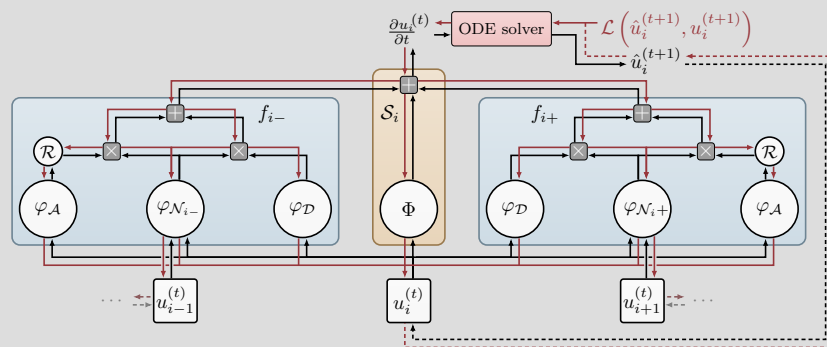




$$\frac{\partial u_i}{\partial t} = - \underbrace{\underbrace{\mathcal{R}(\varphi_A)}_{\mathcal{F}_i = f_{i-} + f_{i+}} \underbrace{\frac{\varphi_{N_{i-}}}{\varphi_{N_{i+}}} \text{ or } \frac{\varphi_{N_{i+}}}{\varphi_{N_{i-}}}}_{\varphi_D}}_{S_i} \frac{\partial u_i}{\partial x} + D(u_i) \frac{\partial^2 u_i}{\partial x^2} + q(u_i)$$

Composing Partial Differential Equations with Physics-Aware Neural Networks

Matthias Karlbauer*, Timothy Praditia*, Sebastian Otte, Sergey Oladyskhin, Wolfgang Nowak, Martin V. Butz

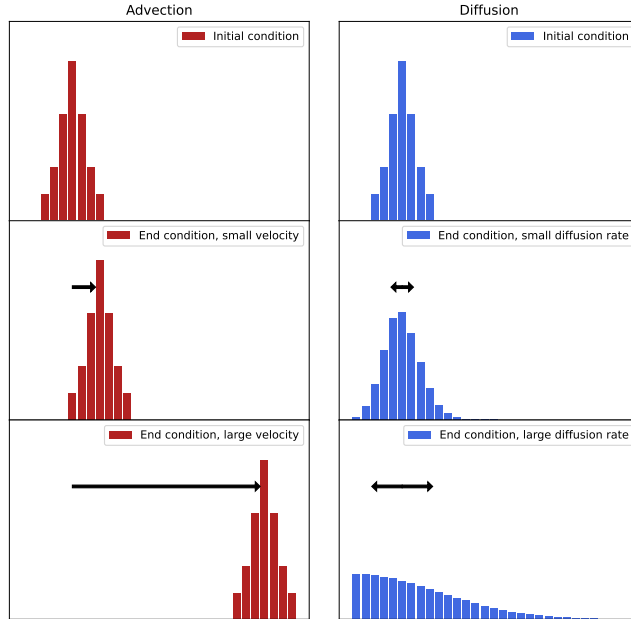
* Equal contribution



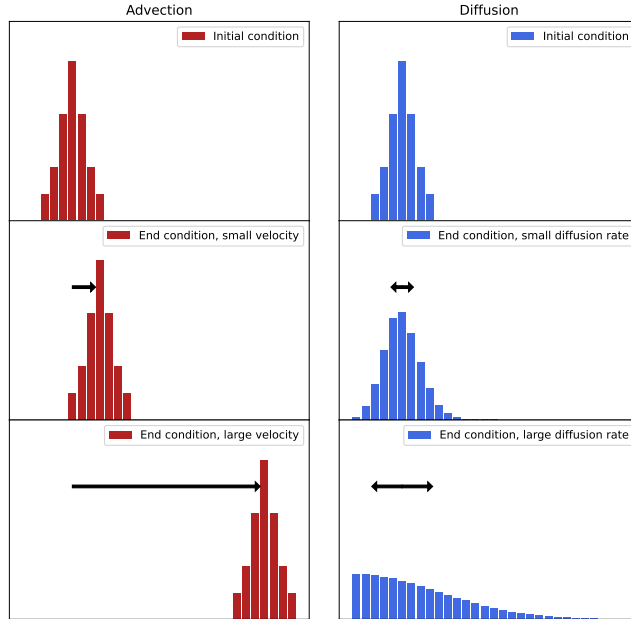
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Advection-Diffusion Processes

