PINN: Final Presentation

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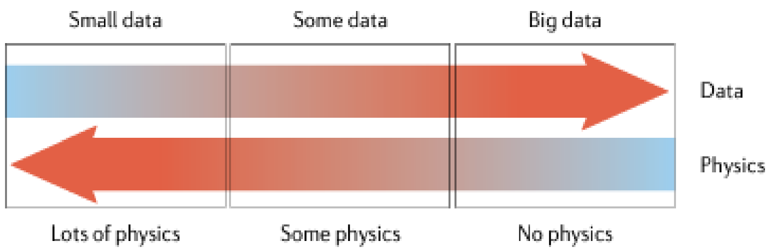
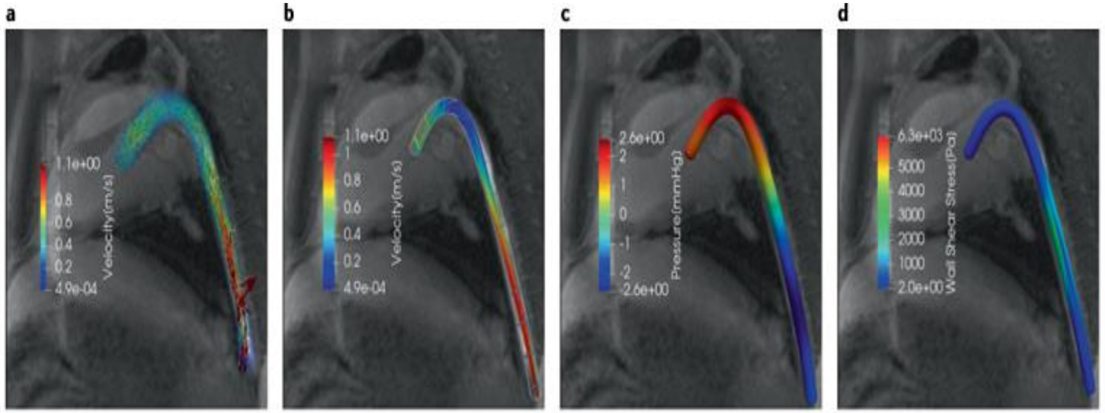
Overview

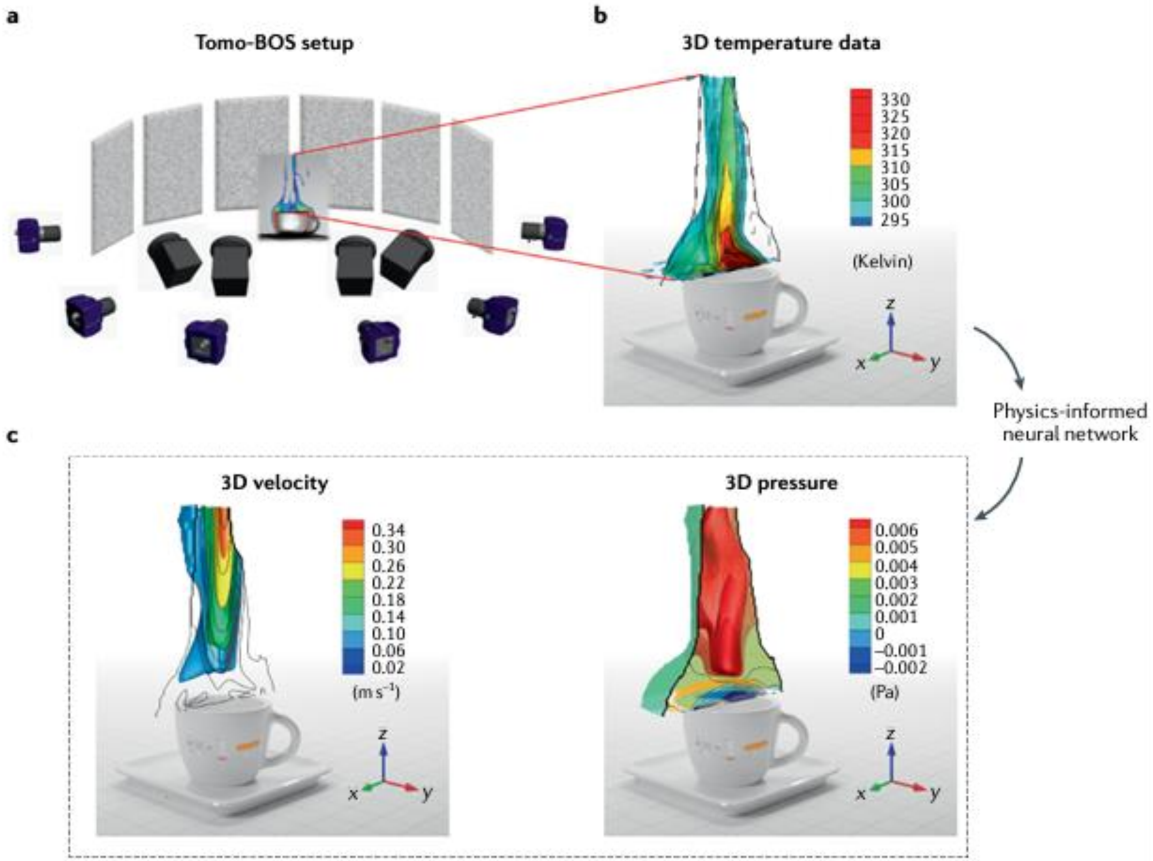
- Background and motivations
  - Hybrid method to attack complicated problems
  - PINN technical details
- Models
  - Burgers’ equation (1D)
  - Diffusion equation (1D vs 2D)
- Result and discussion
  - Data Simulation and PINN results
  - Future Works

