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nPINNS: Nonlocal Physics-Informed Neural Networks

One Nonlocal World
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Outline

- ❑ **Nonlocal Models**
- ❑ **Using computational models in practice**
- ❑ **nPINNS: nonlocal Physics-Informed Neural Networks**
  - ❑ **Data-driven solutions**
  - ❑ **Data-driven discovery**
- ❑ **Example: a nonlocal model for turbulent Couette flow**
- ❑ **Conclusions**

Collaborators and Funding

Dr. Goufei Pang
(Brown)

Dr. Marta D'Elia
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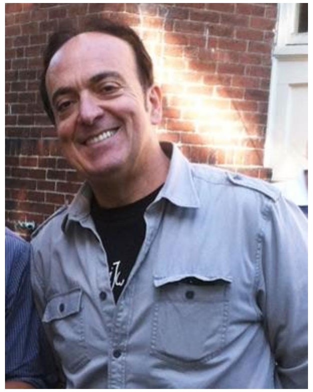

Prof. George Karniadakis
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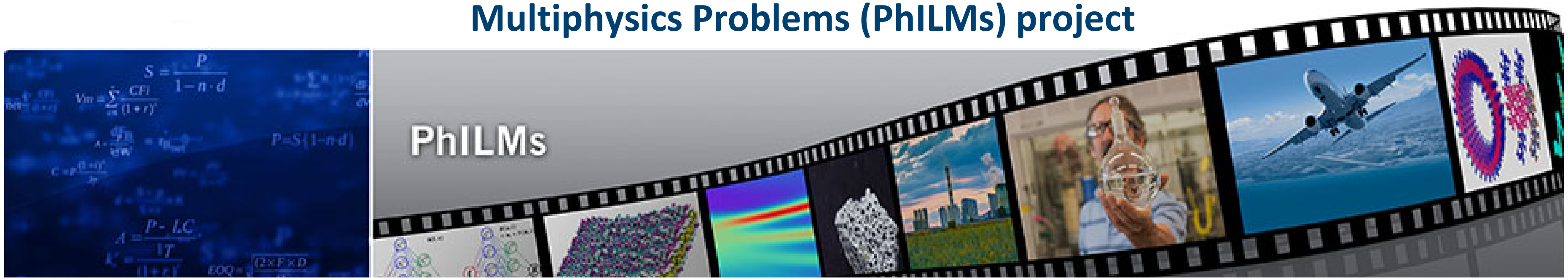

https://www.pnnl.gov/computing/philms/

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Nonlocal Models

- **Nonlocal models describe many phenomena**
  - Multiscale models, fracture & failure, porous media flow, plasma physics, turbulent flow, …

- **Anomalous Diffusion*,****

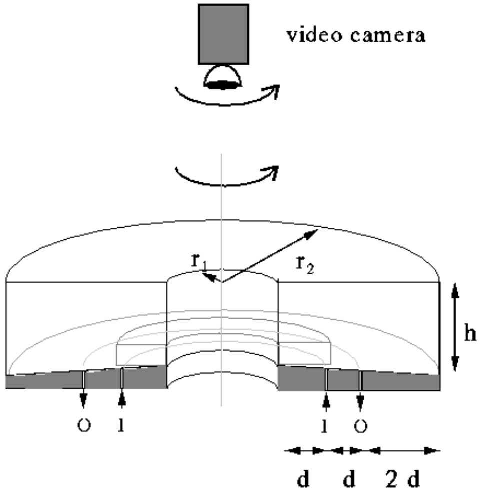


Diagram of chaotic fluid experiment

Cylinder rotates while water pumped in through ring of holes I and out through ring of holes O. Completely filled with water or water-glycerol mixture. Camera records motion of tracers.

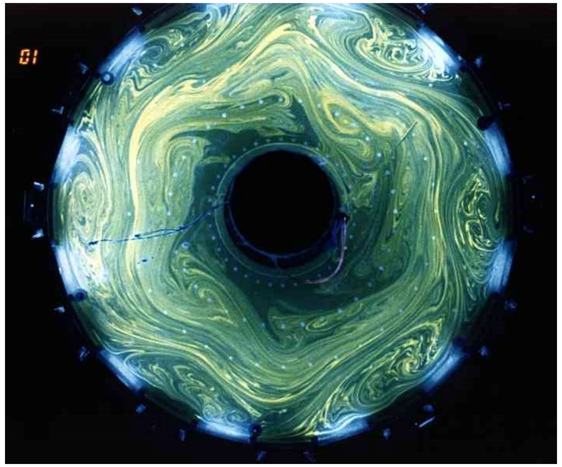
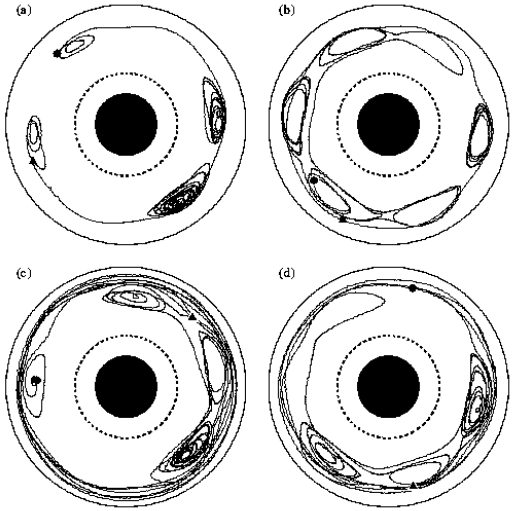


Image of fluid with tracers



Typical particle trajectories

Observations: Long waiting times (in eddies), long jumps

$\sigma^2 \sim t^{1.6 +/- 0.3} \Rightarrow$ superdiffusion

* http://www.physics.emory.edu/faculty/weeks/research/apparatus.html

** TH Solomon, ER Weeks, & HL Swinney, **Observations of anomalous diffusion and Levy flights in a 2-dimensional rotating flow,** Phys. Rev. Lett. **71**, 3975-3979 (1993).

Local and Nonlocal Models

- **Example: Isotropic Elastic Material**

- **Governing equations and parameters**
  - $\rho\ddot{u}(x,t) = \nabla \cdot \sigma(x) + b(x,t)$
  - $\sigma = C:\varepsilon$
  - $C \sim k, \mu$
  - k is bulk modulus, μ is shear modulus

- **Parameters k and μ can be looked up from tables provided by standards organizations.**

- **With appropriate finite element discretization and computational power can achieve highly accurate solutions.**

- **Example: Nonlocal Isotropic Elastic Material**

- **Governing equations and parameters**
  - $\rho\ddot{u}(x,t) = \int_H \left(T[x,t]\langle x'-x\rangle - T[x',t]\langle x-x'\rangle\right) dV_{x'} + b(x,t)$
  - $T[x,t]\langle x'-x\rangle = \left(\frac{3k\theta}{m}\underline{\omega}\underline{x} + \frac{15\mu}{m}\underline{\omega}\underline{e}^d\right)\frac{x'-x}{\|x'-x\|}$
  - k is bulk modulus, μ is shear modulus

- **Parameters k and μ can be looked up from tables provided by standards organizations.**
- **Relationship between functional form of kernel ω and peridynamic horizon δ is in general not specified. I can't just look these up.**

- **In practice:**
  - Choose delta = 3h
  - Choose $\omega \sim 1 / r^{\alpha}$

- **This is not very satisfying…**

Local and Nonlocal Models

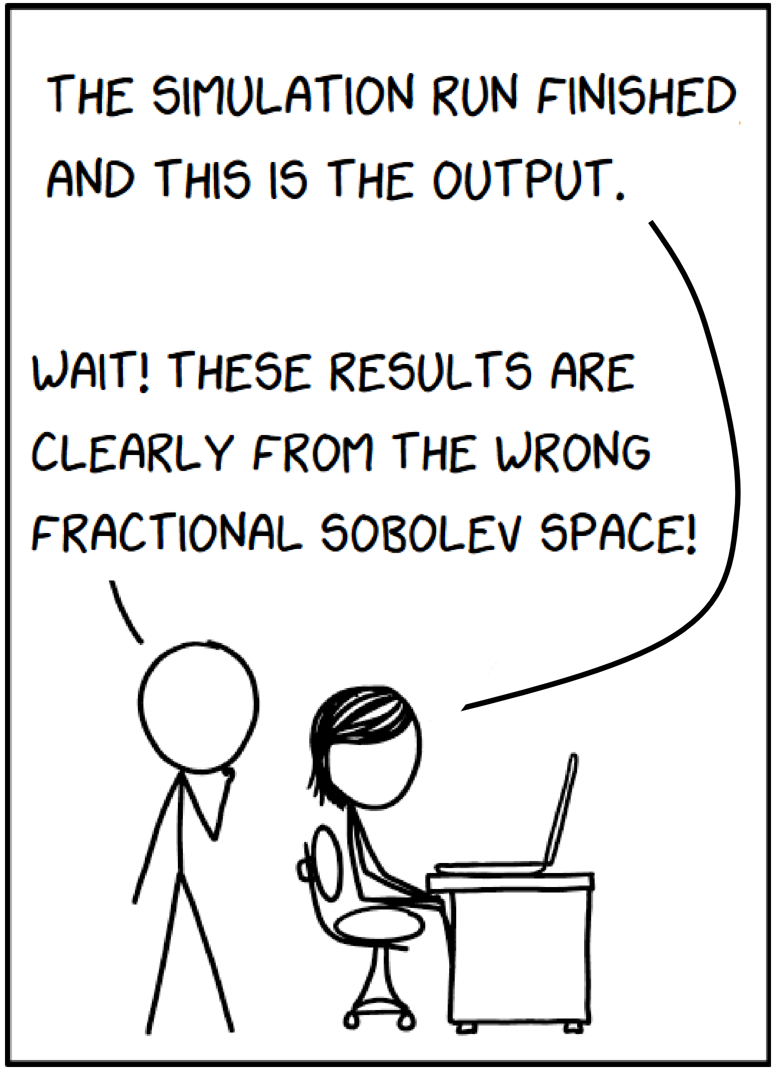
- Perhaps the specific choice of influence function ω and horizon δ is not of practical importance.
- I can calibrate any solid for given ω, δ.

