of RTE solutions[4,5]
- SciML models overcome the ray effect thanks to mesh-free training and inference



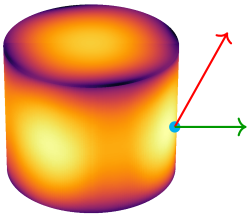
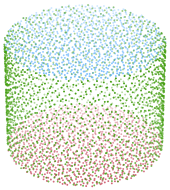
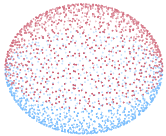
[3] George Em Karniadakis et al. "Physics-informed machine learning". In: *Nature Reviews Physics* 3.6 (2021), pp. 422–440.

[4] Siddhartha Mishra and Roberto Molinaro. "Physics informed neural networks for simulating radiative transfer". In: *J Quant Spectrosc Radiat Transf.* 270 (2021), p. 107705.

[5] Xiaoyi Lu and Yi Wang. "Surrogate modeling for radiative heat transfer using physics-informed deep neural operator networks". In: *Proceedings of the Combustion Institute* 40.1-4 (2024), p. 105282.

RTE dimensions

- Location $\boldsymbol{x} \in \overline{D} = D \cup \partial D$ e.g. $\overline{D}$ a cylinder with surface ∂D enclosing D
- Propagation direction $\boldsymbol{s}$ on unit sphere Ω
- Surface normal $\boldsymbol{n}(\boldsymbol{x})$ at $\boldsymbol{x} \in \partial D$
- Hemisphere of incident rays $\Omega^{\downarrow}(\boldsymbol{x}) = \{\boldsymbol{s} \in \Omega : \boldsymbol{n}(\boldsymbol{x}) \cdot \boldsymbol{s}(\boldsymbol{x}) < 0\}$

RTE integro-differential equation[6]

Governing Equation (GE) and Boundary Condition (BC)

- Location $\boldsymbol{x} \in \overline{D} = D \cup \partial D$. Propagation direction $\boldsymbol{s}$ on unit sphere Ω
- Normal $\boldsymbol{n}(\boldsymbol{x})$ at $\boldsymbol{x} \in \partial D$. Incident hemisphere $\Omega^{\downarrow}(\boldsymbol{x}) = \{\boldsymbol{s} \in \Omega : \boldsymbol{n}(\boldsymbol{x}) \cdot \boldsymbol{s}(\boldsymbol{x}) < 0\}$
- Coefficients $(u^1, \dots, u^5)$. Specular direction $\boldsymbol{s}_s(\boldsymbol{x}, \boldsymbol{s}) = \boldsymbol{s} - 2\boldsymbol{n}(\boldsymbol{x})\,(\boldsymbol{n}(\boldsymbol{x}) \cdot \boldsymbol{s})$

$$
\begin{aligned}
\mathscr{L}_{\mathrm{GE}}\left(I, \left(u^1, \dots, u^5\right), (\boldsymbol{x}, \boldsymbol{s})\right) =& \boldsymbol{s}.\nabla I(\boldsymbol{x}, \boldsymbol{s}) + u^1(\boldsymbol{x}) I(\boldsymbol{x}, \boldsymbol{s}) - u^1(\boldsymbol{x}) u^2(\boldsymbol{x}) = 0 \\
\mathscr{L}_{\mathrm{BC}}\left(I, \left(u^1, \dots, u^5\right), (\boldsymbol{x}, \boldsymbol{s})\right) =& u^2(\boldsymbol{x}) u^3(\boldsymbol{x}) + \frac{u^4(\boldsymbol{x})}{\pi} \int I(\boldsymbol{x}, \boldsymbol{s}') |\boldsymbol{n}(\boldsymbol{x}).\boldsymbol{s}'| \mathrm{d}\Omega^{\downarrow}(\boldsymbol{x}) \\
& + u^5(\boldsymbol{x}) I(\boldsymbol{x}, \boldsymbol{s}_s(\boldsymbol{x}, \boldsymbol{s})) - I(\boldsymbol{x}, \boldsymbol{s}) = 0
\end{aligned}
$$

$$
\begin{cases}
\mathscr{L}_{\mathrm{GE}}\left(I, \left(u^1, \dots, u^5\right), (\boldsymbol{x}, \boldsymbol{s})\right) = 0, & \boldsymbol{x} \in D, \quad \boldsymbol{s} \in \Omega \\
\mathscr{L}_{\mathrm{BC}}\left(I, \left(u^1, \dots, u^5\right), (\boldsymbol{x}, \boldsymbol{s})\right) = 0, & \boldsymbol{x} \in \partial D, \quad \boldsymbol{s} \in \Omega^{\downarrow}(\boldsymbol{x})
\end{cases}
$$

[6] Michael F Modest and Sandip Mazumder. *Radiative heat transfer*. Academic press, 2021.