Motivation



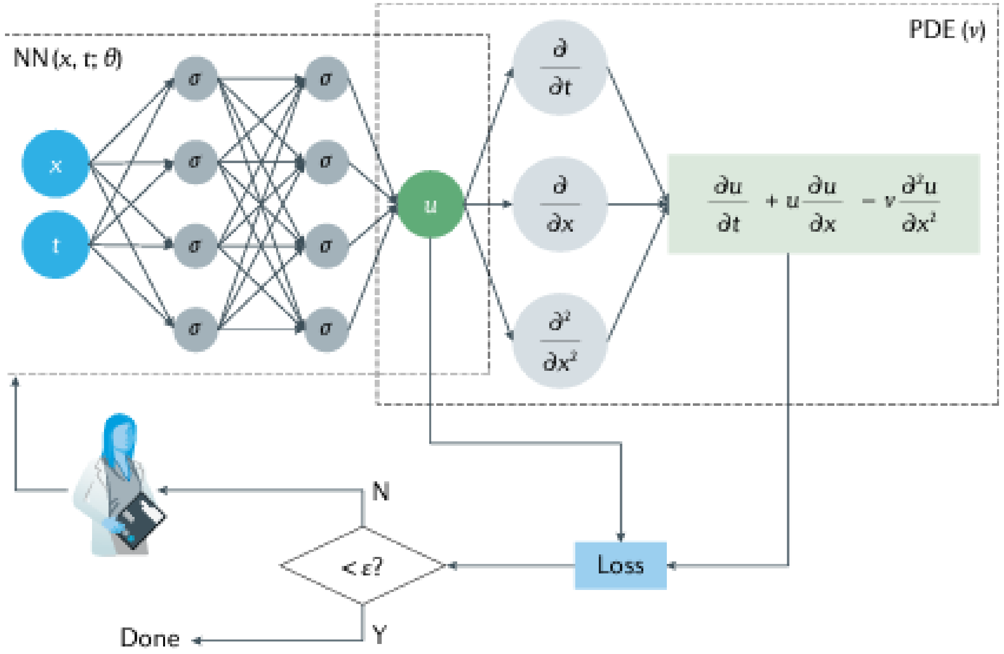


Physics-informed filtering of in-vivo 4D-flow magnetic resonance imaging data of blood flow in a porcine descending aorta (Rassi).
a: Noisy GT Velocity, b: Denoised Velocity, c: Inferred Pressure, d: Inferred Aterial Shear Stress



PINN's generated temperature, velocity, and pressure time series of a coffee cup from background distortion captured by cameras

