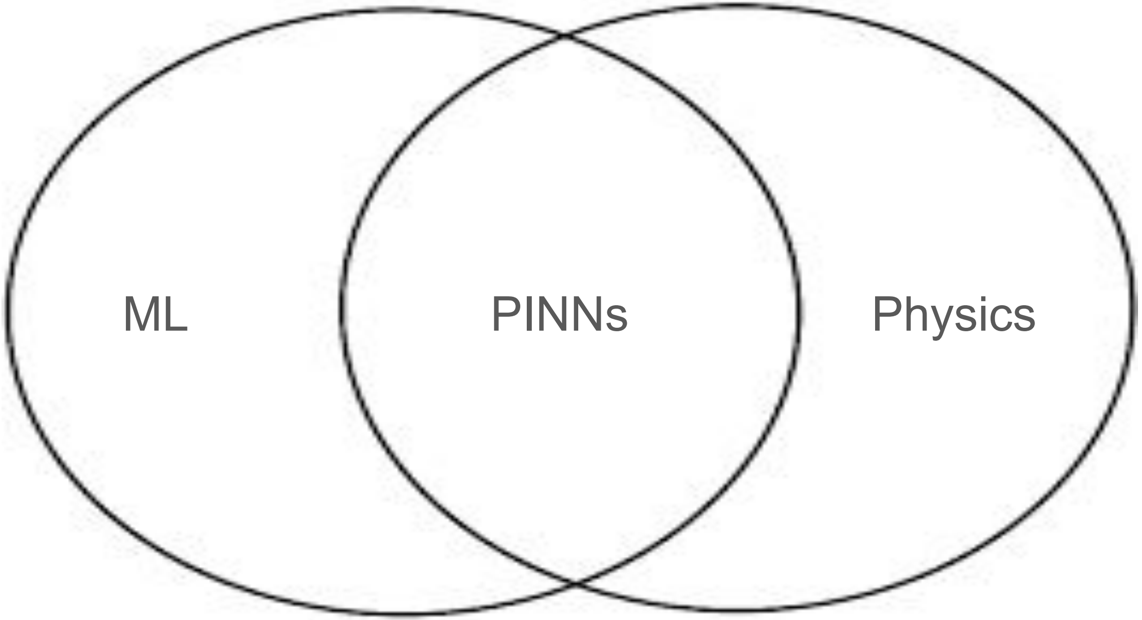
Title and introduction
~ 1 Minute

Physics-informed Neural Networks

A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations

Joel Reimann

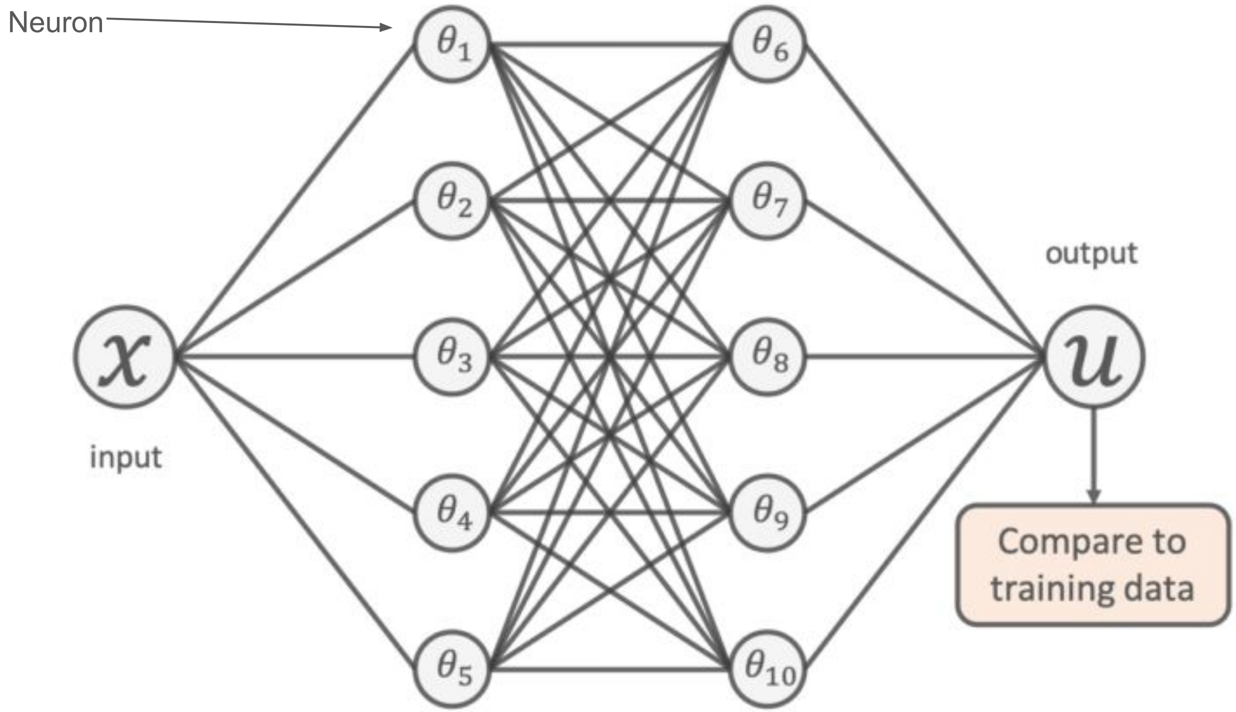
Timon Wattenhofer



A paper by M. Raissi, P. Perdikaris, G.E. Karniadakis

Introductory example
~ 4 min

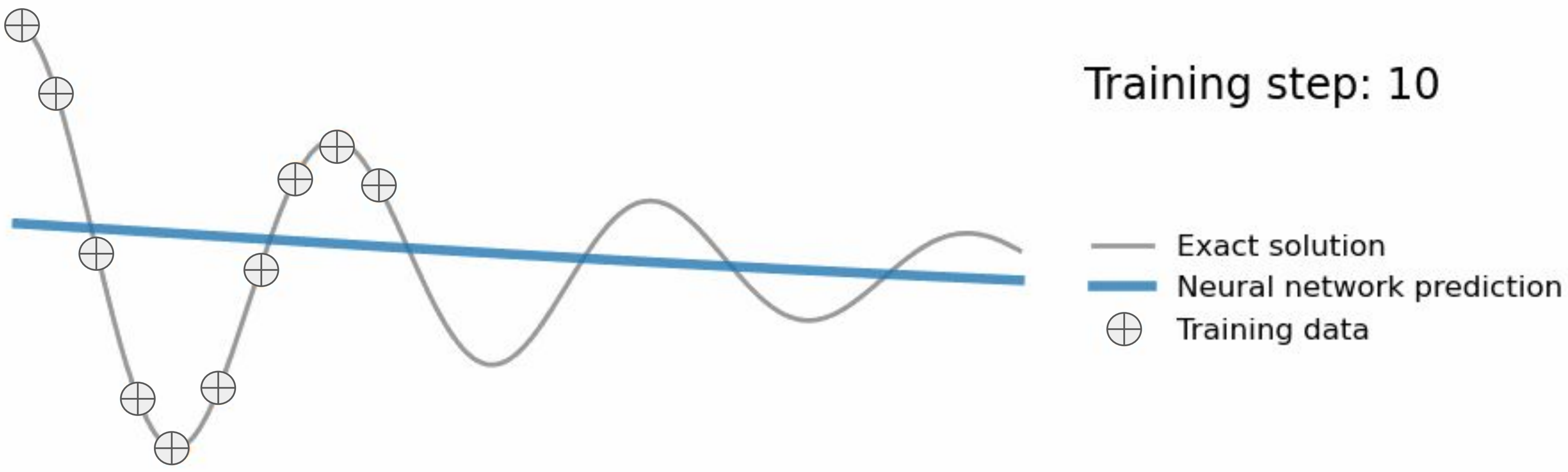
So what exactly is a physics-informed neural network?