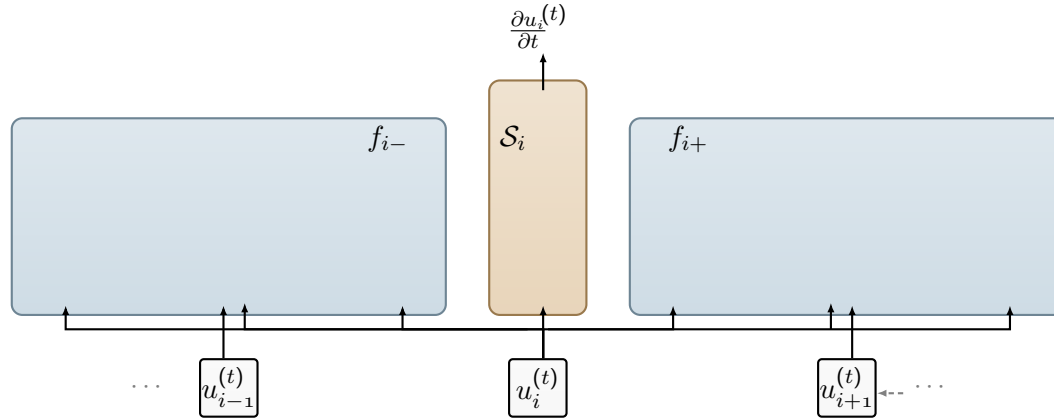


Advection-Diffusion Processes



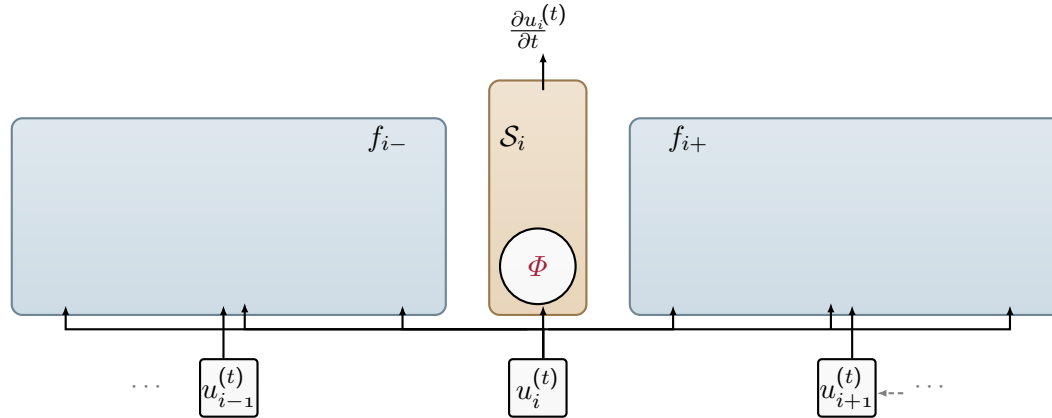
$$\frac{\partial u}{\partial t} = \overbrace{-v(u) \frac{\partial u}{\partial x}}^{\text{Advection}} + \overbrace{D(u) \frac{\partial^2 u}{\partial x^2}}^{\text{Diffusion}}$$

Finite volume Neural Network (FINN)



$$\frac{\partial u_i}{\partial t} = - \underbrace{v(u_i)}_{\text{advection}} + \underbrace{D(u_i)}_{\text{diffusion}} \underbrace{\frac{\partial^2 u_i}{\partial x^2}}_{\text{diffusion}} + \underbrace{q(u_i)}_{\text{source}}$$

Finite volume Neural Network (FINN)

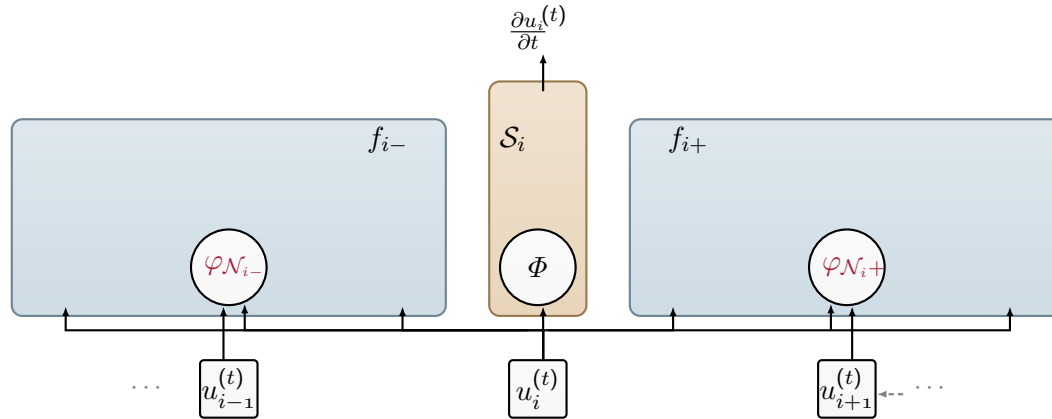


$$\frac{\partial u_i}{\partial t} = - \overbrace{v(u_i)} + \overbrace{\frac{\partial u_i}{\partial x}} + \overbrace{D(u_i)} \overbrace{\frac{\partial^2 u_i}{\partial x^2}} + \overbrace{q(u_i)}^{\Phi}$$

$$\Phi^*(u_i)$$

*Either a learnable parameter, a neural network, or (if known) the physical term.