PINN: Architecture details

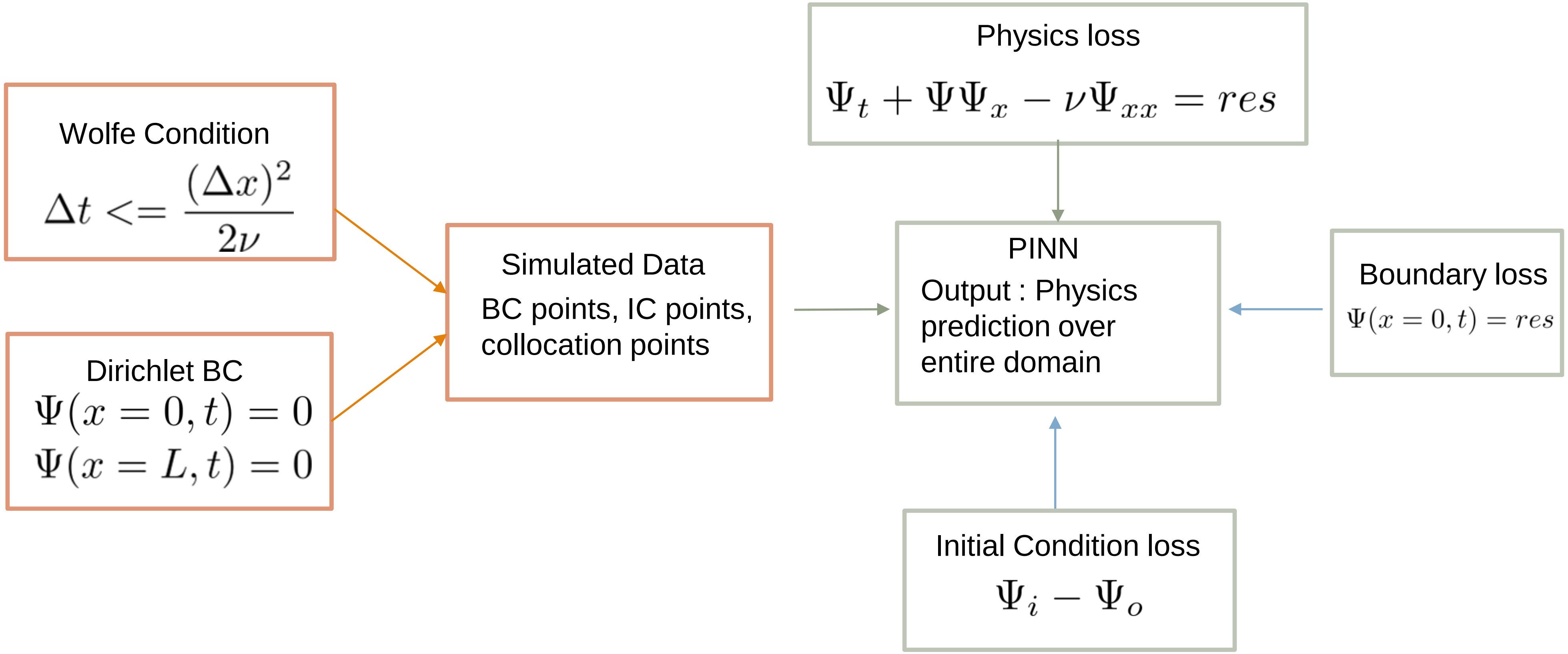


- Specialized loss function:
  - Data driven term
  - Physics driven term
- Data driven term:
  - Fit available data (observations/measurements)
- Physics driven term:
  - Enforce underlying physical laws
- Examples:
  - Burger's (1D)
  - Diffusion (1D)
  - Diffusion (2D)

- Optimizer = LBFGS
  - quasi-Newton approach, full-batch gradient-based optimization algorithm
  - It is commonly used in optimization problems where the number of variables is large

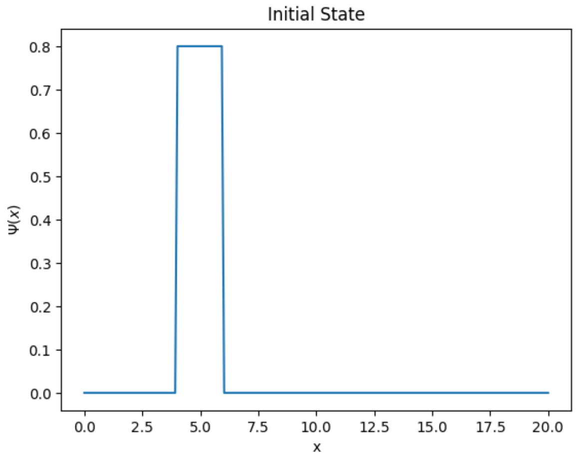
Source: Karniadakis, George & Kevrekidis, Yannis & Lu, Lu & Perdikaris, Paris & Wang, Sifan & Yang, Liu. (2021). Physics-informed machine learning. 1-19. 10.1038/s42254-021-00314-5.