$$\min \frac{1}{N} \sum_{i}^{N} (u_{\mathrm{NN}}(x_i;\theta) - u_{\mathrm{true}}(x_i))^2$$

https://benmoseley.blog/my-research/so-what-is-a-physics-informed-neural-network/

“Naive” purely data-driven model



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$$m\frac{d^2u}{dt^2} + \mu\frac{du}{dt} + ku = 0$$

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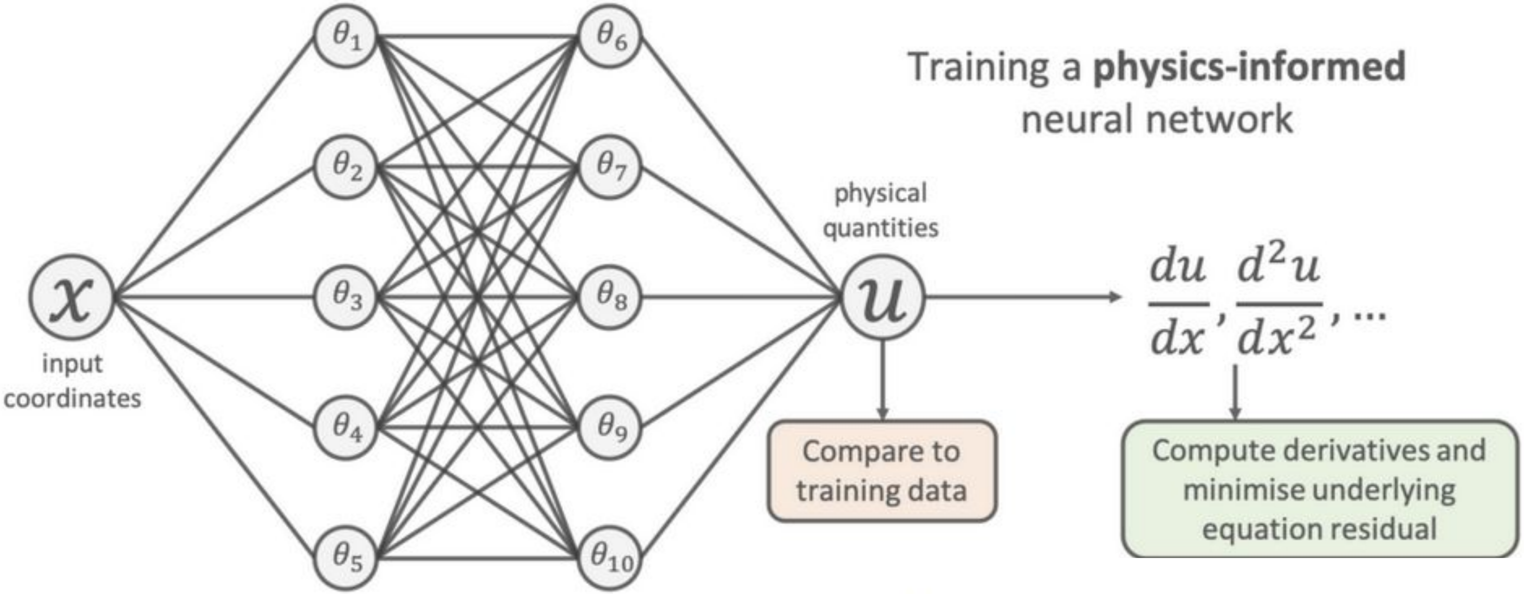
Training a **physics-informed** neural network