Finite volume Neural Network (FINN)



$$\frac{\partial u_i}{\partial t} = - \underbrace{v(u_i)}_{\text{advection}} \underbrace{\left(\overbrace{\varphi_{\mathcal{N}_{i-}}^{\text{or}} \varphi_{\mathcal{N}_{i+}}}^{\varphi_{\mathcal{N}_{i-}} + \varphi_{\mathcal{N}_{i+}}} \right) \frac{\partial u_i}{\partial x}}_{\text{diffusion}} + \underbrace{D(u_i)}_{\text{diffusion}} \underbrace{\left(\overbrace{\varphi_{\mathcal{N}_{i-}} + \varphi_{\mathcal{N}_{i+}}}^{\varphi_{\mathcal{N}_{i-}} + \varphi_{\mathcal{N}_{i+}}} \right) \frac{\partial^2 u_i}{\partial x^2}}_{\text{diffusion}} + \underbrace{q(u_i)}_{\text{source}}$$

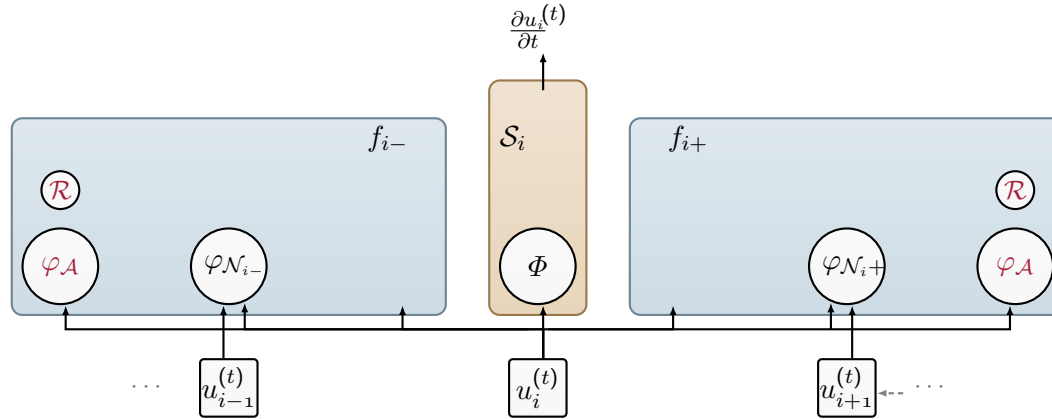
$$\Phi^*(u_i)$$

$$\varphi_{\mathcal{N}_{i-}}^*(u_{i-1}, u_i)$$

$$\varphi_{\mathcal{N}_{i+}}^*(u_{i+1}, u_i)$$

*Either a learnable parameter, a neural network, or (if known) the physical term.

Finite volume Neural Network (FINN)



$$\frac{\partial u_i}{\partial t} = - \underbrace{v(u_i)}_{\mathcal{R}(\varphi_A)} \underbrace{\frac{\partial u_i}{\partial x}}_{\varphi_{\mathcal{N}_{i-}} \text{ or } \varphi_{\mathcal{N}_{i+}}} + D(u_i) \underbrace{\frac{\partial^2 u_i}{\partial x^2}}_{\varphi_{\mathcal{N}_{i-}} + \varphi_{\mathcal{N}_{i+}}} + \underbrace{q(u_i)}_{\Phi}$$

$$\Phi^*(u_i)$$

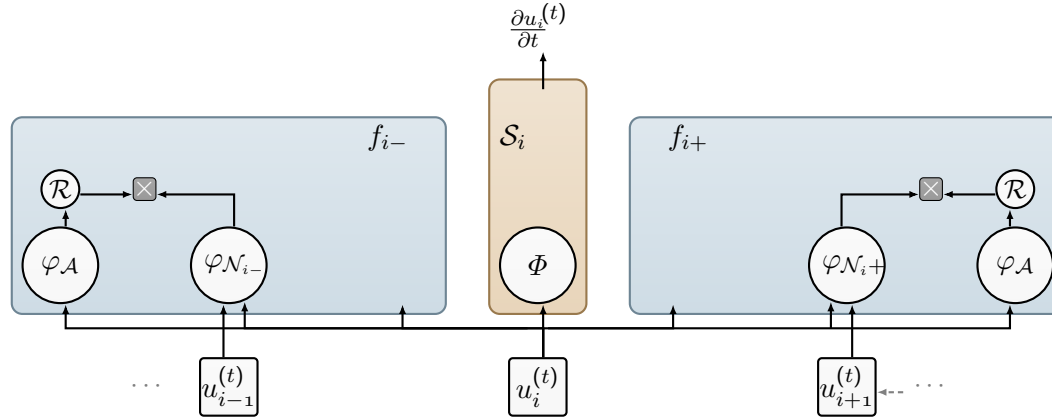
$$\varphi_{\mathcal{N}_{i-}}^*(u_{i-1}, u_i)$$

$$\varphi_{\mathcal{N}_{i+}}^*(u_{i+1}, u_i)$$

$$\mathcal{R} = \begin{cases} \text{ReLU}(\varphi_A) & \text{on } f_{i-} \\ -\text{ReLU}(-\varphi_A) & \text{on } f_{i+} \end{cases} \quad \varphi_A^*(u_i)$$

*Either a learnable parameter, a neural network, or (if known) the physical term.