1D PINN architecture

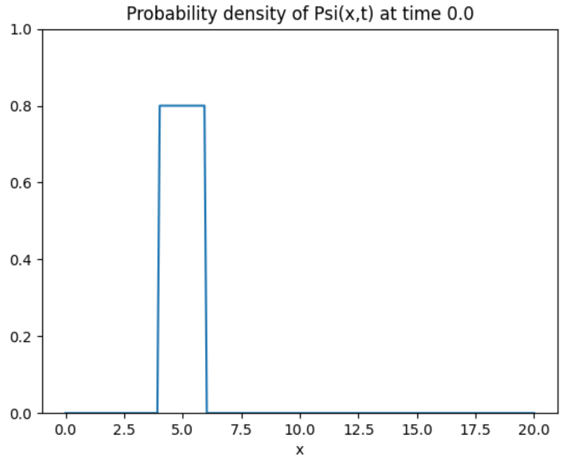


Burger’s equation: $\Psi_t + \Psi\Psi_x - \nu\Psi_{xx} = 0$

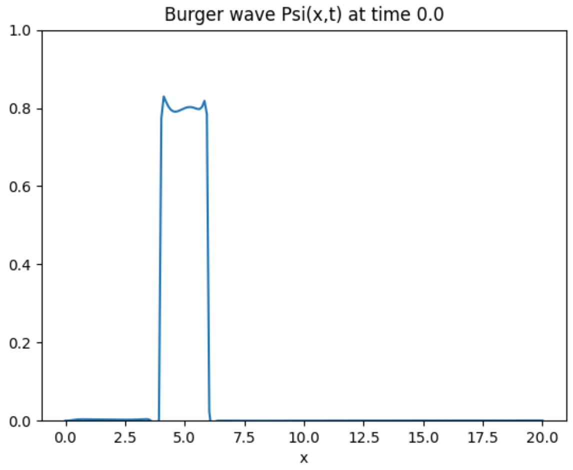
MSE: `0.002 (no and low noise), 0.0922 (high noise)`



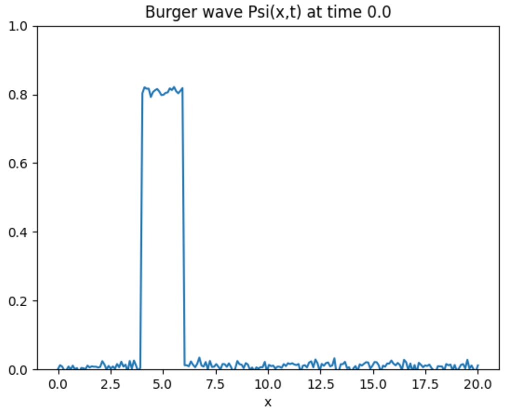
Initial Condition



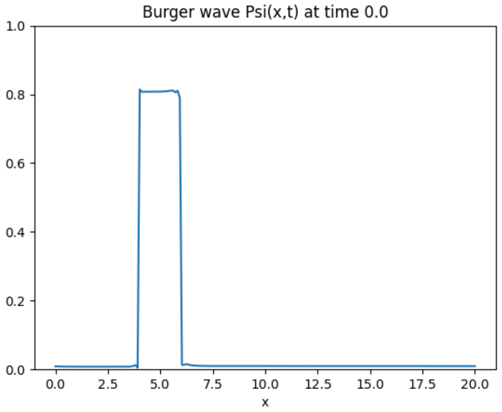
Simulated Ground Truth



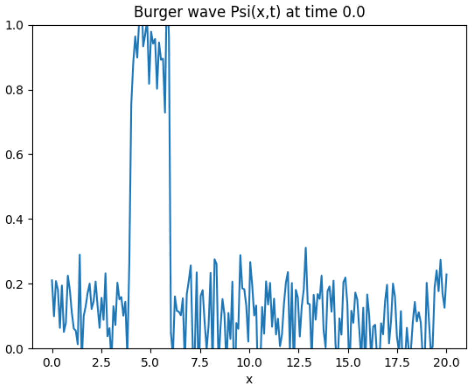
PINN output



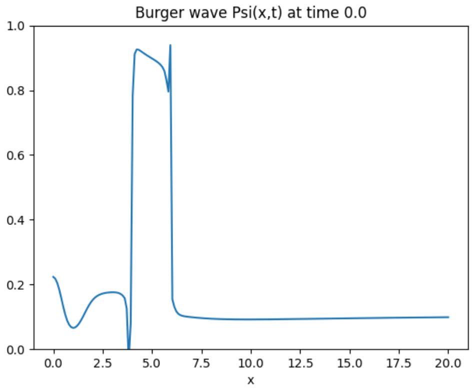
Noisy Ground Truth (low)



Noisy PINN output (low)