$$\min \frac{1}{N}\sum_{i}^{N}\left(u_{\mathrm{NN}}(x_i;\theta) - u_{\mathrm{true}}(x_i)\right)^2$$

$$+\frac{1}{M}\sum_{j}^{M}\left(\left[m\frac{d^2}{dx^2} + \mu\frac{d}{dx} + k\right] u_{\mathrm{NN}}(x_j;\theta)\right)^2$$

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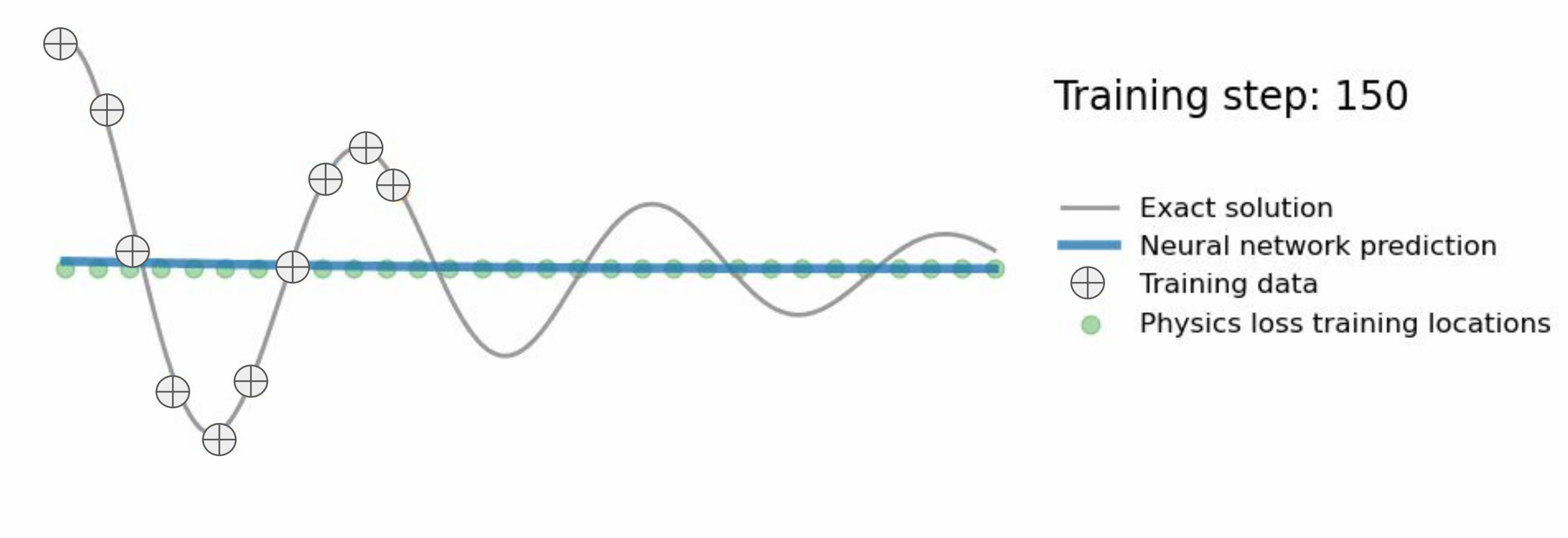
Physics informed neural network



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Motivation, problem statement & related literature
~ 2 min

Motivation and problem presentation

- Physics informed neural networks (**PINNs**)
- Improve ML models with **sparse data** availability
- Direct integration of physical laws through **Partial Differential quations**
- **Bridge the gap** between data-driven ML and physics modeling
- **Performance** improvement with high dimensional data without loss of accuracy

Related literature

- Artificial Neural Networks for Solving Ordinary and Partial Differential Equations (I. E. Lagaris, A. Likas, D. I. Fotiadis, 1997)

- Discovering governing equations from data: Sparse identification of nonlinear dynamical systems (Steven L. Brunton, Joshua L. Proctor, J. Nathan Kutz, 2015)

- Hidden Physics Models: Machine Learning of Nonlinear Partial Differential Equations (Maziar Raissi, George Em Karniadakis, 2017)

