A Neural Surrogate Solver for Radiation Transfer

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Background

Problem

- Simulating industrial-scale fires is computationally expensive
- Solving radiation transfer is one of the most costly part of these simulations

Objective

- Develop a fast neural surrogate solver for large-scale radiation transfer problems
- Overcome numerical issues in traditional methods e.g. the ray effect

Challenges

- Radiative transport equation (RTE): high-dimensional, integro-differential equations

$$s_j\frac{\partial I_\eta}{\partial x_j} = \underbrace{\kappa_\eta I_{b\eta}}_{\text{emission}} - \underbrace{(\kappa_\eta+\sigma_{s\eta})I_\eta}_{\text{absorption}} + \underbrace{\frac{\sigma_{s\eta}}{4\pi}\int_{4\pi} I_\eta(\hat{s}')\Phi(\hat{s}'\to\hat{s})d\Omega_i}_{\text{scattering}},$$

- Radiative properties: millions of spectral lines due to quantized energy transition levels
- Complex geometry, multi-phase flows, multi-physics, and many others

Radiative Transfer Equations

- 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 $\Omega^\downarrow(\boldsymbol{x})=\{\boldsymbol{s}\in\Omega : \boldsymbol{n}(\boldsymbol{x})\cdot\boldsymbol{s}(\boldsymbol{x})<0\}$

Radiative transfer equation (RTE)

$$\mathcal{L}_{\text{RTE}}\left(I,\left(u^1,\dots,u^5\right),(\boldsymbol{x},\boldsymbol{s})\right)=\boldsymbol{s}.\nabla I(\boldsymbol{x},\boldsymbol{s})+u^1(\boldsymbol{x})I(\boldsymbol{x},\boldsymbol{s})-u^1(\boldsymbol{x})u^2(\boldsymbol{x})=0$$

holds for $\boldsymbol{x}\in D$ and $\boldsymbol{s}\in\Omega$.

Boundary Condition (BC)

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

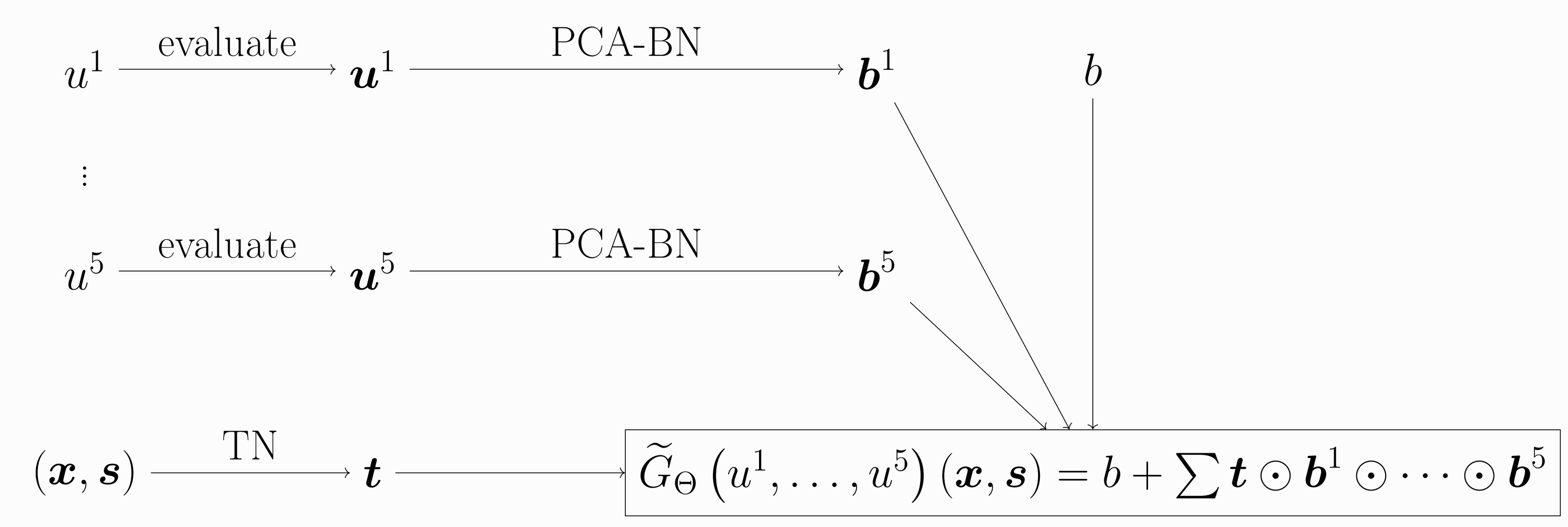
holds for $\boldsymbol{x}\in\partial D$ and $\boldsymbol{s}\in\Omega^\downarrow(\boldsymbol{x})$ with $\boldsymbol{s}_s(\boldsymbol{x},\boldsymbol{s})=\boldsymbol{s}-2\boldsymbol{n}(\boldsymbol{x})\left(\boldsymbol{n}(\boldsymbol{x})\cdot\boldsymbol{s}\right)$