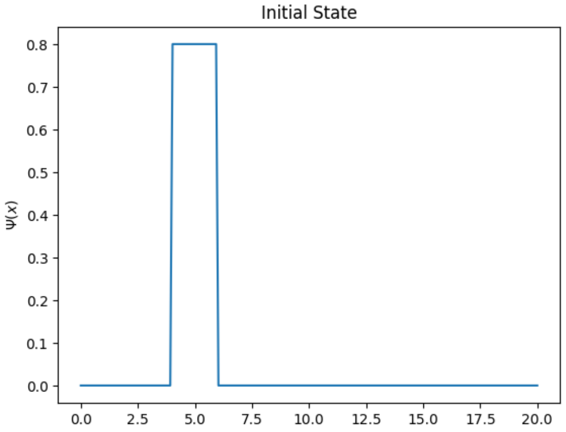


Noisy Ground Truth (high)

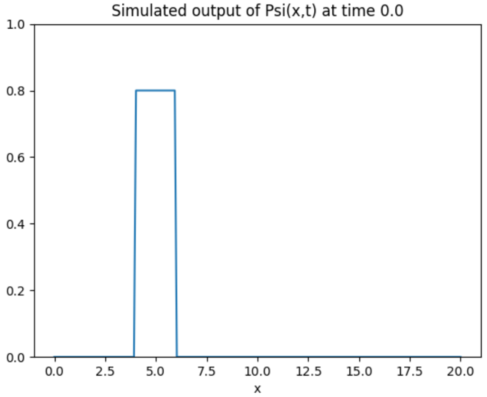


Noisy PINN output (high)

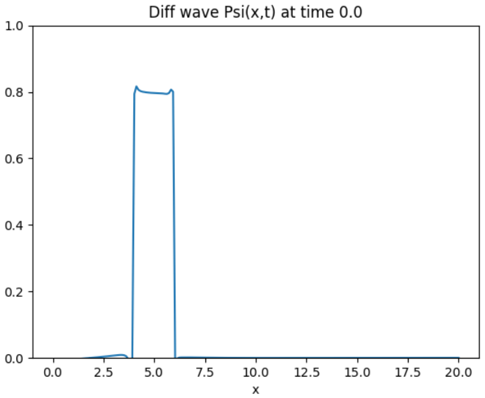
Burger's equation: $\Psi_t + \Psi\Psi_x - \nu\Psi_{xx} = 0$ $\xrightarrow{\Psi\Psi_x << 1}$ Diffusion equation: $\Psi_t - \nu\Psi_{xx} = 0$