Data-driven solutions of PDEs
~ 6 min

Example

1D Nonlinear Schrodinger Equation:

$$i\partial_t \psi = -\frac{1}{2}\partial_x^2 \psi + \kappa |\psi|^2 \psi$$

$$\Rightarrow -0.5\frac{d^2}{dx^2}h - |h|^2 h = i\frac{d}{dt}h \quad \textit{for} \quad x \in [-5, 5], t \in [0, \frac{\pi}{2}]$$

$$\Rightarrow f = ih_t + 0.5h_{xx} + |h|^2 h$$

Initial / Boundary-conditions

$$h(0, x) = 2sech(x)$$

$$h(t, -5) = h(t, 5)$$

$$\frac{d}{dt}h(t, -5) = \frac{d}{dt}h(t, 5)$$

Error → Solution

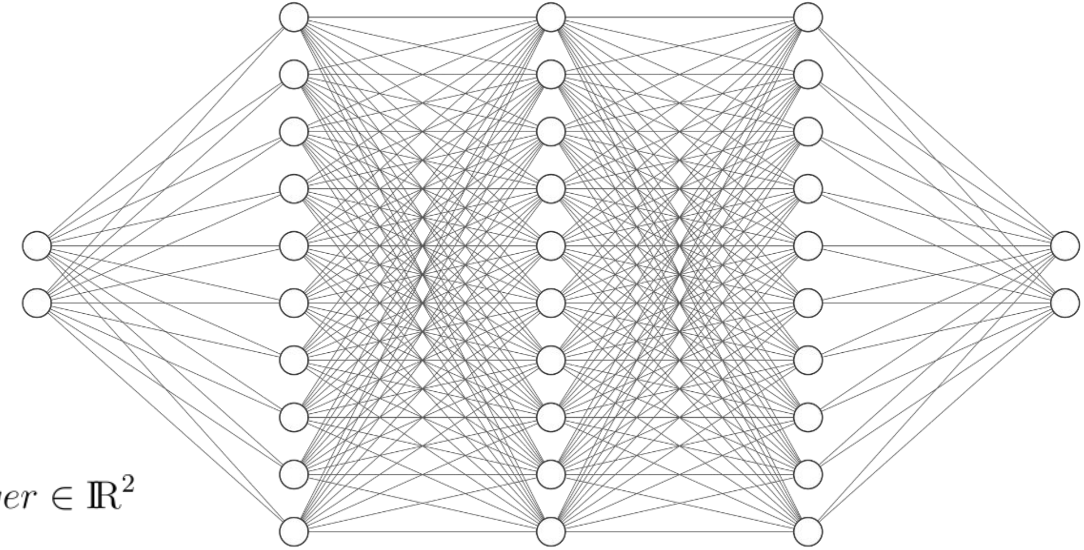
$$MSE = MSE_0 + MSE_b + MSE_f$$

$MSE_0 :=$ *Error for initial state [h(0,x)]*

$MSE_b :=$ *Error for 1st,2nd boundary condition [h(t,-5)]*