Finite volume Neural Network (FINN)

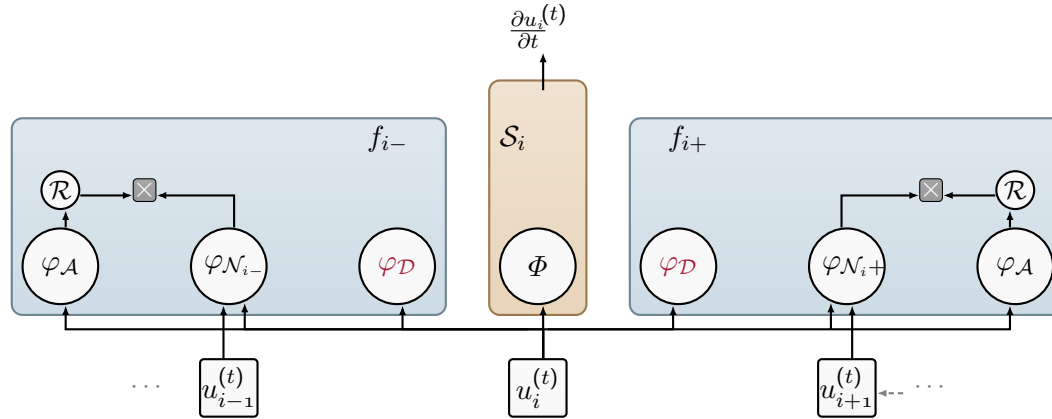


$$\frac{\partial u_i}{\partial t} = - \underbrace{v(u_i)}_{\mathcal{R}(\varphi_A)} \underbrace{\frac{\partial u_i}{\partial x}}_{\varphi_{N_{i-}} \text{ or } \varphi_{N_{i+}}} + \underbrace{D(u_i)}_{\varphi_{N_{i-}} + \varphi_{N_{i+}}} \underbrace{\frac{\partial^2 u_i}{\partial x^2}}_{\Phi} + q(u_i)$$

$$\Phi^*(u_i) \quad \varphi_{N_{i-}}^*(u_{i-1}, u_i) \quad \varphi_{N_{i+}}^*(u_{i+1}, u_i) \quad \mathcal{R} = \begin{cases} \text{ReLU}(\varphi_A) & \text{on } f_{i-} \\ -\text{ReLU}(-\varphi_A) & \text{on } f_{i+} \end{cases} \quad \varphi_A^*(u_i)$$

*Either a learnable parameter, a neural network, or (if known) the physical term.

Finite volume Neural Network (FINN)

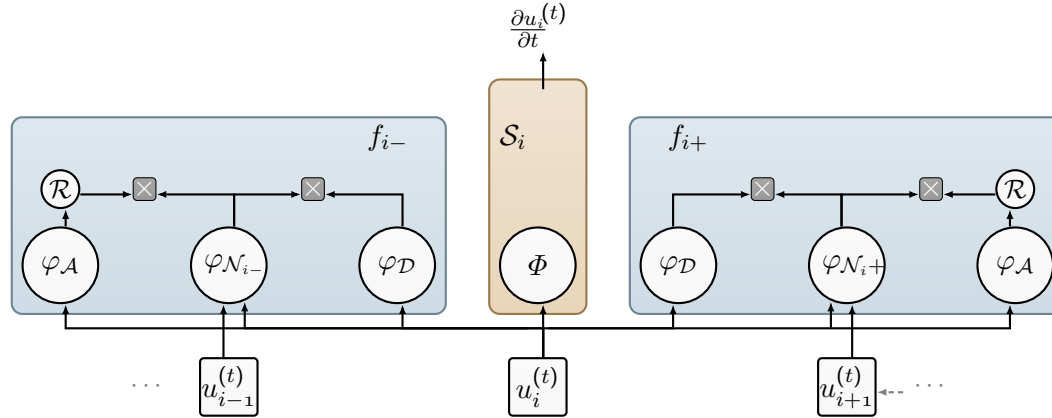


$$\frac{\partial u_i}{\partial t} = - \underbrace{\underbrace{\mathcal{R}(\varphi_A)}_{\varphi_{\mathcal{N}_{i-}} \text{ or } \varphi_{\mathcal{N}_{i+}}} \frac{\partial u_i}{\partial x} + \underbrace{\varphi_D}_{D(u_i)} \frac{\partial^2 u_i}{\partial x^2}}_{\Phi} + q(u_i)$$

$$\Phi^*(u_i) \quad \varphi_{\mathcal{N}_{i-}}^*(u_{i-1}, u_i) \quad \varphi_{\mathcal{N}_{i+}}^*(u_{i+1}, u_i) \quad \mathcal{R} = \begin{cases} \text{ReLU}(\varphi_A) & \text{on } f_{i-} \\ -\text{ReLU}(-\varphi_A) & \text{on } f_{i+} \end{cases} \quad \begin{matrix} \varphi_A^*(u_i) \\ \varphi_D^*(u_i) \end{matrix}$$

*Either a learnable parameter, a neural network, or (if known) the physical term.