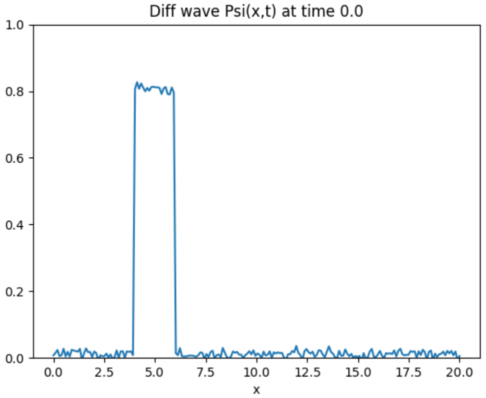
Initial Condition



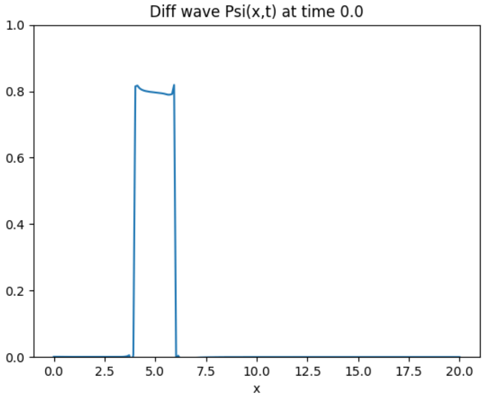
Ground truth



PINN prediction



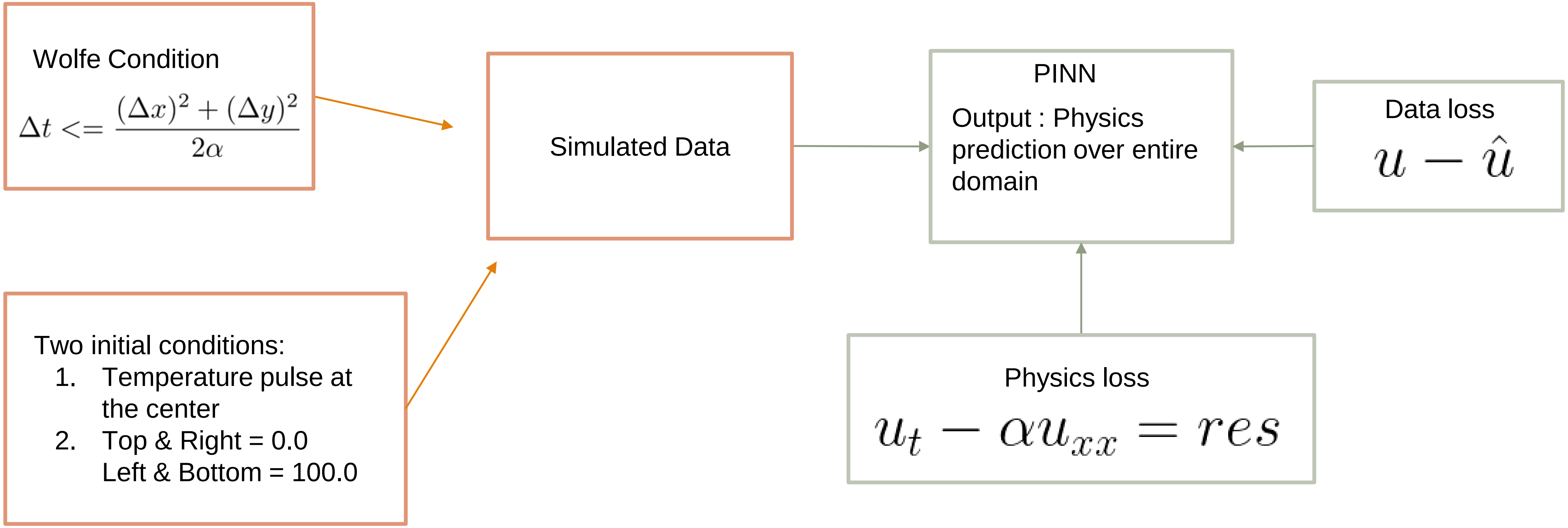
noise corrupted ground truth



Noisy PINN prediction

MSE: `0.001 (no and low noise)`

Diffusion in 2D



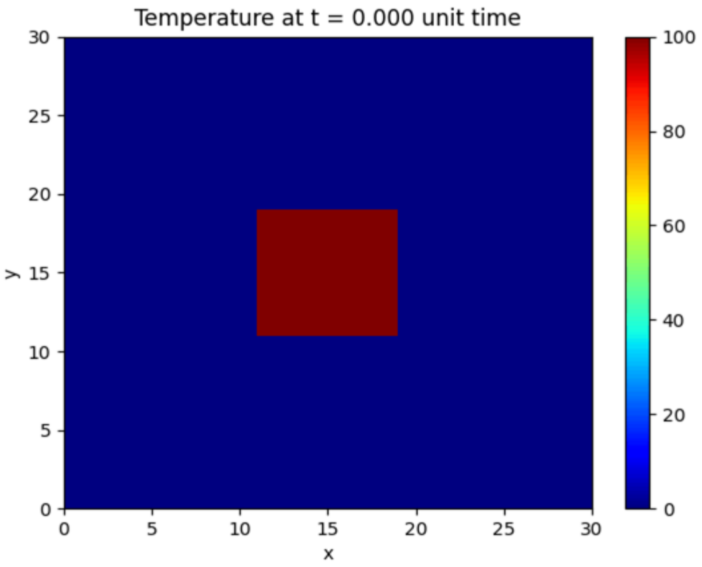
2D Diffusion Simulation

2D Diffusion Equation:

$$\frac{\partial u}{\partial t} = \alpha \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$

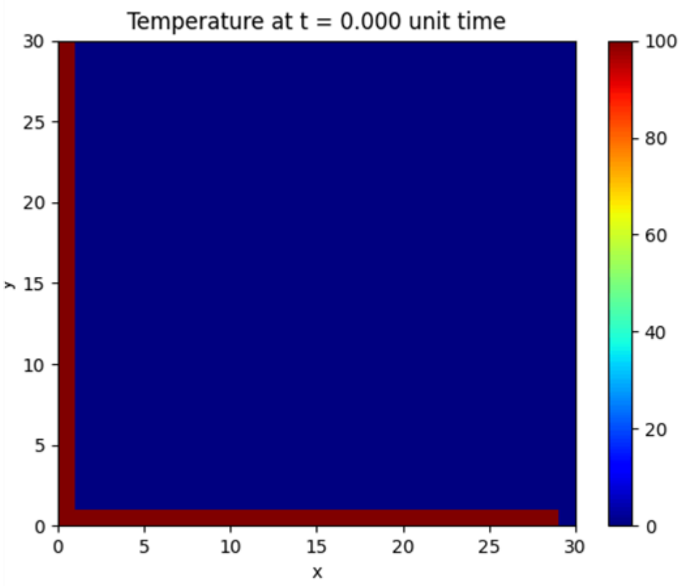
$\alpha = 1$ ⇨ Generalization for any system