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

Principal Component Analysis - Deep Operator Networks

Solution operator $G:(u^1,\dots,u^5)\mapsto I$ approximated by 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)** $\mathcal{B}_{\Theta_j}^j:\boldsymbol{u}^j\mapsto\mathcal{B}_{\Theta_j}^j(\mathsf{P}_j^\intercal\boldsymbol{u}^j-\boldsymbol{\mu}^j)=:\boldsymbol{b}^j\in\mathbb{R}^c$
- **TN (Trunk Net)** $\mathcal{T}_{\Theta_0}:(\boldsymbol{x},\boldsymbol{s})\mapsto\mathcal{T}_{\Theta_0}(\boldsymbol{x},\boldsymbol{s})=:\boldsymbol{t}\in\mathbb{R}^c$



Hybrid Physics-Informed Data-Driven Loss

$$\omega_{\text{GE}}\left\|\mathcal{L}_{\text{GE}}\left(\widetilde{G}_\Theta,\mathcal{D}_{\text{GE}}^{\text{RC}}\right)\right\|+\omega_{\text{BC}}\left\|\mathcal{L}_{\text{BC}}\left(\widetilde{G}_\Theta,\mathcal{D}_{\text{BC}}^{\text{RC}}\right)\right\|+\omega_{\text{data}}\left\|\mathcal{L}_{\text{data}}\left(\widetilde{G}_\Theta,\mathcal{D}_{\text{data}}^{\text{RC}}\right)\right\|$$

$$\mathcal{D}_{\text{GE}}^{\text{RC}}=\mathcal{D}^{\text{RC}}\times\mathcal{D}_{\text{GE}}\qquad\mathcal{D}_{\text{BC}}^{\text{RC}}=\mathcal{D}^{\text{RC}}\times\mathcal{D}_{\text{BC}}\qquad\mathcal{D}_{\text{data}}^{\text{RC}}=\mathcal{D}^{\text{RC}}\times\mathcal{D}_{\text{data}}$$