Scientific machine learning (SciML) model

principal component analysis (PCA) - deep operator networks (DeepONets)

Solution operator $G : (u^1, \dots, u^5) \mapsto I$ approximated by PCA-DeepONet $\widetilde{G}_\Theta$

- **Sensor Values:** $\boldsymbol{u}^j = \left(u^j\left(\boldsymbol{x}_1^j\right), \dots, u^j\left(\boldsymbol{x}_{n_j}^j\right)\right)$ at sensor locations $\{\boldsymbol{x}_i^j\}_{i=1}^{n_j} \subset \overline{D}$
- **PCA-BN (Branch Net)** $\mathcal{B}^j_{\Theta_j} : \boldsymbol{u}^j \mapsto \mathcal{B}^j_{\Theta_j}(\mathsf{P}_j^\mathsf{T}\boldsymbol{u}^j - \boldsymbol{\mu}^j) =: \boldsymbol{b}^j \in \mathbb{R}^c$,
  PCA projection matrix $\mathsf{P}_j \in \mathbb{R}^{n_j \times \hat{n}_j}$ with $\hat{n}_j \ll n_j$
- **TN (Trunk Net)** $\mathcal{T}_{\Theta_0} : (\boldsymbol{x}, \boldsymbol{s}) \mapsto \mathcal{T}_{\Theta_0}(\boldsymbol{x}, \boldsymbol{s}) =: \boldsymbol{t} \in \mathbb{R}^c$

$$
\begin{tikzcd}
u^1 \arrow[r, "\text{evaluate}"] & \boldsymbol{u}^1 \arrow[r, "\text{PCA-BN}"] & \boldsymbol{b}^1 \arrow[dddr] & b \arrow[ddd] \\
\vdots & \vdots & \vdots & \\
u^5 \arrow[r, "\text{evaluate}"] & \boldsymbol{u}^5 \arrow[r, "\text{PCA-BN}"] & \boldsymbol{b}^5 \arrow[dr] & \\
(\boldsymbol{x}, \boldsymbol{s}) \arrow[r, "\text{TN}"] & \boldsymbol{t} \arrow[rr] & & \boxed{\widetilde{G}_\Theta\left(u^1, \dots, u^5\right)(\boldsymbol{x}, \boldsymbol{s}) = b + \sum \boldsymbol{t} \odot \boldsymbol{b}^1 \odot \cdots \odot \boldsymbol{b}^5}
\end{tikzcd}
$$

DeepONet training

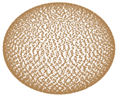
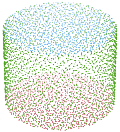
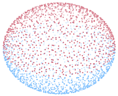
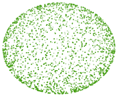
hybrid physics-informed data-driven loss

$$\mathscr{L}(\Theta) = \omega_{\mathrm{GE}} \left\| \mathscr{L}_{\mathrm{GE}}\left(\tilde{G}_\Theta, \mathcal{D}^{\mathrm{RC}}_{\mathrm{GE}}\right)\right\| + \omega_{\mathrm{BC}} \left\| \mathscr{L}_{\mathrm{BC}}\left(\tilde{G}_\Theta, \mathcal{D}^{\mathrm{RC}}_{\mathrm{BC}}\right)\right\| + \omega_{\mathrm{data}} \left\| \mathscr{L}_{\mathrm{data}}\left(\tilde{G}_\Theta, \mathcal{D}^{\mathrm{RC}}_{\mathrm{data}}\right)\right\|$$

dataset: $\mathcal{D}^{\mathrm{RC}}_{\mathrm{GE}} = \mathcal{D}^{\mathrm{RC}} \times \mathcal{D}_{\mathrm{GE}}$ $\quad \mathcal{D}^{\mathrm{RC}}_{\mathrm{BC}} = \mathcal{D}^{\mathrm{RC}} \times \mathcal{D}_{\mathrm{BC}}$ $\quad \mathcal{D}^{\mathrm{RC}}_{\mathrm{data}} = \mathcal{D}^{\mathrm{RC}} \times \mathcal{D}_{\mathrm{data}}$