Finite volume Neural Network (FINN)

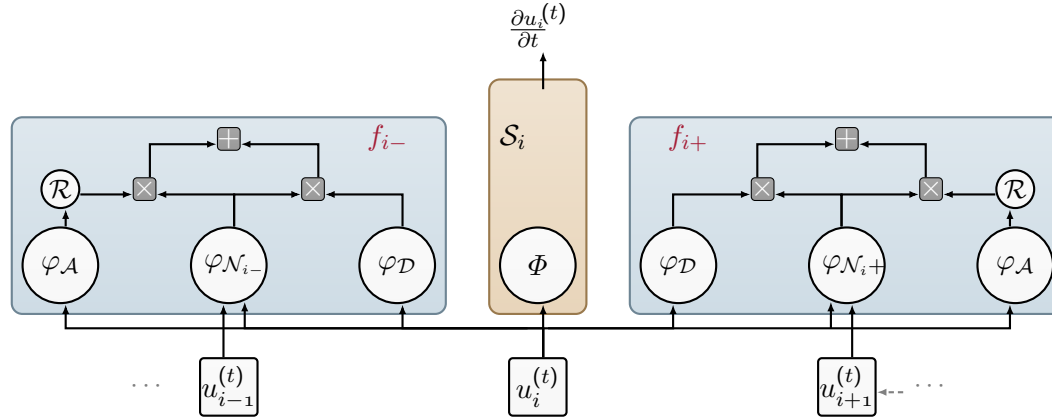


$$\frac{\partial u_i}{\partial t} = - \underbrace{v(u_i)}_{\mathcal{R}(\varphi_A)} \underbrace{\frac{\partial u_i}{\partial x}}_{\varphi_{\mathcal{N}_{i-}} \text{ or } \varphi_{\mathcal{N}_{i+}}} + \underbrace{D(u_i)}_{\varphi_D} \underbrace{\frac{\partial^2 u_i}{\partial x^2}}_{\varphi_{\mathcal{N}_{i-}} + \varphi_{\mathcal{N}_{i+}}} + \underbrace{q(u_i)}_{\Phi}$$

$$\Phi^*(u_i) \quad \varphi_{\mathcal{N}_{i-}}^*(u_{i-1}, u_i) \quad \varphi_{\mathcal{N}_{i+}}^*(u_{i+1}, u_i) \quad \mathcal{R} = \begin{cases} \text{ReLU}(\varphi_A) & \text{on } f_{i-} & \varphi_A^*(u_i) \\ -\text{ReLU}(-\varphi_A) & \text{on } f_{i+} & \varphi_D^*(u_i) \end{cases}$$

*Either a learnable parameter, a neural network, or (if known) the physical term.

Finite volume Neural Network (FINN)



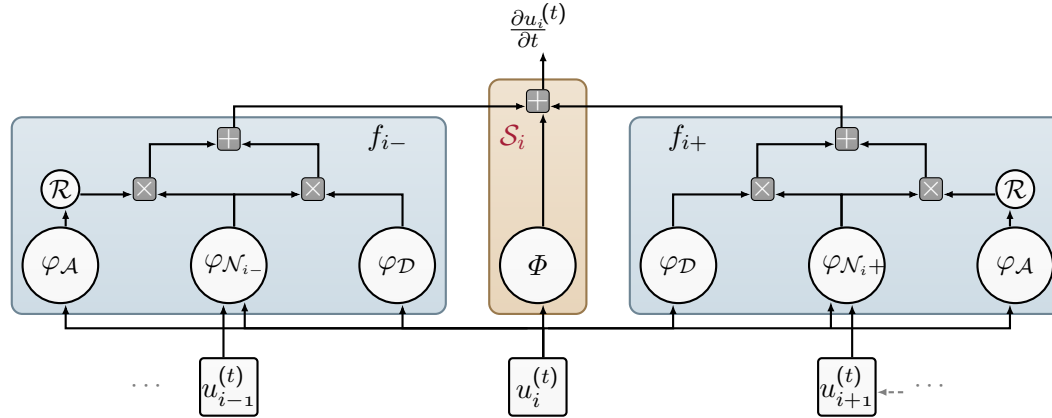
$$\frac{\partial u_i}{\partial t} = - \underbrace{v(u_i)}_{\mathcal{R}(\varphi_A)} \underbrace{\frac{\partial u_i}{\partial x}}_{\varphi_{\mathcal{N}_{i-}} \text{ or } \varphi_{\mathcal{N}_{i+}}} + \underbrace{D(u_i)}_{\varphi_D} \underbrace{\frac{\partial^2 u_i}{\partial x^2}}_{\varphi_{\mathcal{N}_{i-}} + \varphi_{\mathcal{N}_{i+}}} + \underbrace{q(u_i)}_{\Phi}$$