Finite Differencing



Pulse at the center

(IC 1)



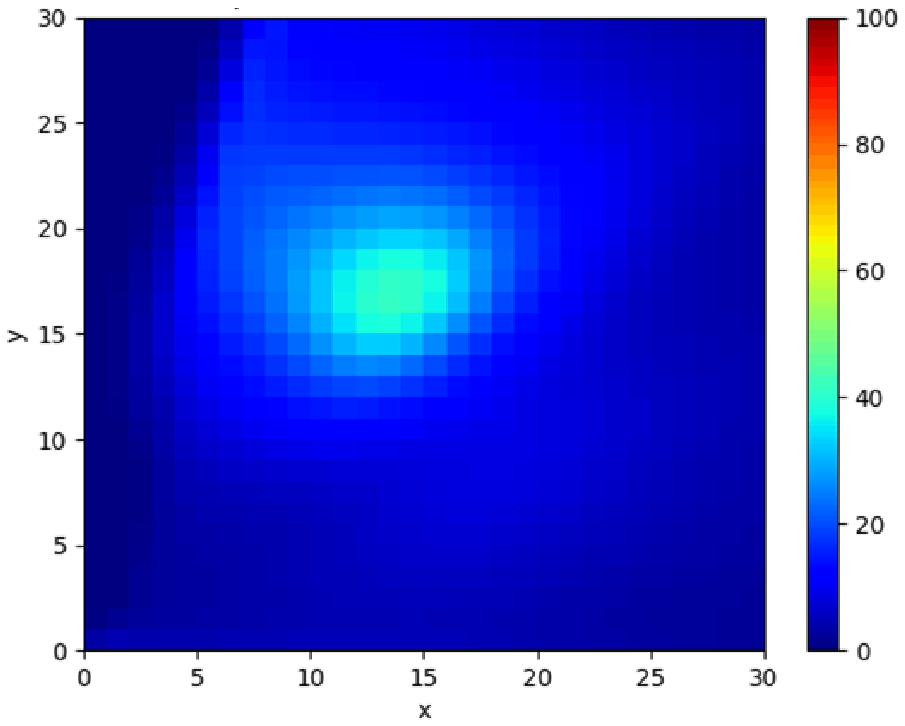
IC → Left, Bottom =100

Top,

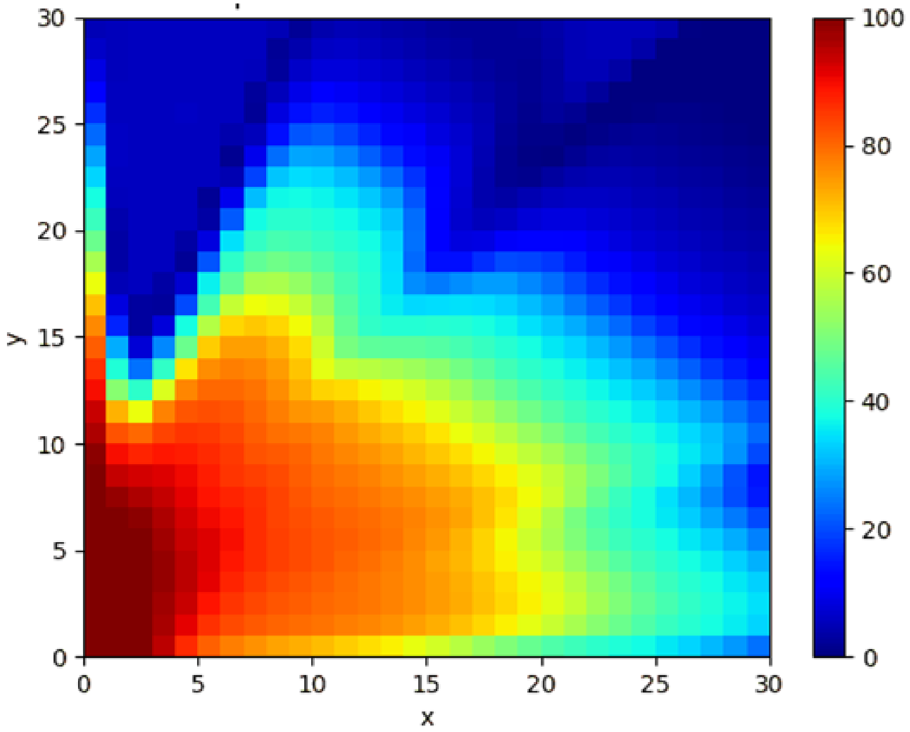
Right = 0

(IC 2)