- $\mathcal{D}^{\mathrm{RC}} = \{(u^1_r, u^2_r, u^3_r, u^4_r, u^5_r)\}_{r=1}^{R}$ realizations of random coefficients
- $\mathcal{D}_{\mathrm{GE}} \subset D \times \Omega$ collocation points for GE loss
- $\mathcal{D}_{\mathrm{BC}} \subset \{(\boldsymbol{x}, \boldsymbol{s}) \in \partial D \times \Omega : \boldsymbol{s} \in \Omega^{\downarrow}(\boldsymbol{x})\}$ collocation points for BC loss
- $\mathcal{D}_{\mathrm{data}} \subset \overline{D} \times \Omega$ the mesh of a traditional solver e.g. finite volume method

$\mathscr{L}_{\mathrm{data}}$ the residual between the DeepONet prediction and the traditional solver solution

Quantities of interest

approximated using Gauss-Legendre quadrature or (Quasi-)Monte Carlo

- Incident radiation

$$G(\boldsymbol{x}) = \int I(\boldsymbol{x}, \boldsymbol{s}) \mathrm{d}\Omega, \qquad \boldsymbol{x} \in D$$

- Radiative Heat Flux

$$\boldsymbol{q}(\boldsymbol{x}) = \int I(\boldsymbol{x}, \boldsymbol{s}) \boldsymbol{s} \mathrm{d}\Omega, \qquad \boldsymbol{x} \in D$$

- Net Radiative Heat Flux

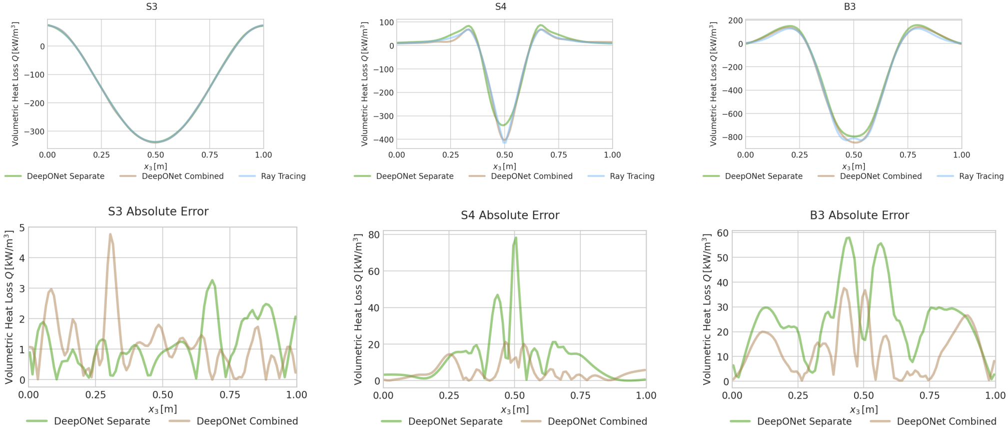
$$\boldsymbol{n}(\boldsymbol{x}) \cdot \boldsymbol{q}(\boldsymbol{x}) = \int I(\boldsymbol{x}, \boldsymbol{s}) \boldsymbol{s} \mathrm{d}\Omega^{\downarrow}(\boldsymbol{x}), \qquad \boldsymbol{x} \in \partial D$$

- Volumetric Heat Loss

$$Q(\boldsymbol{x}) = \nabla \cdot \boldsymbol{q}(\boldsymbol{x}), \qquad \boldsymbol{x} \in D$$

Parallel planes

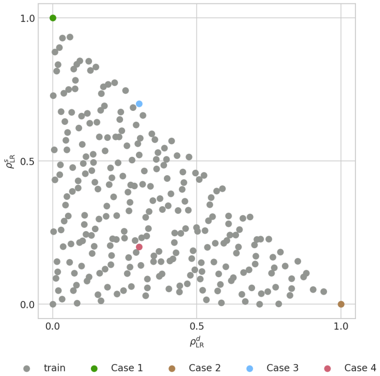
Non-gray gas with RCSLW model in `radlib`[7]

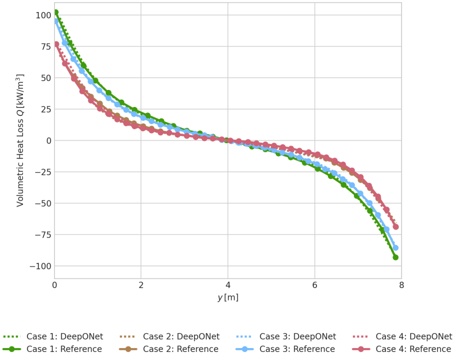


[7] Victoria B Stephens et al. "RadLib: A radiative property model library for CFD". In: *Comput. Phys. Commun.* 272 (2022), p. 108227.