$$\underbrace{\mathcal{F}_i = f_{i-} + f_{i+}}_{\text{Total Flux}}$$

$$\Phi^*(u_i) \quad \varphi_{\mathcal{N}_{i-}}^*(u_{i-1}, u_i) \quad \varphi_{\mathcal{N}_{i+}}^*(u_{i+1}, u_i) \quad \mathcal{R} = \begin{cases} \text{ReLU}(\varphi_A) & \text{on } f_{i-} & \varphi_A^*(u_i) \\ -\text{ReLU}(-\varphi_A) & \text{on } f_{i+} & \varphi_D^*(u_i) \end{cases}$$

*Either a learnable parameter, a neural network, or (if known) the physical term.

Finite volume Neural Network (FINN)

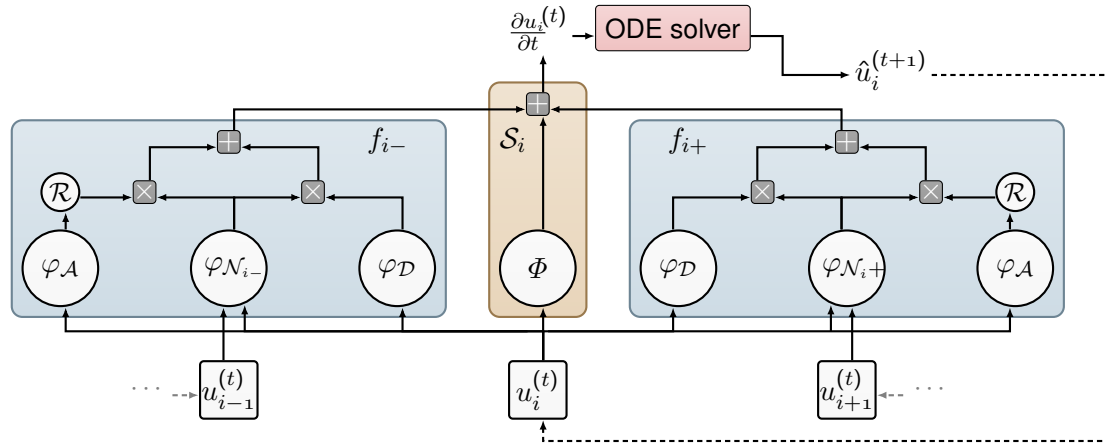


$$\frac{\partial u_i}{\partial t} = - \underbrace{\underbrace{\mathcal{R}(\varphi_A)}_{\varphi_{N_{i-}} \text{ or } \varphi_{N_{i+}}} \frac{\partial u_i}{\partial x} + \underbrace{\varphi_D}_{\varphi_{N_{i-}} + \varphi_{N_{i+}}} \frac{\partial^2 u_i}{\partial x^2}}_{\mathcal{F}_i = f_{i-} + f_{i+}} + \underbrace{q(u_i)}_{\Phi}$$

$$\Phi^*(u_i) \quad \varphi_{N_{i-}}^*(u_{i-1}, u_i) \quad \varphi_{N_{i+}}^*(u_{i+1}, u_i) \quad \mathcal{R} = \begin{cases} \text{ReLU}(\varphi_A) & \text{on } f_{i-} & \varphi_A^*(u_i) \\ -\text{ReLU}(-\varphi_A) & \text{on } f_{i+} & \varphi_D^*(u_i) \end{cases}$$

*Either a learnable parameter, a neural network, or (if known) the physical term.

Finite volume Neural Network (FINN)



$$\frac{\partial u_i}{\partial t} = - \underbrace{v(u_i)}_{\mathcal{R}(\varphi_{\mathcal{A}})} \underbrace{\frac{\partial u_i}{\partial x}}_{\substack{\varphi_{\mathcal{N}_{i-}} \\ \text{or} \\ \varphi_{\mathcal{N}_{i+}}}} + \underbrace{D(u_i)}_{\varphi_{\mathcal{D}}} \underbrace{\frac{\partial^2 u_i}{\partial x^2}}_{\substack{\varphi_{\mathcal{N}_{i-}} \\ + \\ \varphi_{\mathcal{N}_{i+}}}} + \underbrace{q(u_i)}_{\Phi}$$