- This raises several questions:
  - Is the choice of influence function or horizon important?
  - Does choice of these parameters make a difference in getting a physically correct answer or a physically incorrect answer?
  - Is any specific choice just as good as any other? Is there a single best choice for a specific application? Are there families of good choices?
  - How do you tell?

- **Data-driven methods present the opportunity to discover these parameters from data.**

- Let's talk about Physics-Informed Neutal Networks (PINNs), both for (1) data-driven solution to PDEs, and (2) data-driven discovery of model parameters.

PERIDYNAMIC SIMULATION*



Said no engineer ever…

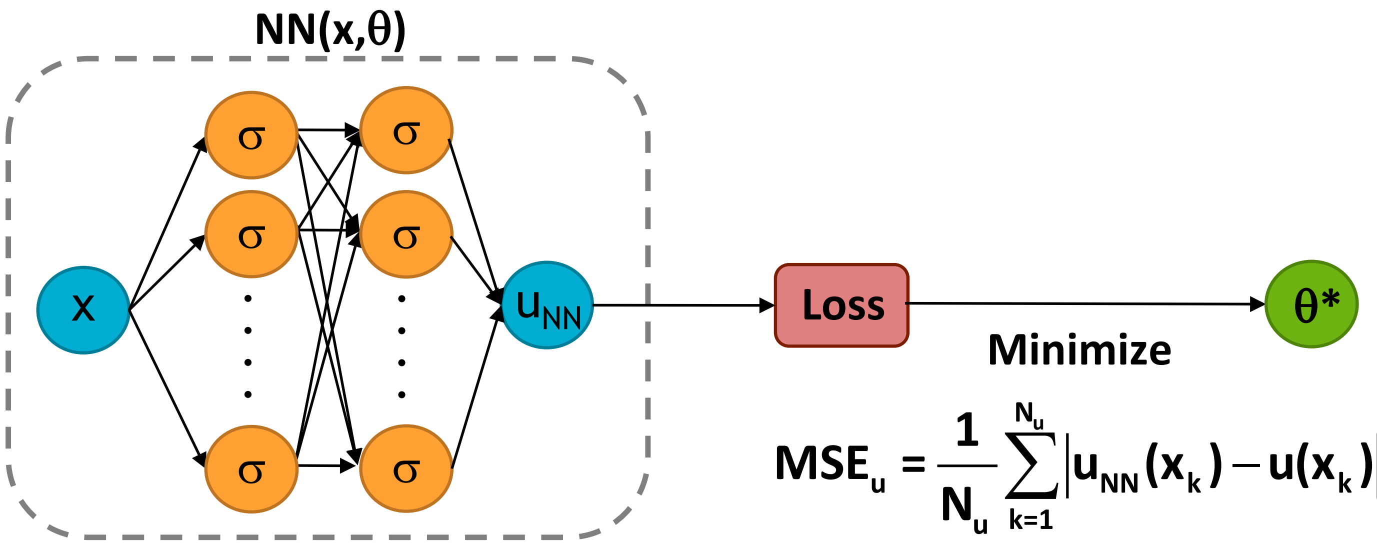
*Apologies to Randall Munroe & XKCD!

Train a Neural Network to Solve a PDE (Naïve Approach)

- Train deep neural network (DNN) to solve this PDE:

$$f\left(x;\frac{\partial u}{\partial x_1},\cdots,\frac{\partial u}{\partial x_d};\frac{\partial^2 u}{\partial x_1 \partial x_1},\cdots,\frac{\partial^2 u}{\partial x_1 \partial x_d};\cdots;\lambda\right)=0$$

- Traditional approach: Train network minimizing loss based on provided training data



$$MSE_u = \frac{1}{N_u}\sum_{k=1}^{N_u}\left|u_{NN}(x_k) - u(x_k)\right|^2$$

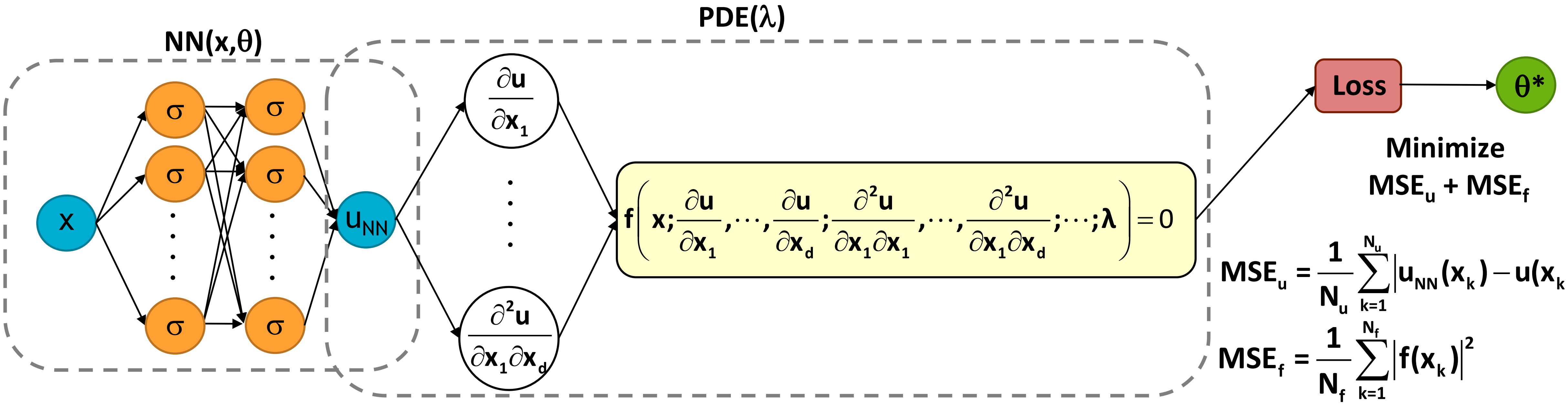
- In practice, this requires lots of data
- There is no explicit notion of governing physics anywhere in this system.

PINNs*: Train a Neural Network to Solve a PDE

- Train deep neural network (DNN) to solve this PDE:

$$f\left(x;\frac{\partial u}{\partial x_1},\cdots,\frac{\partial u}{\partial x_d};\frac{\partial^2 u}{\partial x_1 \partial x_1},\cdots,\frac{\partial^2 u}{\partial x_1 \partial x_d};\cdots;\lambda\right)=0$$

- Physics-Informed Neural Network (PINN) explicitly incorporates physics by constraining network output



Minimize
$MSE_u + MSE_f$

$$MSE_u = \frac{1}{N_u}\sum_{k=1}^{N_u}\left|u_{NN}(x_k)-u(x_k)\right|^2$$

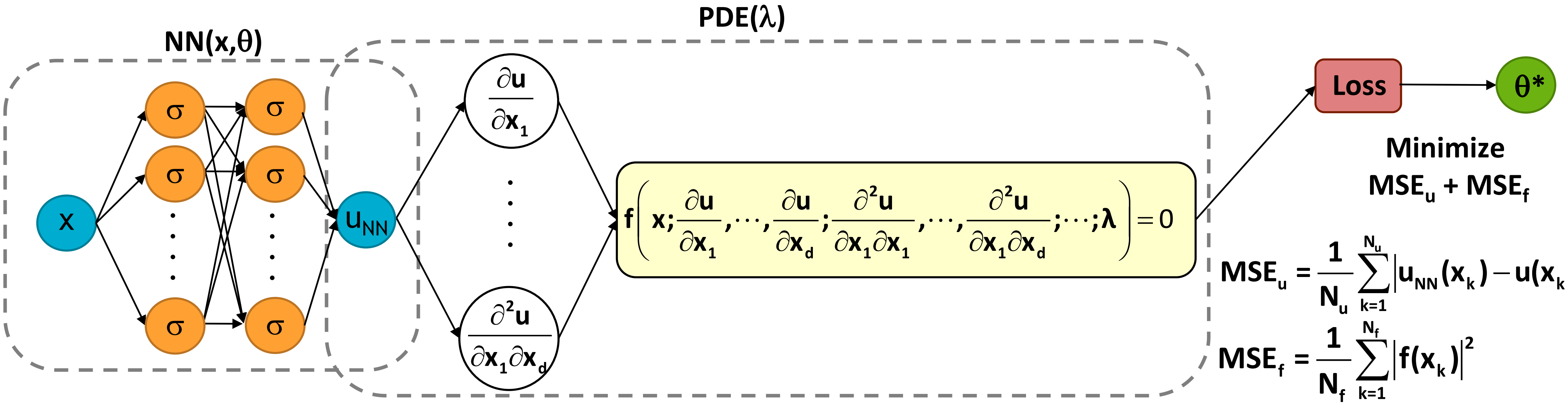
$$MSE_f = \frac{1}{N_f}\sum_{k=1}^{N_f}\left|f(x_k)\right|^2$$

- In general, this requires much less data and can produce highly accurate solutions.