Results : 2D Diffusion PINN Model



(a)



(b)

Model Outputs for (a) IC 1 and (b) IC 2

Conclusion

1. PINN performs well as a hybrid method: data augmentation, denoising
2. PINN's performance is dependent on loss structure
    a. BC and IC losses
    b. Physics model (wrong model can be misleading)
3. Limitation: high noise, initial condition dependent generalization, prediction

Future improvements

- Improve PINN models
  - Add boundary and initial losses
  - Conservation laws
    - Mass and momentum
  - Different architectures
  - Hyper parameter tuning

- Adapt PINNs for systems in complex space

- Adapt PINNs for data with different noise sources

References

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PINN architecture references

Physics Architecture guide

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Raissi, Maziar, Paris Perdikaris, and George Em Karniadakis. "Physics Informed Deep Learning (Part I): Data-driven Solutions of Nonlinear Partial Differential Equations." arXiv preprint arXiv:1711.10561 (2017).

Raissi, Maziar, Paris Perdikaris, and George Em Karniadakis. "Physics Informed Deep Learning (Part II): Data-driven Discovery of Nonlinear Partial Differential Equations." arXiv preprint arXiv:1711.10566 (2017).

Github references, both sources are from researchers affiliated with George Karniadakis of Brown University (No codes were taken, but their works were studied to reverse engineer the physics data preprocessing):

https://github.com/maziarraissi/PINNs

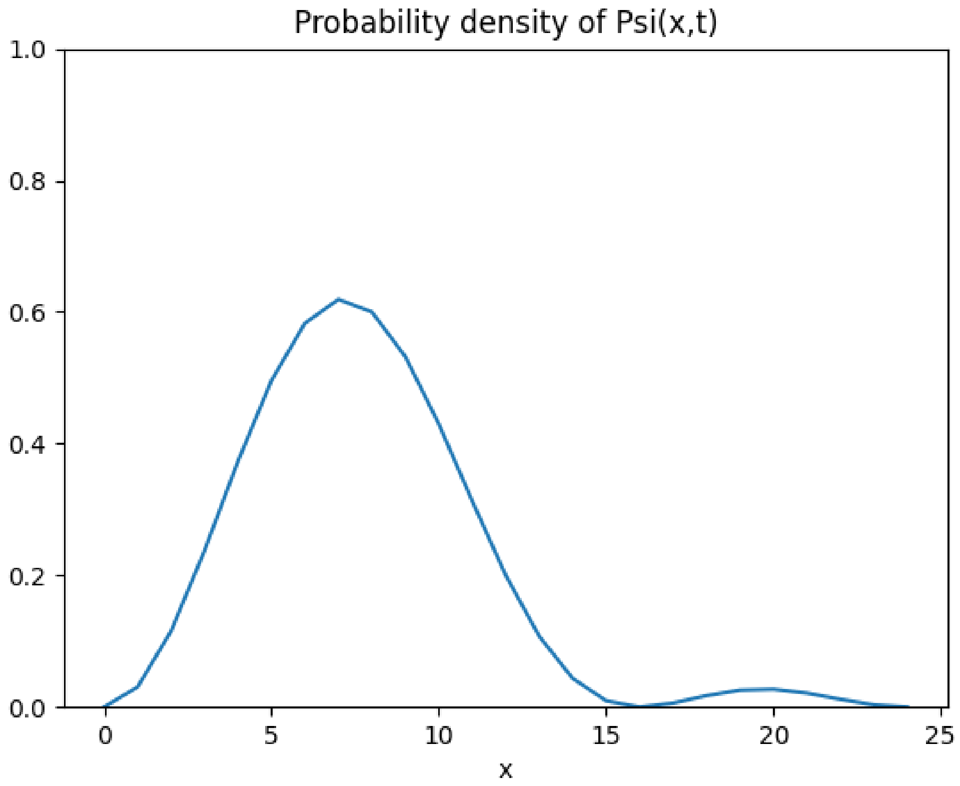
https://github.com/jdtoscano94/Learning-Python-Physics-Informed-Machine-Learning-PINNs-DeepONets/tree/main/PINNs

1D Schrodinger Eq:

- Schrodinger wave function in Planck unit:

$$i\frac{d\Psi}{dt} = -\frac{1}{2}\frac{d^2\Psi}{dx^2} + V(x)\Psi(x)$$

- All physical information can be inferred through Psi(x,t): probabilities of energy, momentum, positions
- <A> = <Psi|A|Psi>
- For the case of 1-D infinite potential box, we can ignore the potential term V(x)



Data Simulation and PINN architecture