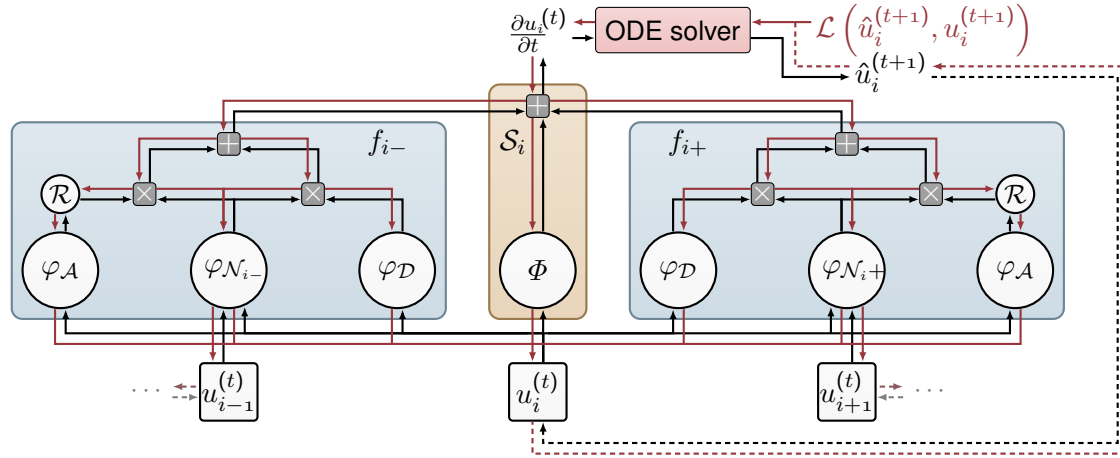
$$\underbrace{\hspace{15em}}_{\mathcal{F}_i = f_{i-} + f_{i+}}$$

$$\underbrace{\hspace{15em}}_{\mathcal{S}_i}$$

$$\Phi^*(u_i) \quad \begin{array}{l} \varphi_{\mathcal{N}_{i-}}^*(u_{i-1}, u_i) \\ \varphi_{\mathcal{N}_{i+}}^*(u_{i+1}, u_i) \end{array} \quad \mathcal{R} = \begin{cases} \text{ReLU}(\varphi_{\mathcal{A}}) & \text{on } f_{i-} & \varphi_{\mathcal{A}}^*(u_i) \\ -\text{ReLU}(-\varphi_{\mathcal{A}}) & \text{on } f_{i+} & \varphi_{\mathcal{D}}^*(u_i) \end{cases}$$

* Either a learnable parameter, a neural network, or (if known) the physical term.

Finite volume Neural Network (FINN)



$$\frac{\partial u_i}{\partial t} = - \underbrace{v(u_i) \frac{\partial u_i}{\partial x} + D(u_i) \frac{\partial^2 u_i}{\partial x^2} + q(u_i)}_{\mathcal{F}_i = f_{i-} + f_{i+}} + \underbrace{\mathcal{R}(\varphi_A)}_{\varphi_{\mathcal{N}_{i-}} \text{ or } \varphi_{\mathcal{N}_{i+}}} + \underbrace{\varphi_{\mathcal{D}}}_{\varphi_{\mathcal{N}_{i+}} + \varphi_{\mathcal{N}_{i-}}} + \underbrace{\Phi}_{\Phi}$$

$$\Phi^*(u_i) \quad \varphi_{\mathcal{N}_{i-}}^*(u_{i-1}, u_i) \quad \varphi_{\mathcal{N}_{i+}}^*(u_{i+1}, u_i) \quad \mathcal{R} = \begin{cases} \text{ReLU}(\varphi_A) & \text{on } f_{i-} & \varphi_A^*(u_i) \\ -\text{ReLU}(-\varphi_A) & \text{on } f_{i+} & \varphi_D^*(u_i) \end{cases}$$

*Either a learnable parameter, a neural network, or (if known) the physical term.



Benchmark: 2D Burgers' equation



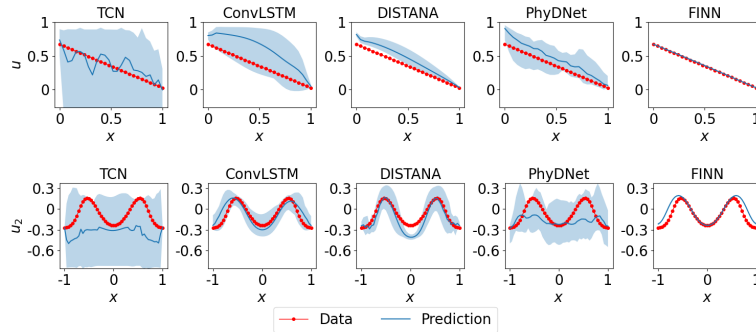
Applications

Ongoing work

Applications

Ongoing work

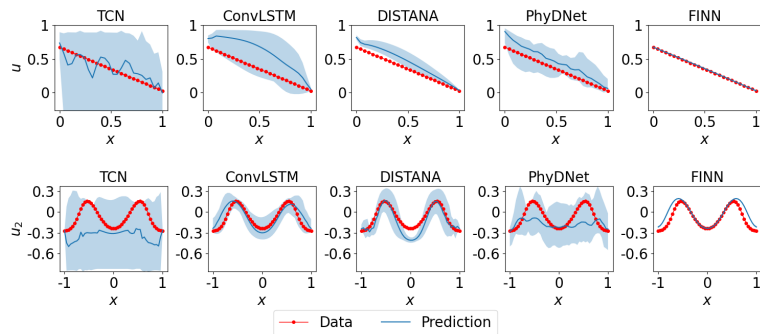
► Characterization of substance diffusion