* M. Raissi, P. Perdikaris, G.E. Karniadakis, Physics-informed neural networks: a deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, J. Comput. Phys. 378 (2019) 686-707.

PINNs*: Train a Neural Network to Solve a PDE

- PINNs can be used in two ways:
  - **Data-driven solutions to PDEs** (i.e., λ is known and we seek u(x)).
  - **Data-driven discovery of PDEs** (i.e., λ is unknown and we seek u(x) and λ). In this case, λ becomes a parameter of our PINN.



$$MSE_u = \frac{1}{N_u}\sum_{k=1}^{N_u}\left|u_{NN}(x_k) - u(x_k)\right|^2$$

$$MSE_f = \frac{1}{N_f}\sum_{k=1}^{N_f}\left|f(x_k)\right|^2$$

* M. Raissi, P. Perdikaris, G.E. Karniadakis, Physics-informed neural networks: a deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, J. Comput. Phys. 378 (2019) 686-707.

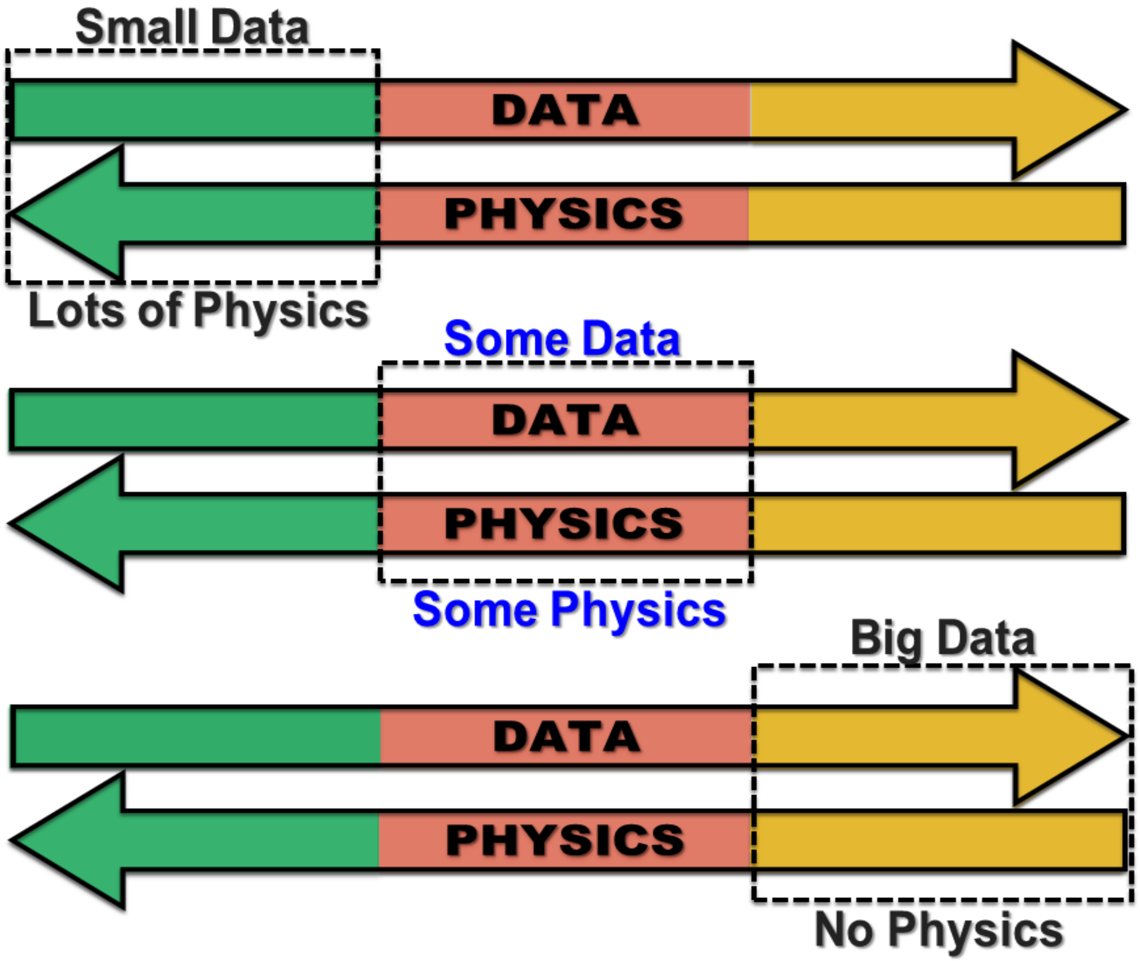
Knowledge of Physics vs. Data

- **PINNs = Neural Networks + Data + Physical Laws**

- **How much do we know about governing physics?**
- **How much data do we have?**

- **An alphabet of PINNS has been developed:**
  - cPINNs: conservative PINNs
  - vPINNs: variations PINNs
  - pPINNs: parareal PINNs
  - sPINNs: stochastic PINNs
  - fPINNs: fractional PINNs
  - LesPINNs: LES PINNs
  - **nPINNs: Nonlocal PINNs**
  - xPINNs: eXtended PINNs

- Next: **Universal Nonlocal Laplace Operator**



Universal Nonlocal Laplace Operator

- Given broad spectrum of experimental data, we desire flexible operator.
  - i.e., operator discovery using parameterized classical Laplacian with data governed by a nonlocal Laplacian will not work well. But we don't know in advance the functional form data obeys.

- Use this operator*:

$$-\mathcal{L}_{\delta,\alpha}u(x) = C_{\delta,\alpha}\int_{B_\delta(x)} \frac{u(y)-u(x)}{\|y-x\|_2^{d+\alpha}} \quad \forall x \in \Omega$$

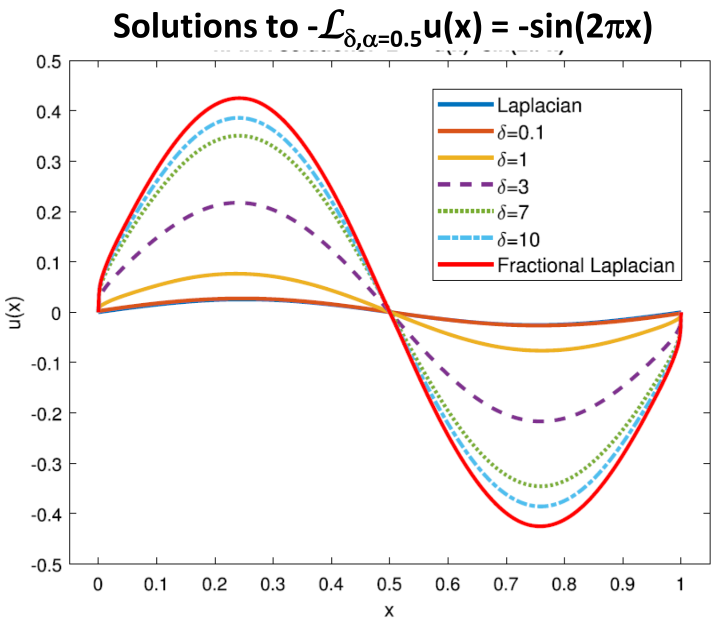
- So that these properties are satisfied:

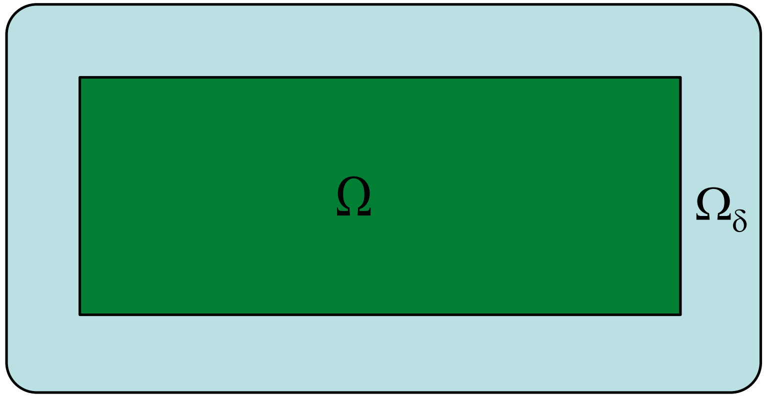
$$\lim_{\delta\to 0}\left(-\mathcal{L}_{\delta,\alpha}\right)u(x) = -\Delta u(x) \qquad \forall \alpha \in (0,2) \qquad \text{(Classical Laplacian)}$$

$$\lim_{\delta\to \infty}\left(-\mathcal{L}_{\delta,\alpha}\right)u(x) = \left(-\Delta\right)^{\alpha/2}u(x) \qquad \forall \alpha \in (0,2) \qquad \text{(Fractional Laplacian)}$$

- Apply nPINNs to this problem:

$$\begin{aligned} -\mathcal{L}_{\delta,\alpha}u(x) &= f(x) \quad x \in \Omega \\ u(x) &= g(x) \quad x \in \Omega_\delta \end{aligned}$$





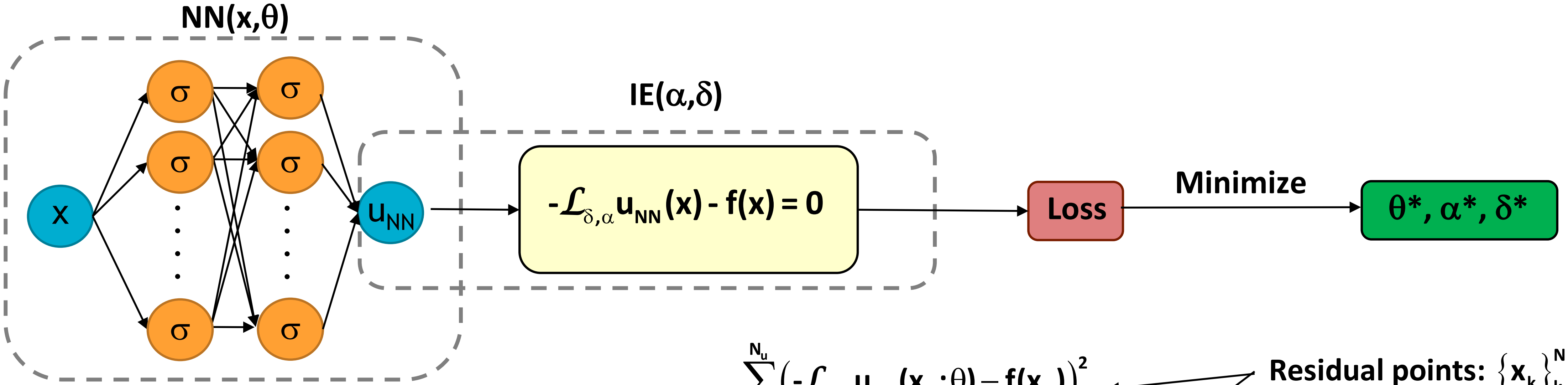
* This operator bridges fractional and local operators. For more on related unification results, see M. D'Elia, M. Gulian, H. Olson, G. E. Karniadakis. A Unified Theory of Fractional, Nonlocal, and Weighted Nonlocal Vector Calculus, 2020 arXiv:2005.07686.

Nonlocal Physics-Informed Neural Networks (nPINNs)

- **nPINNS can be summarized in 3 steps:**

1. **Collect observations or high fidelity simulations of the solution, u_{obs}**
2. **Approximate the solution with a fully connected NN: $u(x) \approx u_{NN}(x; \theta)$**
3. **Minimize the loss function with respect to the unknown parameters**

$$\begin{aligned} -\mathcal{L}_{\delta,\alpha} u(x) &= f(x) \quad x \in \Omega \\ u(x) &= g(x) \quad x \in \Omega_\delta \end{aligned}$$



- **Forward mode (data-driven solution):** $\text{Loss}(\theta) = \dfrac{\sum_{k=1}^{N_u} \left(-\mathcal{L}_{\delta,\alpha} u_{NN}(x_k;\theta) - f(x_k)\right)^2}{\sum_{k=1}^{N_u} f(x_k)^2}$

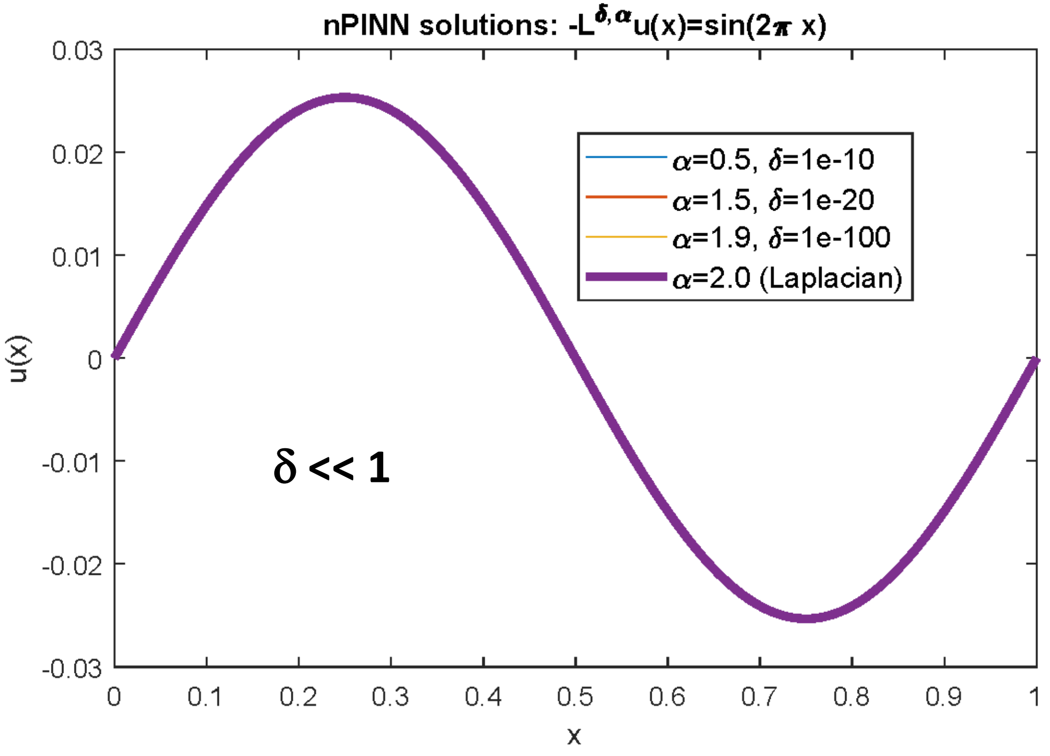
Residual points: $\{x_k\}_{k=1}^{N}$

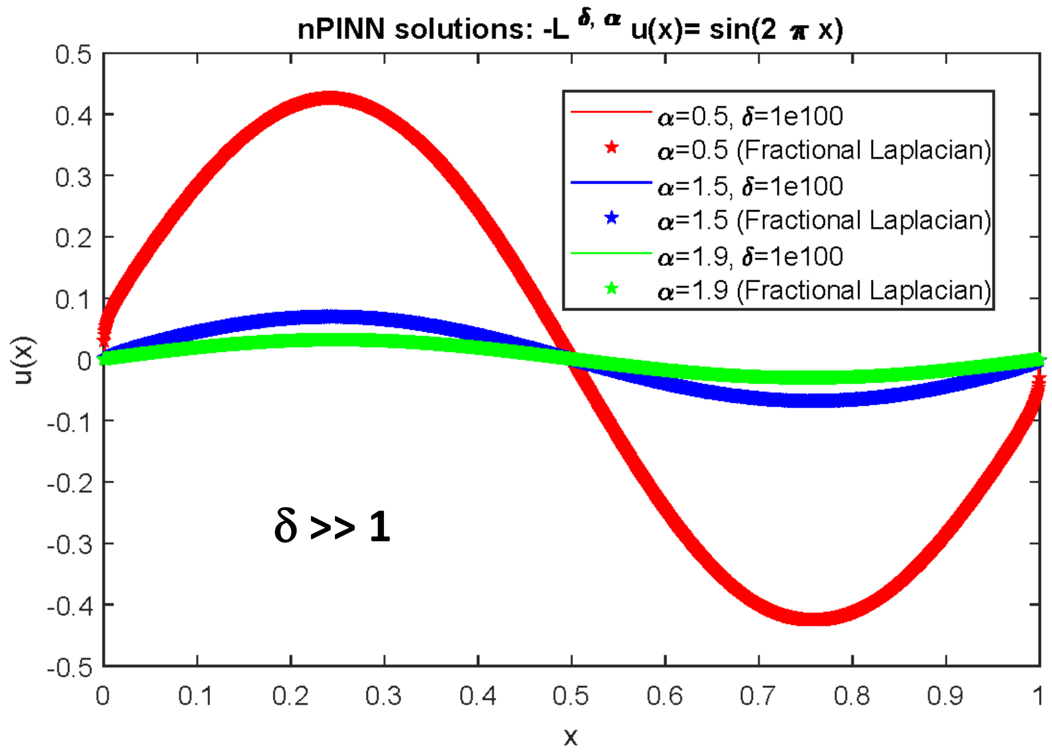
Observation points: $\{\hat{x}_k\}_{k=1}^{N}$