$MSE_f :=$ *Error for PDE [f(t,x)]*

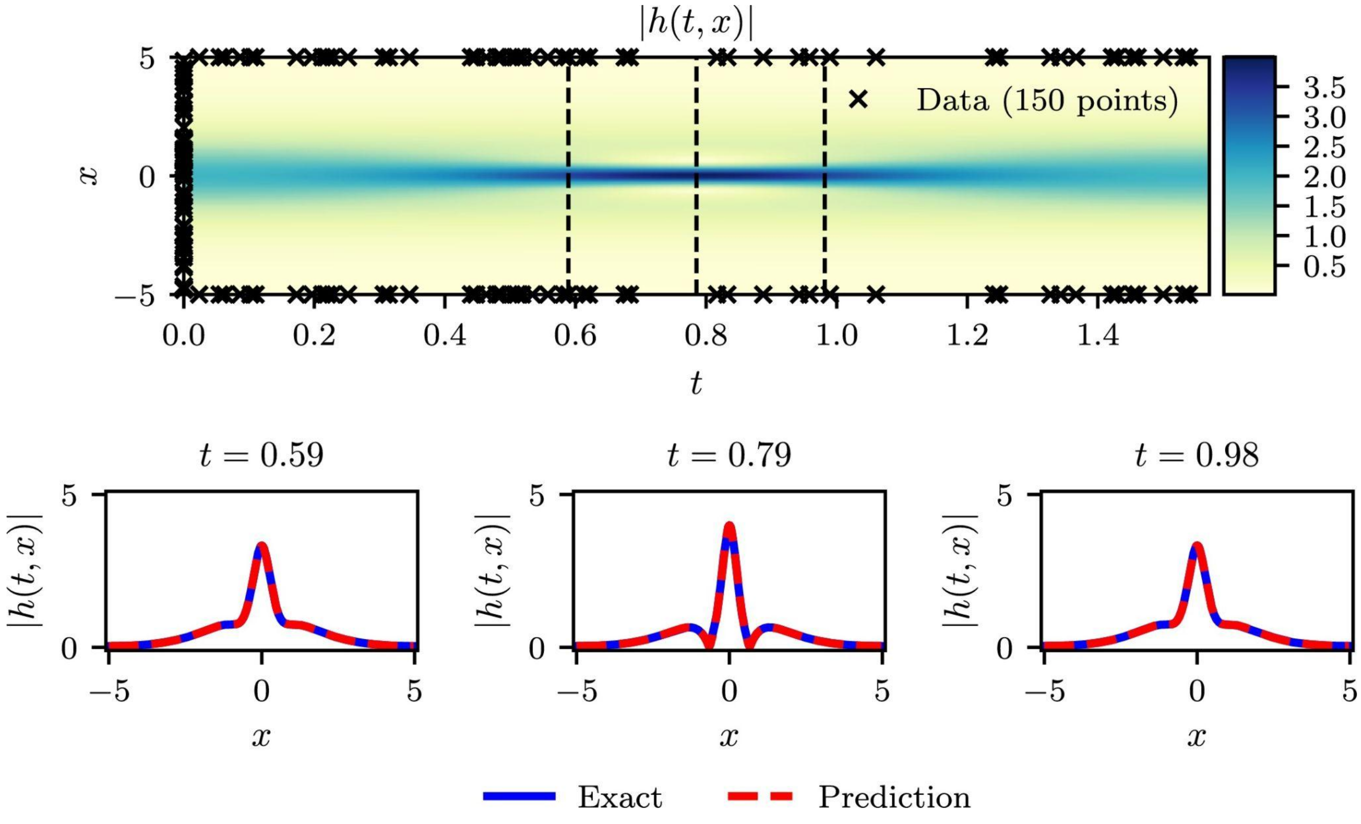
Neural Network



$Input/Output\_Layer \in \mathbb{R}^2$

$Hidden\_Layer \in \mathbb{R}^{100}$

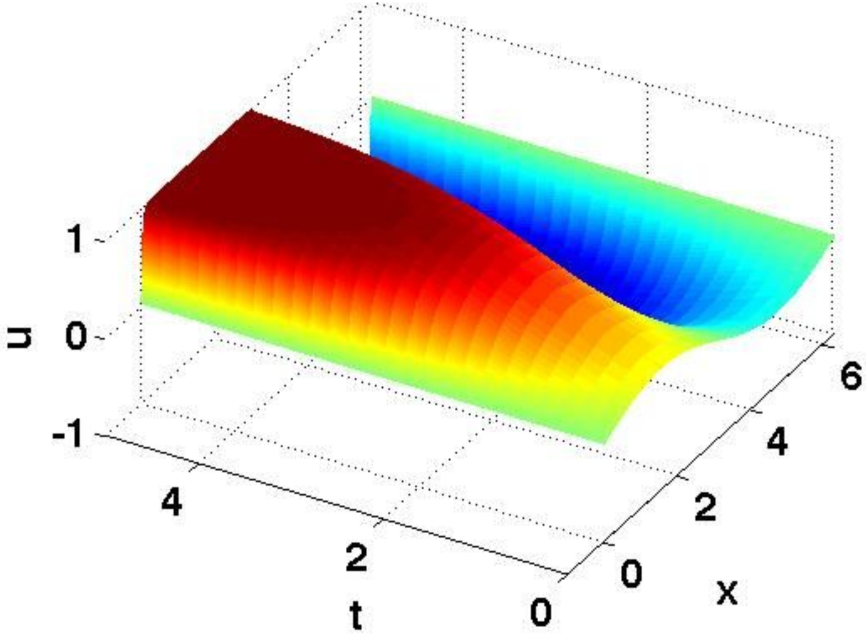
Results



Demonstration
~ 5 min

Demonstration

Discrete Equation

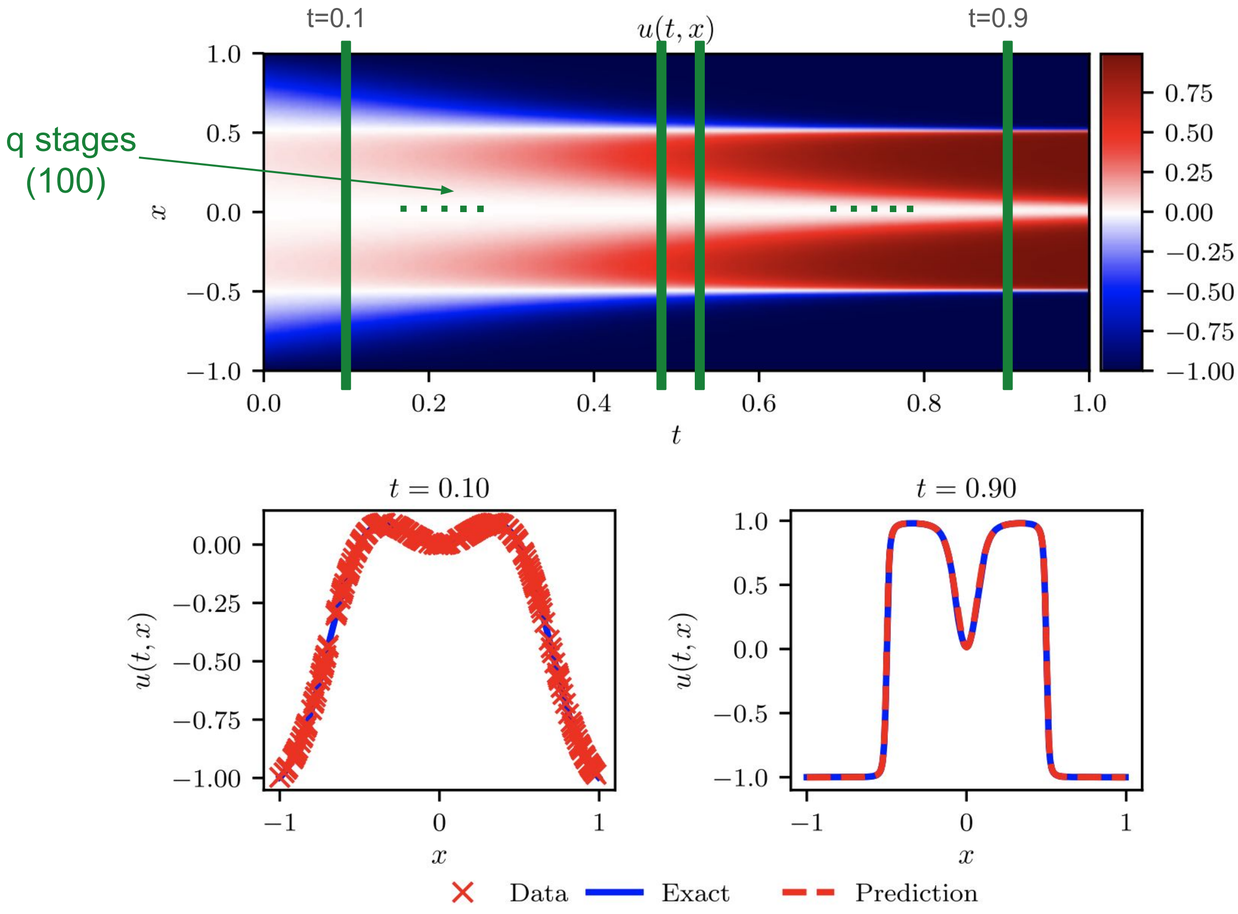


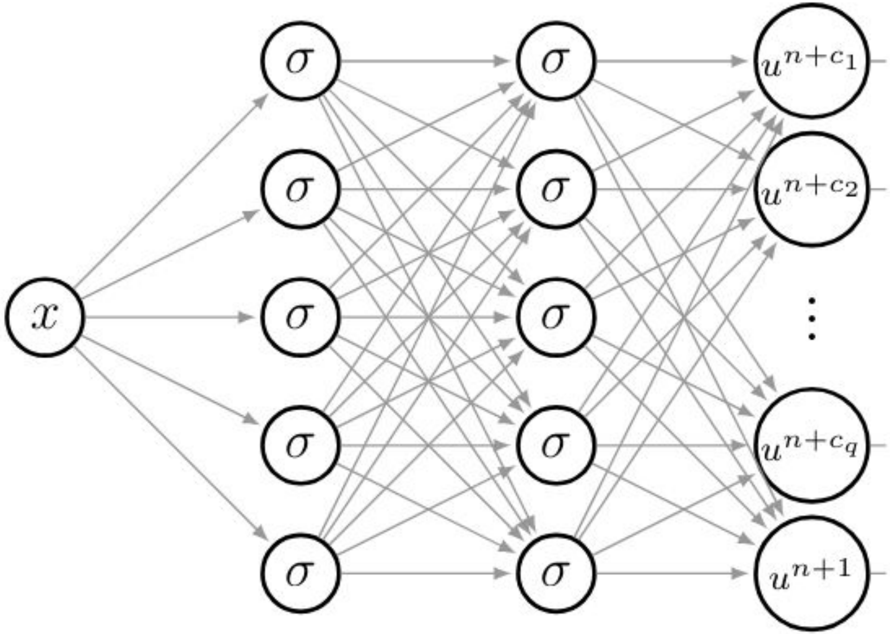
Discrete Equation: Allen-Cahn

http://open.umich.edu/education/lsa/resources/psnm/2012
Gong Chen, Brandon Cloutier, Ning Li, Benson K. Muite and Paul Rigge

Allen-Cahn Equation

$$u_t - 0.0001u_{xx} + 5u^3 - 5u = 0, \quad x \in [-1, 1], \quad t \in [0, 1],$$
$$u(0, x) = x^2 \cos(\pi x),$$
$$u(t, -1) = u(t, 1),$$
$$u_x(t, -1) = u_x(t, 1).$$


t=0.1
u(t, x)
t=0.9
q stages
(100)
1.0
0.5
0.0
−0.5
−1.0
x
0.0
0.2
0.4
0.6
0.8
1.0
t
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
t = 0.10
t = 0.90
u(t, x)
x
Data
Exact
Prediction



$$u_1^n = u^{n+c_1} - \Delta t \sum_{j=1}^{q} a_{1j} g\left[u^{n+c_j}\right]$$

$$u_2^n = u^{n+c_2} - \Delta t \sum_{j=1}^{q} a_{2j} g\left[u^{n+c_j}\right]$$

$$\vdots$$

$$u_q^n = u^{n+c_q} - \Delta t \sum_{j=1}^{q} a_{qj} g\left[u^{n+c_j}\right]$$

$$u_{q+1}^n = u^{n+1} - \Delta t \sum_{j=1}^{q} b_j g\left[u^{n+c_j}\right]$$

Source: Stefan Kollmannsberger & Davide D’Angella & Moritz Jokeit & Leon Herrmann: *Deep Learning in Computational Mechanics,* 2021 Springer p.74