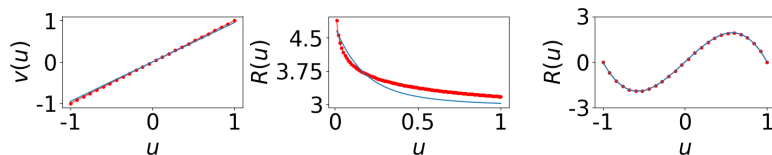
Applications

Ongoing work

► Characterization of substance diffusion

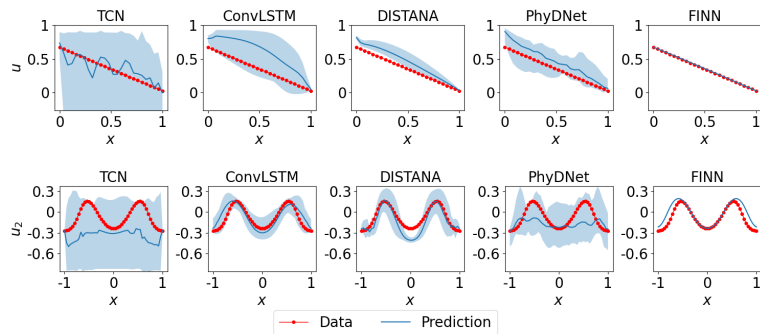


► Determination of unknown functions

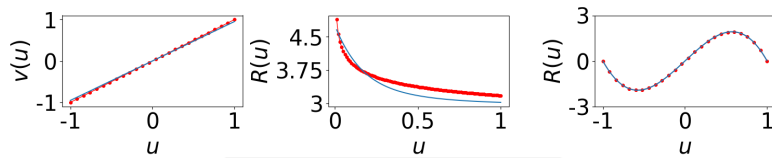


Applications

► Characterization of substance diffusion

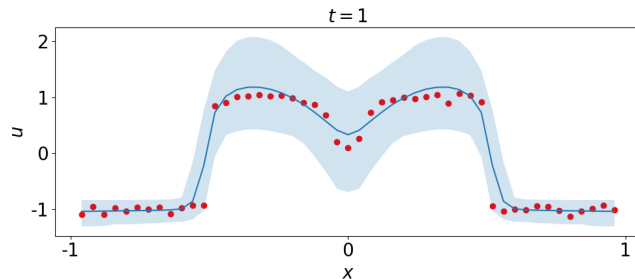


► Determination of unknown functions



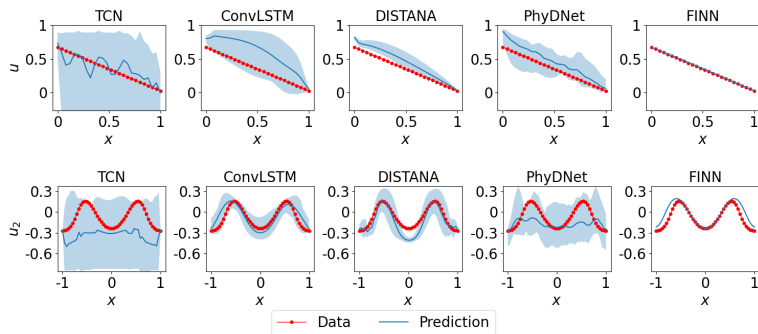
Ongoing work

► Direct uncertainty estimates

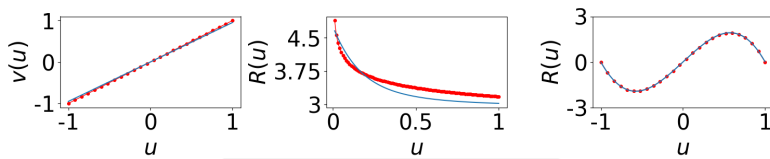


Applications

► Characterization of substance diffusion

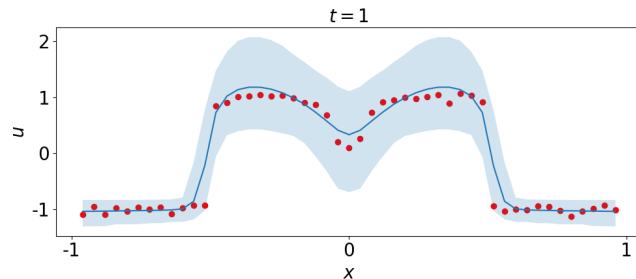


► Determination of unknown functions



Ongoing work

► Direct uncertainty estimates



► Inference of boundary conditions