- **Inverse mode (data-driven discovery):** $\text{Loss}(\theta,\delta,\alpha) = \dfrac{\sum_{k=1}^{N_u} \left(-\mathcal{L}_{\delta,\alpha} u_{NN}(x_k;\theta) - f(x_k)\right)^2}{\sum_{k=1}^{N_u} f(x_k)^2} + \dfrac{\sum_{k=1}^{N_u} \left(u_{NN}(\hat{x}_k;\theta) - u_{obs}(\hat{x}_k)\right)^2}{\sum_{k=1}^{N_u} u_{obs}(\hat{x}_k)^2}$

Computational Results: Data Driven Solutions

- nPINNs solutions show universal Laplace operator reproduces classical and fractional Laplacians





$$\lim_{\delta\to 0}\left(-\mathcal{L}_{\delta,\alpha}\right)u(x) = -\Delta u(x) \qquad \forall\alpha\in(0,2)$$

(Classical Laplacian)

$$\lim_{\delta\to\infty}\left(-\mathcal{L}_{\delta,\alpha}\right)u(x) = \left(-\Delta\right)^{\alpha/2}u(x) \quad \forall\alpha\in(0,2)$$

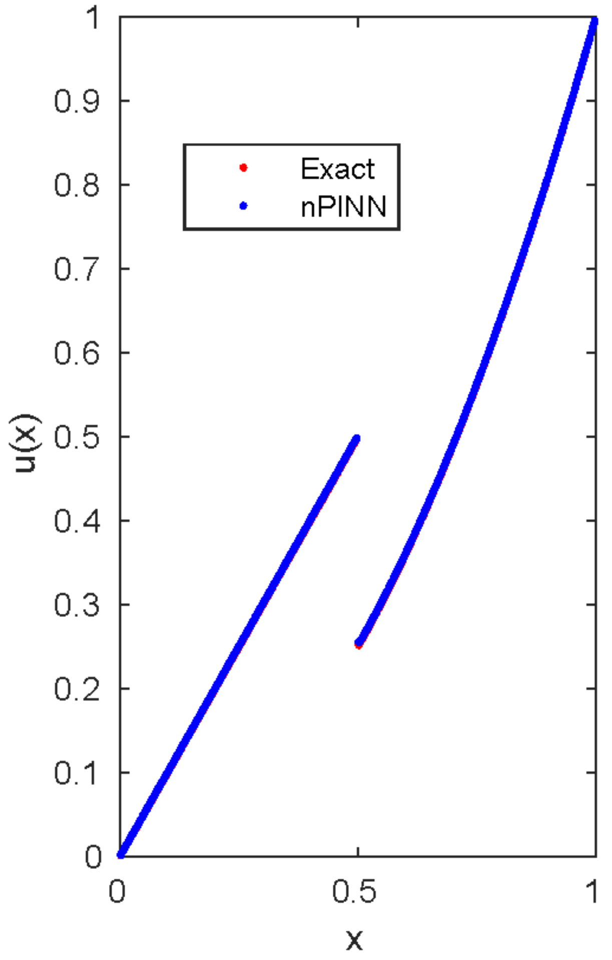
(Fractional Laplacian)

Computational Results: Data Driven Solutions

- **nPINNs can reproduce discontinuous solutions (α=0, δ = 0.3)***

$$u(x) = \begin{cases} x & x \in [-\delta, 0.5) \\ x^2 & x \in (0.5, 1+\delta] \end{cases}$$

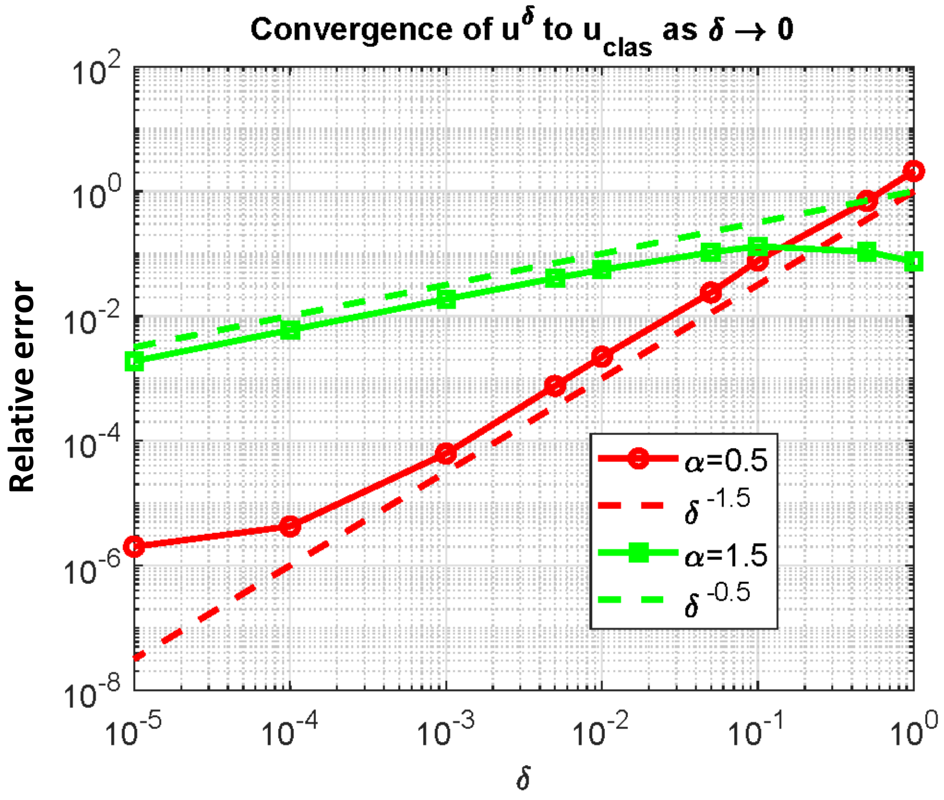
$$f(x) = \begin{cases} 0 & x \in [0, 0.5-\delta) \\ -\frac{2}{\delta^2}\left[\frac{1}{2}\delta^2 - \delta + \frac{3}{8} + (2\delta - \frac{3}{2} - \ln\delta)x + (\frac{3}{2} + x^2\ln\delta - (x^2 - x)\ln\frac{1}{2} - x\right] & x \in [0.5-\delta, 0.5) \\ -\frac{2}{\delta^2}\left[\frac{1}{2}\delta^2 - \delta - \frac{3}{8} + (2\delta + \frac{3}{2} + x\ln\delta) - (\frac{3}{2} + x^2\ln\delta + (x^2 - x)\ln x - \frac{1}{2}\right] & x \in (0.5, 0.5+\delta) \\ -2 & x \in [0.5+\delta, 1.0], \end{cases}$$



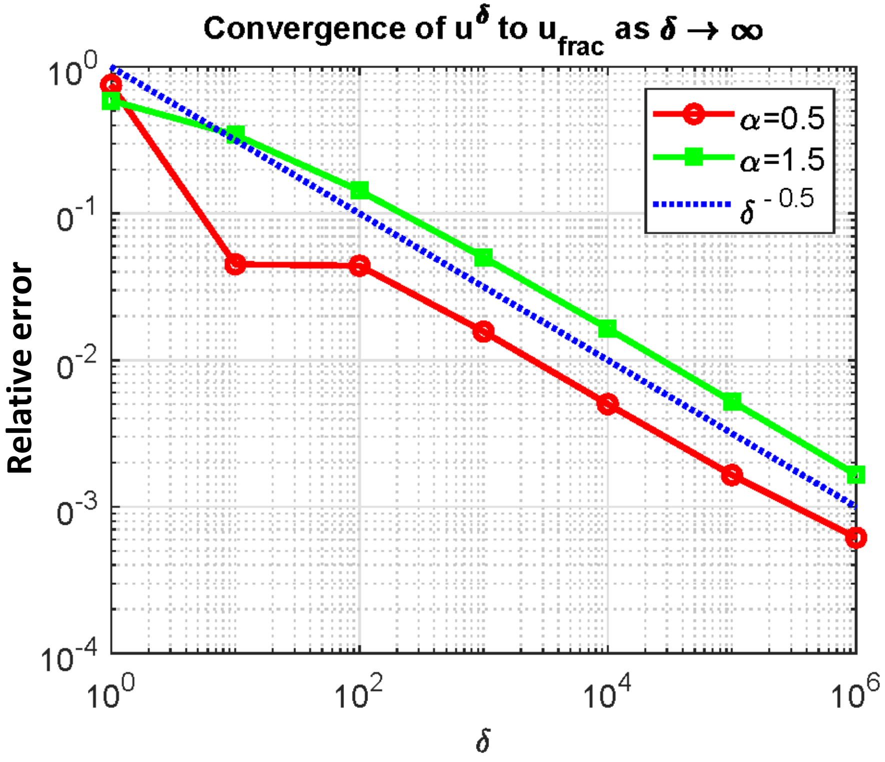
*X. Chen, M. Gunzburger, Continuous and discontinuous finite element methods for a peridynamics model of mechanics, Comput. Methods Appl. Mech. Eng. 200(9-12) (2011) 1237-1250.