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

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

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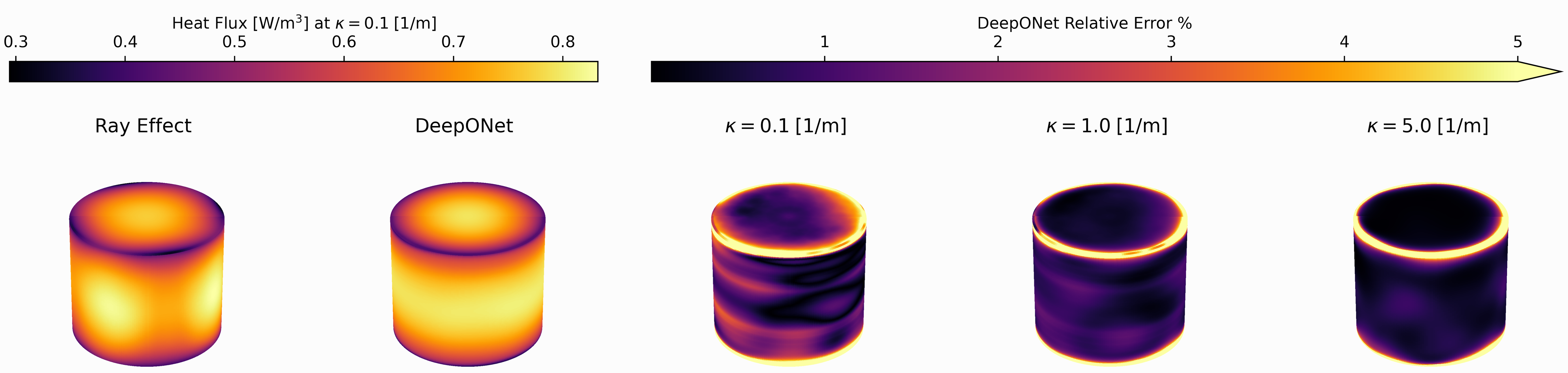
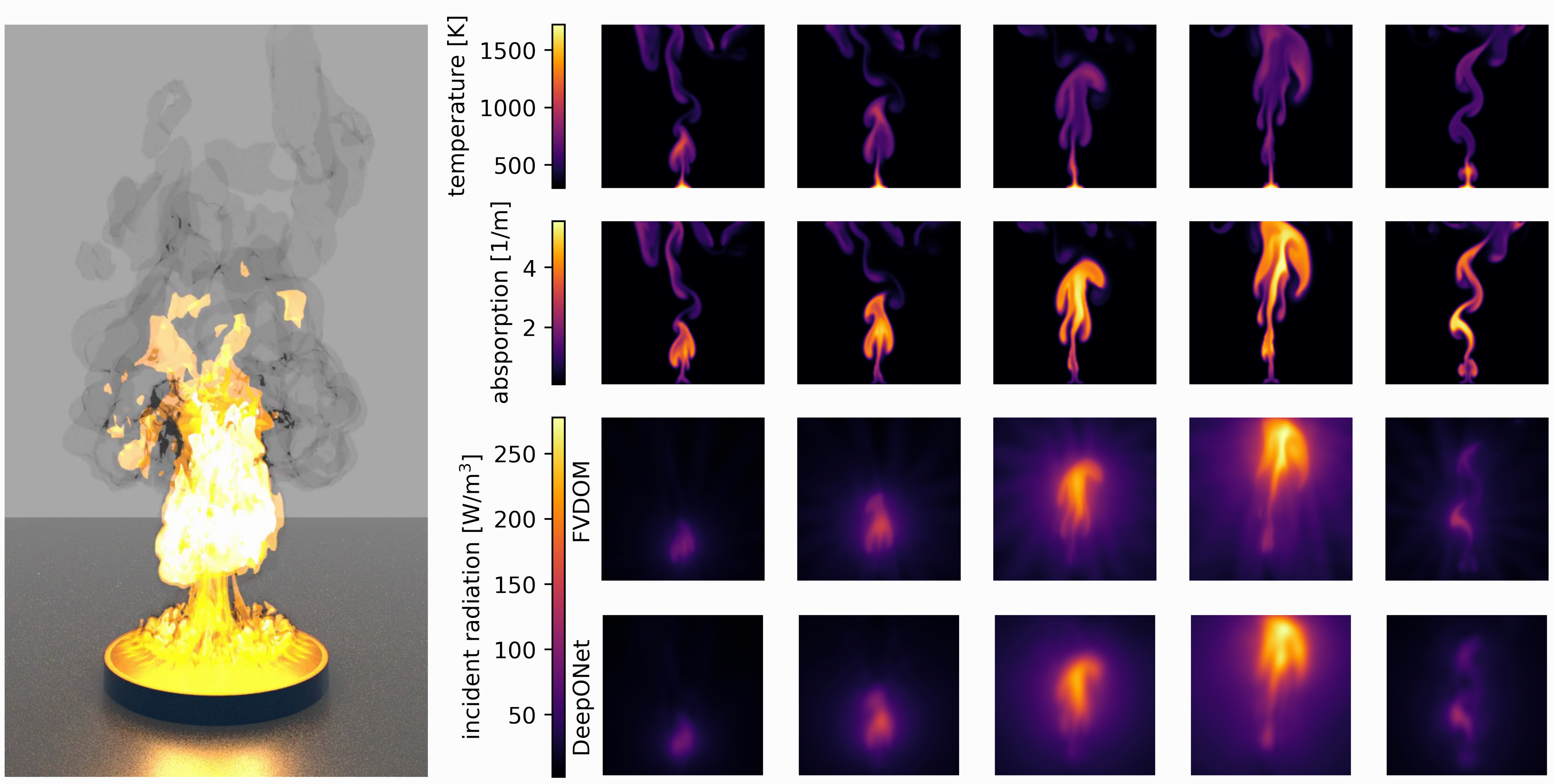
Radiation in a cylindrical enclosure



- The heat flux $\boldsymbol{n}(\boldsymbol{x}).\int\boldsymbol{s}I(\boldsymbol{x},\boldsymbol{s})\mathrm{d}\Omega^\downarrow(\boldsymbol{s})$ is approximated by numerically integrating DeepONet predictions over incident propagation directions $\boldsymbol{s}\in\Omega^\downarrow(\boldsymbol{x})$.
- Solving the RTE along a small number of solid angles leads to the ray effect.
- DeepONet can infer radiative intensity along any direction and eliminates the ray effect.

Radiation in pool fires



- The DeepONet predicts the radiative intensity I from the temperatures T and absorption coefficients κ generated by `FireFOAM`.
- The training data contains 365K snapshots of (T,κ) pairs generated from a `FireFOAM` solver.
- The incident radiation $\int I(\boldsymbol{x},\boldsymbol{s})\mathrm{d}\Omega$ is compared to the numerical solutions of traditional discrete-ordinate method.