Solution

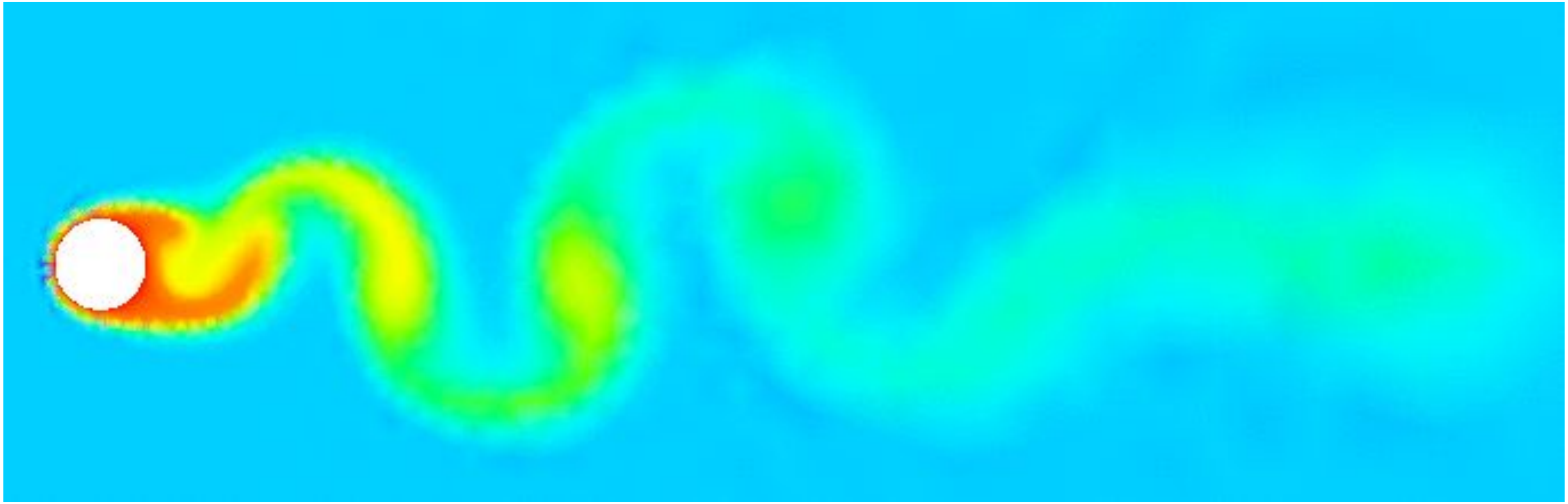
$$SSE = SSE_n + SSE_b,$$

SSE_b = Boundary Condition Error

SSE_n = Difference between predicted $u^{n+c_i}, ..., u^{n+1}$ and u^n

Data driven discovery of PDEs / inverse problem ~ 6 Min

Data-Driven Discovery with PINNs



Data-Driven discovery with PINNs: Navier-Stokes equation

$$f := u_t + \lambda_1(uu_x + vu_y) + p_x - \lambda_2(u_{xx} + u_{yy}),$$
$$g := v_t + \lambda_1(uv_x + vv_y) + p_y - \lambda_2(v_{xx} + v_{yy}),$$

$$u_x + v_y = 0.$$

$$u = \psi_y, \quad v = -\psi_x,$$

$$\{t^i, x^i, y^i, u^i, v^i\}_{i=1}^N$$

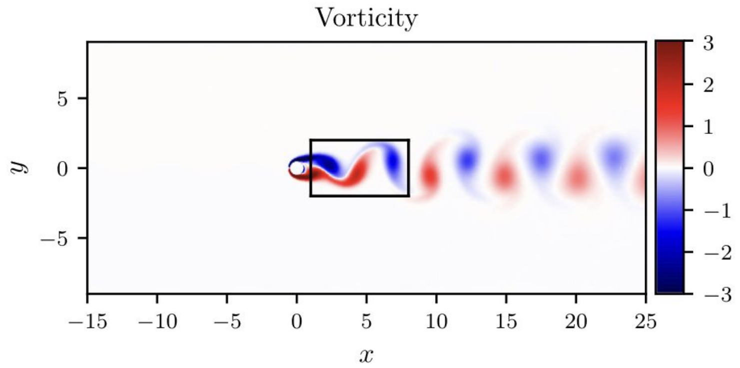
Data-Driven discovery with PINNs: Navier-Stokes equation

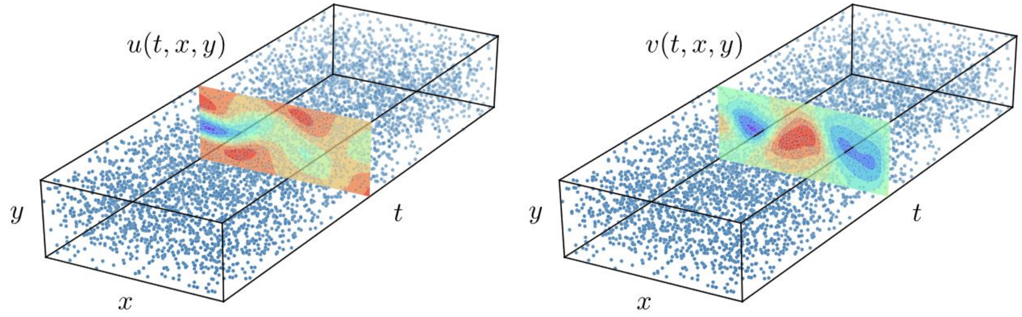
$$[\psi(t,x,y) \quad p(t,x,y)] \quad [f(t,x,y) \quad g(t,x,y)]$$