Computational Results: Data Driven Solutions

- Convergence of nPINN solution to solution of classical Laplacian ($\delta \to 0$) and fractional Laplacian ($\delta \to \infty$)



$$\left|\left(-\mathcal{L}_{\delta,\alpha}\right)u(x)-\left(-\Delta\right)u(x)\right| \sim \delta^{2-\alpha} \quad \text{as } \delta \to 0$$



$$\left|\left(-\mathcal{L}_{\delta,\alpha}\right)u(x)-\left(-\Delta\right)^{\alpha/2}u(x)\right| \sim \delta^{\max\{\alpha-2,-\alpha\}} \quad \text{as } \delta \to \infty$$

Computational Results: Data Driven Discovery

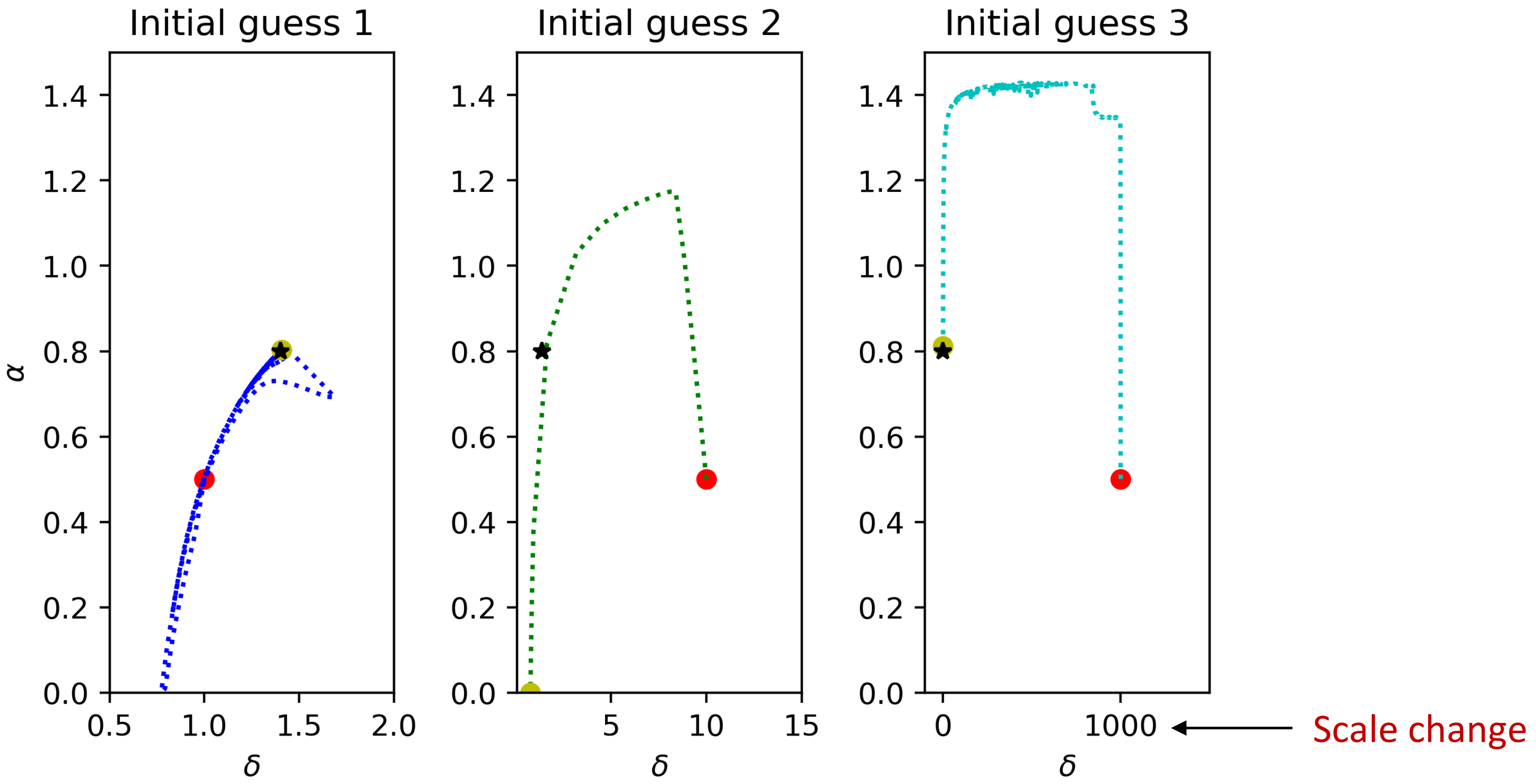
- nPINNs can discover parameterized operator from data: Seek $(\delta,\alpha) \in (0,\infty) \times (0,2)$.
- $\Omega = (0,1)$, $g(x) = 0$, $f(x) = \sin(2\pi x)$
- Training data: 100 uniformly spaced points in $\Omega \cup \Omega_\delta$
- Optimal $(\delta^*,\alpha^*) = (1.4, 0.8)$

$$-\mathcal{L}_{\delta,\alpha} u(x) = f(x) \quad x \in \Omega$$
$$u(x) = g(x) \quad x \in \Omega_\delta$$

● Initial guess

● Converged value

★ True solution



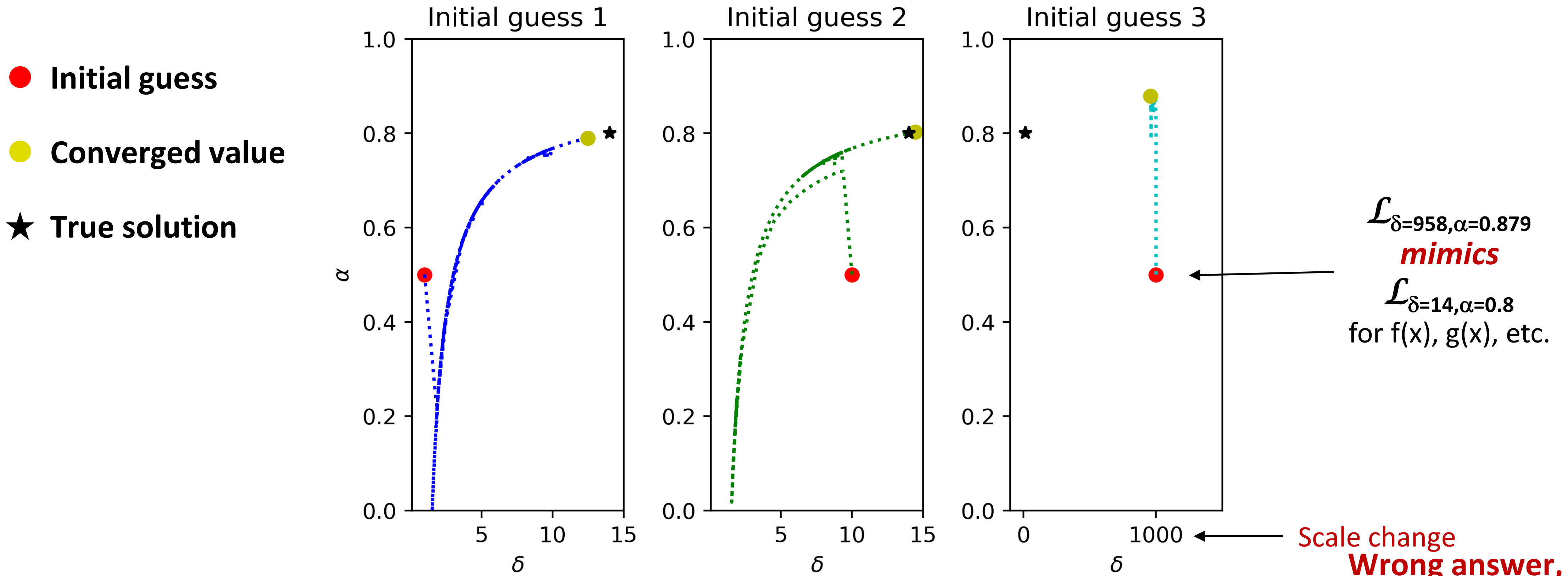
Initial guesses: $(\delta_1,\alpha_1) = (1,0.5)$ $(\delta_2,\alpha_2) = (10,0.5)$ $(\delta_3,\alpha_3) = (1000,0.5)$

Relative errors: $e_1 = 2.64\times10^{-4}$ $e_2 = 1.43\times10^{-2}$ $e_3 = 2.69\times10^{-4}$

Computational Results: Data Driven Discovery

- nPINNs can discover parameterized operator from data: Seek $(\delta,\alpha) \in (0,\infty)\ (0,2)$.
- $\Omega = (0,1)$, $g(x) = 0$, $f(x) = \sin(2\pi x)$
- Training data: 100 uniformly spaced points in $\Omega \cup \Omega_\delta$
- Optimal $(\delta^*,\alpha^*) = (14.0, 0.8)$ ← Increase δ^* by 10× from previous example

$$-\mathcal{L}_{\delta,\alpha} u(x) = f(x) \quad x \in \Omega$$
$$u(x) = g(x) \quad x \in \Omega_\delta$$



Initial guesses: $(\delta_1,\alpha_1) = (1,0.5)$ $(\delta_2,\alpha_2) = (10,0.5)$ $(\delta_3,\alpha_3) = (1000,0.5)$

Relative errors: $e_1 = 5.46\times10^{-4}$ $e_2 = 1.06\times10^{-4}$ $e_3 = 8.17\times10^{-4}$

Wrong answer, but comparable error!