Rectangular enclosure with random boundary conditions[8]

unknown constant coefficients $(\epsilon_{\mathrm{LR}}, \rho^d_{\mathrm{LR}}, \rho^s_{\mathrm{LR}})$ satisfying $\epsilon_{\mathrm{LR}} + \rho^d_{\mathrm{LR}} + \rho^s_{\mathrm{LR}} = 1$

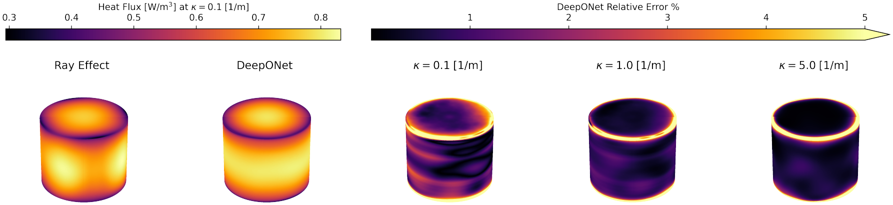




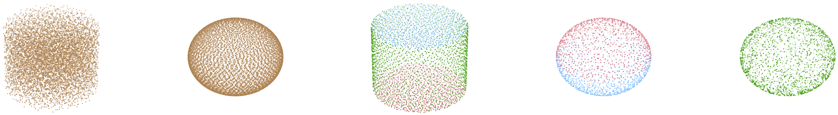
[8] Wenjun Ge, Michael F Modest, and Somesh P Roy. "Development of high-order PN models for radiative heat transfer in special geometries and boundary conditions". In: *Journal of Quantitative Spectroscopy and Radiative Transfer* 172 (2016), pp. 98–109.

Cylinder problem

gray gas with unknown constant absorption κ

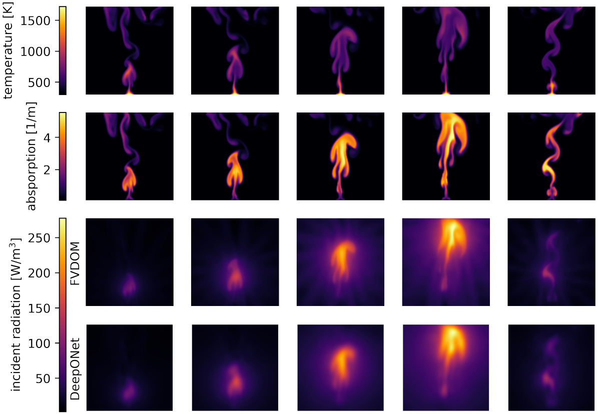


- L_2 relative errors of less than 2% were achieved at each held out $\kappa \in \{0.1, 1, 5\}$
- Overcomes the ray effect of Finite Volume Discrete Ordinates Method (FVDOM)
- Non-trivial to generate uniformly distributed collocation points below



Pool fire simulation in FireFOAM

unknown temperature and absorption coefficients



- Overcomes the ray effect of Finite Volume Discrete Ordinates Method (FVDOM)
- 4000 coefficient realizations, 365K collocation points, 3.1M DeepONet parameters

Conclusions

Presented

- Trained DeepONets to model radiative transfer with unknown coefficients
- Utilized SOA DeepONet enhancements: PCA, physics-informed loss
- Applied to a variety of problems including a medium scale pool fire in `FireFOAM`
- Overcame the ray effect common in traditional solvers e.g. FVDOM

In the works

- Show computational speedup when replacing traditional solver with DeepONet
- Open source `RTENet` software framework built on `PyTorch Lightning`
- Poster at NeurIPS 2024 D3S3 workshop following

  Aleksei Sorokin, Xiaoyi Lu, and Yi Wang. "A neural surrogate solver for radiation transfer". In: *NeurIPS 2024 Workshop on Data-driven and Differentiable Simulations, Surrogates, and Solvers*. 2024. URL: https://openreview.net/forum?id=SHidR8UMKo

Thank you for listening!

References I

[1] Wenjun Ge, Michael F Modest, and Somesh P Roy. “Development of high-order PN models for radiative heat transfer in special geometries and boundary conditions”. In: *Journal of Quantitative Spectroscopy and Radiative Transfer* 172 (2016), pp. 98–109.

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