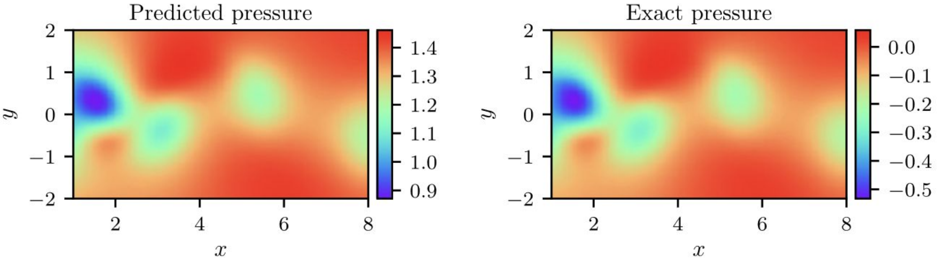
$$MSE := \frac{1}{N}\sum_{i=1}^{N}\left(|u(t^i,x^i,y^i) - u^i|^2 + |v(t^i,x^i,y^i) - v^i|^2\right)$$

$$+ \frac{1}{N}\sum_{i=1}^{N}\left(|f(t^i,x^i,y^i)|^2 + |g(t^i,x^i,y^i)|^2\right).$$

Continuous Time Model: Navier-Stokes in Fluid Dynamics

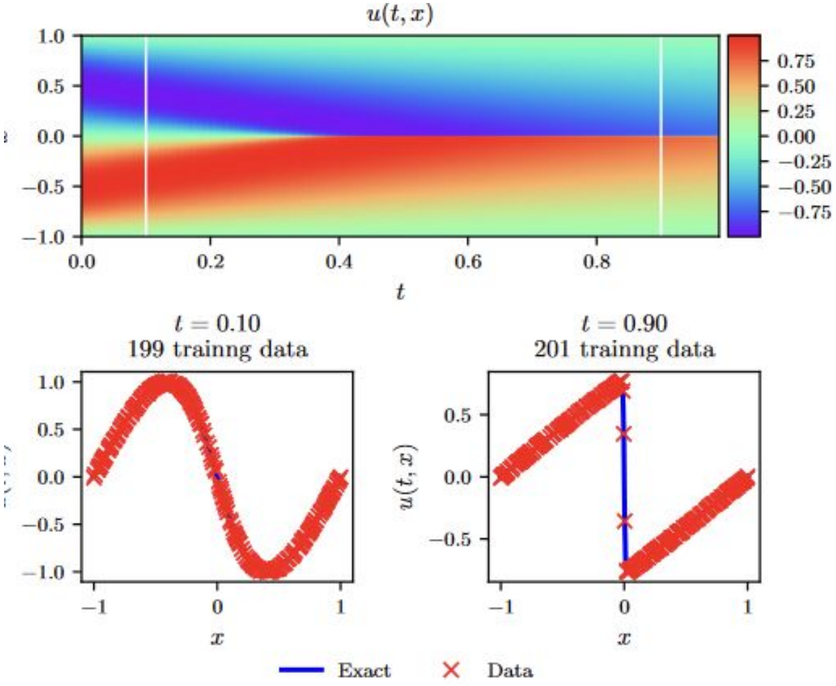






Correct PDE	$u_t + (uu_x + vu_y) = -p_x + 0.01(u_{xx} + u_{yy})$ $v_t + (uv_x + vv_y) = -p_y + 0.01(v_{xx} + v_{yy})$
Identified PDE (clean data)	$u_t + 0.999(uu_x + vu_y) = -p_x + 0.01047(u_{xx} + u_{yy})$ $v_t + 0.999(uv_x + vv_y) = -p_y + 0.01047(v_{xx} + v_{yy})$
Identified PDE (1% noise)	$u_t + 0.998(uu_x + vu_y) = -p_x + 0.01057(u_{xx} + u_{yy})$ $v_t + 0.998(uv_x + vv_y) = -p_y + 0.01057(v_{xx} + v_{yy})$

Discrete Time Model: Burgers equation



$$u_t + \lambda_1 u u_x - \lambda_2 u_{xx} = 0$$

Correct PDE	$u_t + uu_x - 0.0031831u_{xx} = 0$
Identified PDE (clean data)	$u_t + 0.99915uu_x - 0.0031794u_{xx} = 0$
Identified PDE (1% noise)	$u_t + 1.00042uu_x - 0.0032098u_{xx} = 0$

Comparison to traditional methods, critique & conclusion
~ 5 Min

Comparison

- Surrogate Modeling

- Numerical Methods (FDM, FEM…)

Conclusion

+ PINNs excel in **sparse data**, robust against noise

+ Potentially surpass classical methods with Runge-Kutta integration (Sec 4.2)

+ **Computational Cost** (High dimensional PDEs)

- True paradigm shift or an incremental update over traditional models?

- Paper did not provide detailed comparison with other models, s.a. FEM

- Reliability

Q & A
~ 15 Min

Q & A

Sources

- sciencedirect.com/science/article/abs/pii/S0021999118307125
- open.umich.edu/education/lsa/resources/psnm/2012 Bong Chen, Brandon Cloutier, Ning Li, Benson K. Muite and Paul Rigge
- benmoseley.blog/my-research/so-what-is-a-physics-informed-neural-network/
- Stefan Kollmannsberger & Davide D’Angella & Moritz Jokeit & Leon, Herrmann: Deep Learning in Computational Mechanics, 2021 Springer p.74