Turbulence Modeling of Couette Flow

- **1D equation for Couette flow**

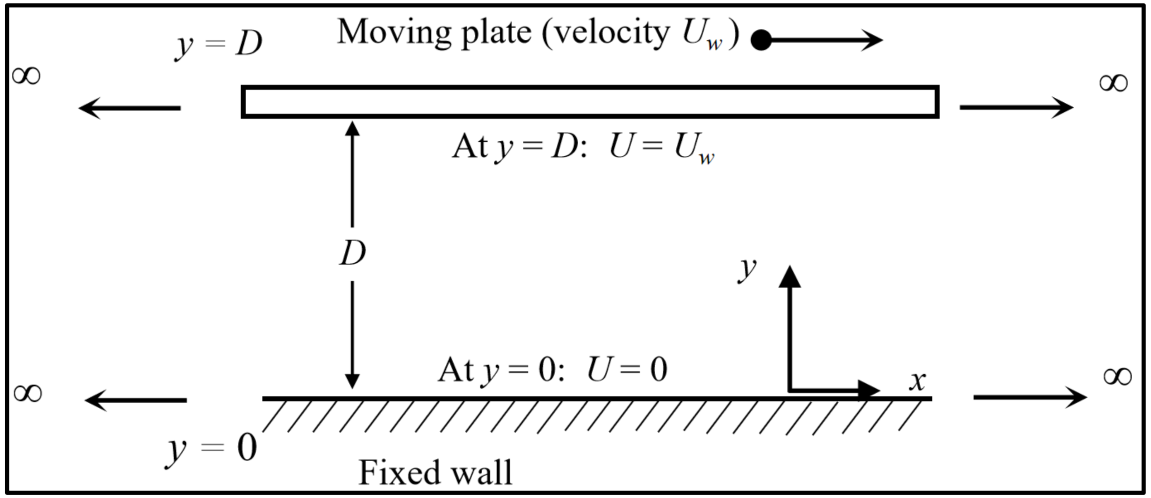
$$\frac{d}{dy^+}\left(\frac{dU^+}{dy^+} - \left(\overline{uv}\right)^+\right) = 0, \quad y^+ \in [0, 2Re_\tau]$$

dimensionless total shear stress — dimensionless Reynolds stress

U+, y+ are dimensionless variables based on wall units

- **Total shear stress equation**

$$\frac{dU^+}{dy^+} - \left(\overline{uv}\right)^+ = 1, \quad y^+ \in [0, 2Re_\tau]$$



- **Propose new nonlocal model for Couette flow:**

$$\tilde{\mathcal{L}}_{\delta,\alpha} U^+ = 1, \quad \delta > 0,\ \alpha(y^+) \in (0,1)$$

- **New operator is not the operator $\mathcal{L}_{\delta,\alpha}$ we explored previously!**

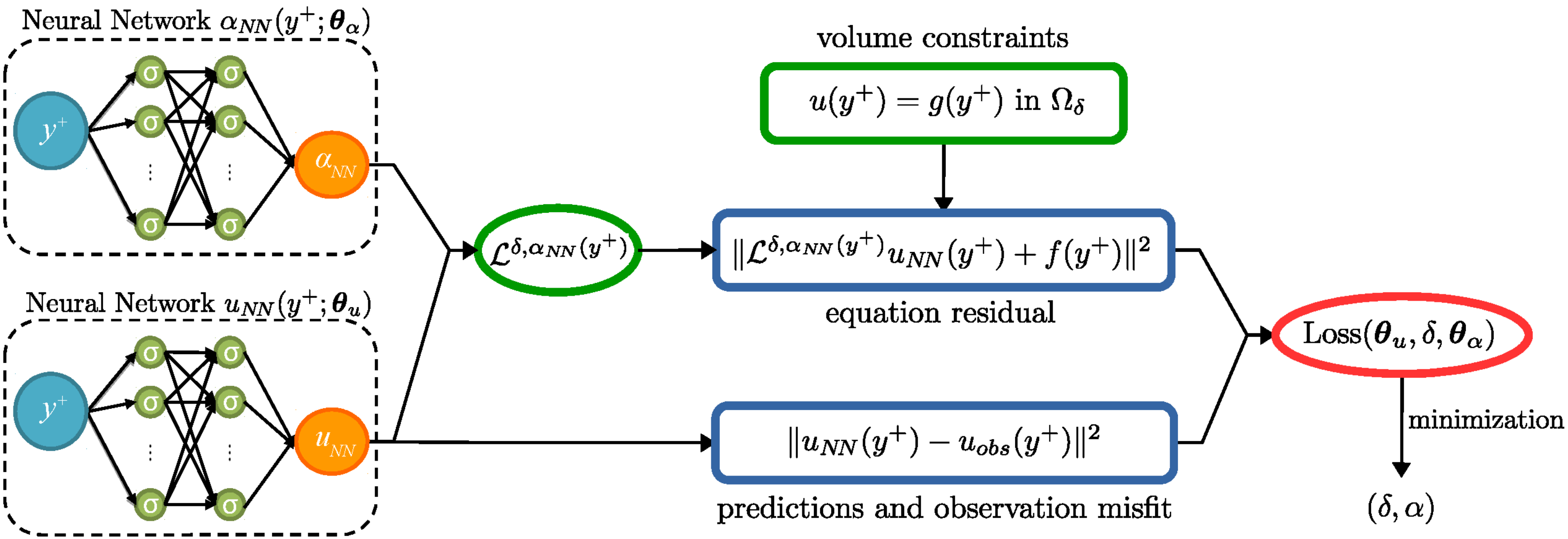
$$\lim_{\delta\to\infty}\left(\tilde{\mathcal{L}}_{\delta,\alpha}\right)U^+ \to$$ **Combinaton of Caputo fractional derivatives**

$$\lim_{\alpha(y^+)\to 1,\delta\to\infty}\left(-\mathcal{L}_{\delta,\alpha}\right)U^+ = \frac{dU^+}{dy^+}$$

Reduces to local model only in viscous sublayer where Reynolds stress << 1.

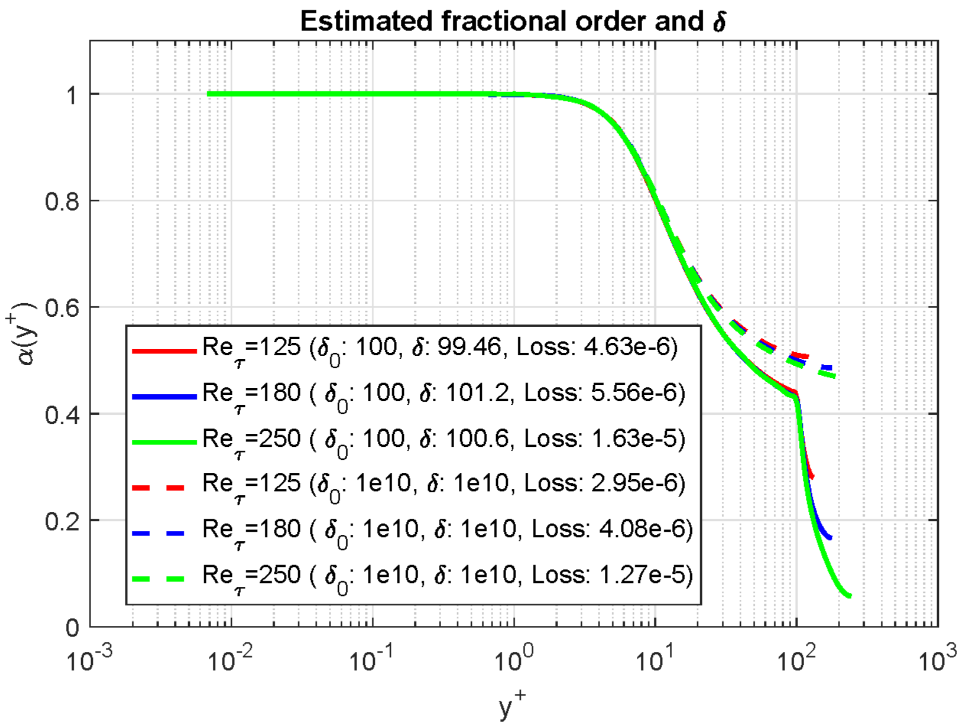
Turbulence Modeling of Couette Flow

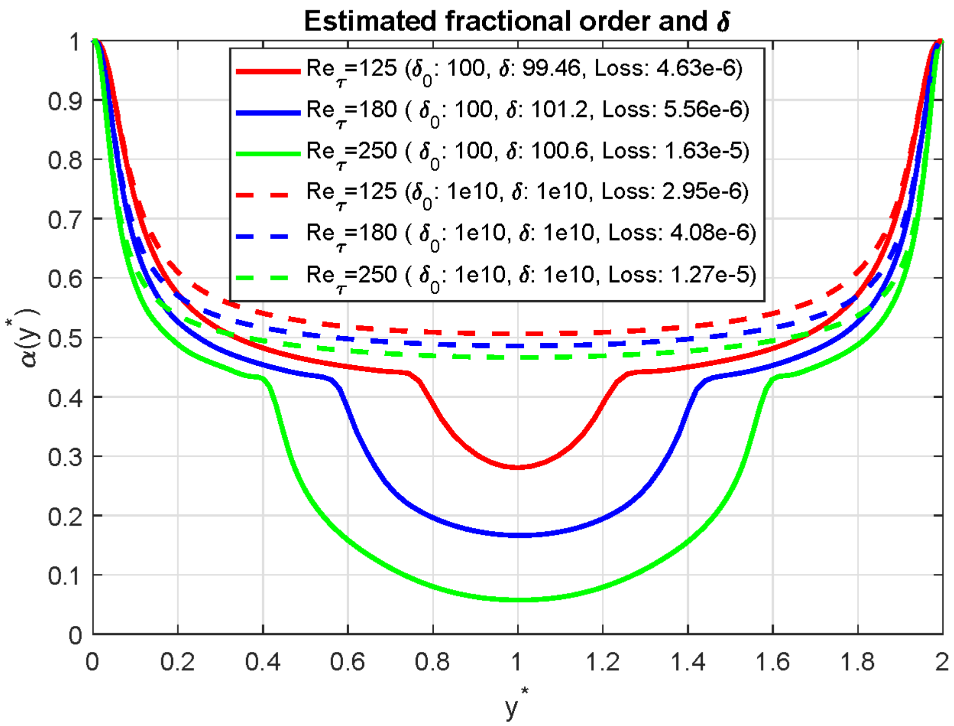
- ❑ **Use nPINN to jointly estimate δ = 0.3, α(y+). Use separate neural networks for U, α.**
- ❑ **Train using DNS data* for three different Reynolds numbers, Re_τ = 125, 180, 250.**



*V. Avsarkisov, S. Hoyas, M. Oberlack, Jose Pedro Garcia-Galache, Turbulent plane Couette flow at moderately high Reynolds number, J. Fluid Mech. 751 (2014).

Turbulence Modeling of Couette Flow

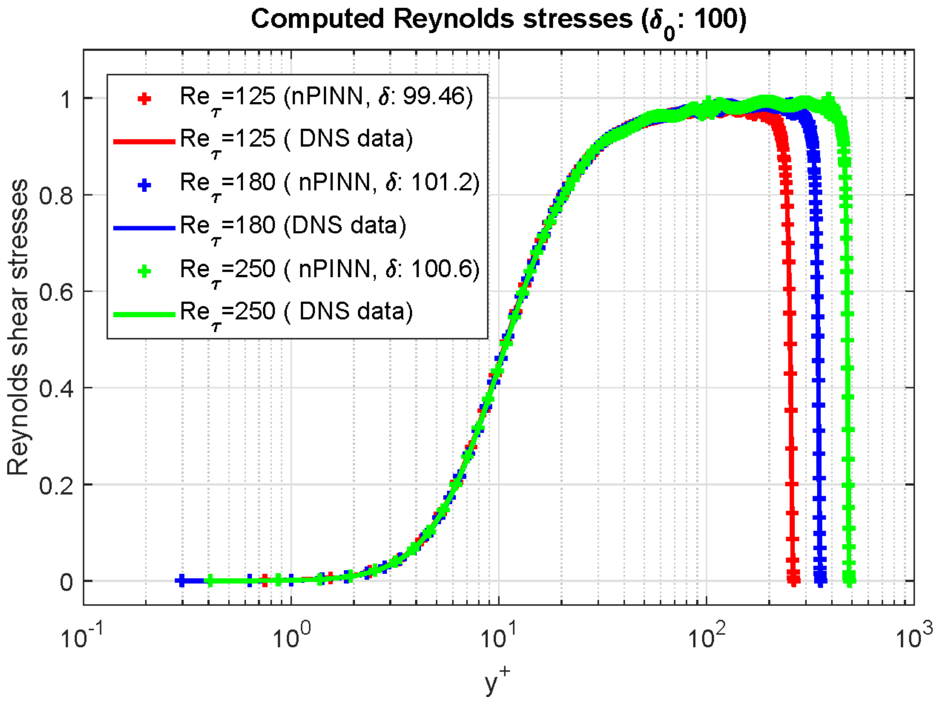


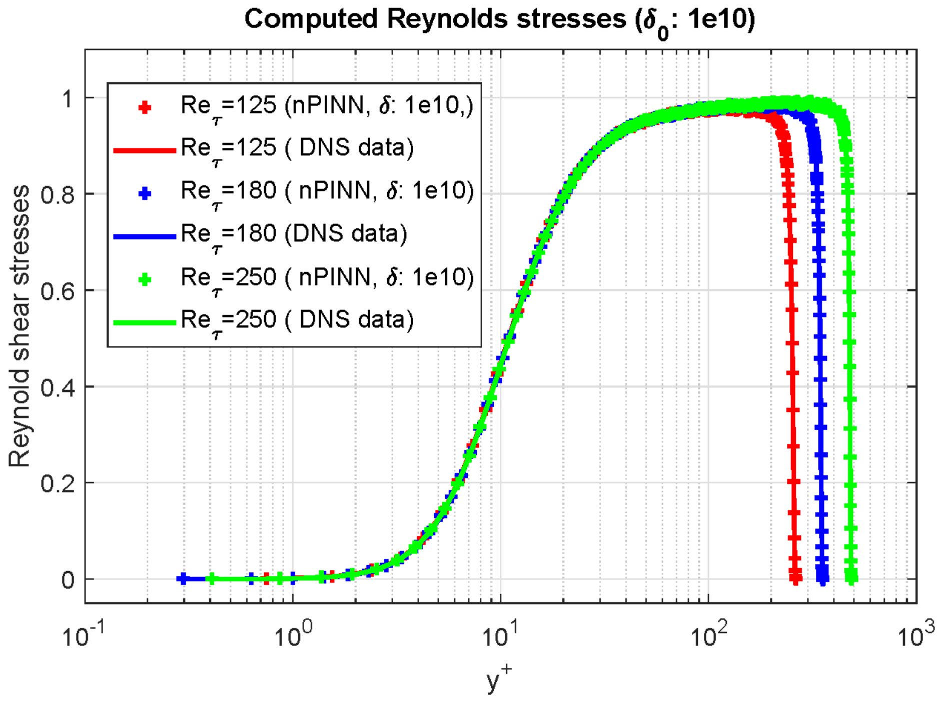


Observations:

- ❑ **Loss function not sensitive to changes in δ.**
- ❑ **Estimated fractional order profiles $\alpha(y^+)$ on top of each other independent of δ, Re_τ. Suggests existence of universal fractional order $\alpha(y^+)$ that reproduces DNS data independent of these Reynolds numbers.**
- ❑ **Fractional order $\approx$ 1 near walls. Agrees with limit behavior for small Reynolds stress.**
- ❑ **Fractional orders different for $y^+ > 20$, but with similar losses. Operators are distinct, but action on velocity is essentially the same (Mimic operator).**

Turbulence Modeling of Couette Flow





Observations:

- ❑ **Computed Reynolds stresses on top of those reported from DNS dataset.**
- ❑ **Very different values of δ produce same stresses. These and other results (not shown) imply larger values of δ are more physically meaningful, and there is a threshold above which the nPINN reaches the same accuracy.**

Summary

- Nonlocal Models
- Using computational models in practice
- nPINNS: nonlocal Physics-Informed Neural Networks
  - Data-driven solutions
  - Data-driven discovery
- Example: a nonlocal model for turbulent Couette flow
- Conclusions