DeepONet: Learning nonlinear operators

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Conference on the Numerical Solution of Differential and Differential-Algebraic Equations
Sept 7, 2021

From function to operator

- Function: $\mathbb{R}^{d_1} \to \mathbb{R}^{d_2}$

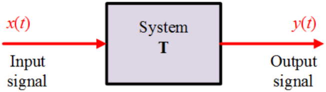
  e.g., image classification:  $\mapsto$ 5

- Operator: function (∞-dim) $\mapsto$ function (∞-dim)

  e.g., derivative (local): $x(t) \mapsto x'(t)$

  e.g., integral (global): $x(t) \mapsto \int K(s,t)x(s)ds$

  e.g., dynamic system:



  e.g., biological system

  e.g., social system

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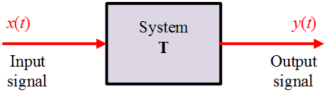
  e.g., dynamic system: 

  e.g., biological system

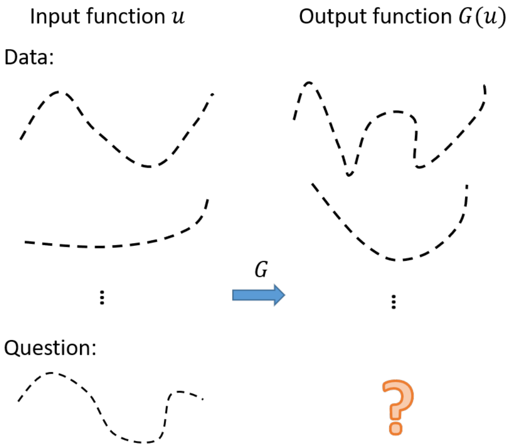
  e.g., social system

  $\Rightarrow$ Can we learn operators via neural networks?

  $\Rightarrow$ How?

Problem setup

$G : u \in V \subset C(K_1) \mapsto G(u) \in C(K_2)$
$G(u) : y \in \mathbb{R}^d \mapsto G(u)(y) \in \mathbb{R}$



Universal Approximation Theorem for Operator

$G : u \in V \subset C(K_1) \mapsto G(u) \in C(K_2)$
$G(u) : y \in \mathbb{R}^d \mapsto G(u)(y) \in \mathbb{R}$

Theorem (Chen & Chen, 1995)

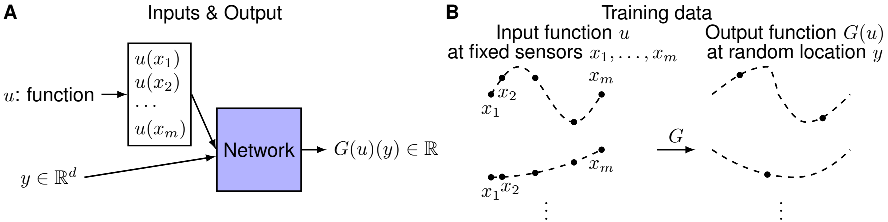
Suppose that σ is a continuous non-polynomial function, X is a Banach Space, $K_1 \subset X$, $K_2 \subset \mathbb{R}^d$ are two compact sets in X and $\mathbb{R}^d$, respectively, V is a compact set in $C(K_1)$, G is a continuous operator, which maps V into $C(K_2)$.
Then for any $\epsilon > 0$, there are positive integers n, p, m, constants $c_i^k, \xi_{ij}^k, \theta_i^k, \zeta_k \in \mathbb{R}$, $w_k \in \mathbb{R}^d$, $x_j \in K_1$, $i = 1, \ldots, n$, $k = 1, \ldots, p$, $j = 1, \ldots, m$, such that

$$\left| G(u)(y) - \sum_{k=1}^{p} \sum_{i=1}^{n} c_i^k \sigma \left(\sum_{j=1}^{m} \xi_{ij}^k u(x_j) + \theta_i^k \right) \sigma(w_k \cdot y + \zeta_k) \right| < \epsilon$$

holds for all $u \in V$ and $y \in K_2$.

Problem setup

$G : u \in V \subset C(K_1) \mapsto G(u) \in C(K_2)$
$G(u) : y \in \mathbb{R}^d \mapsto G(u)(y) \in \mathbb{R}$



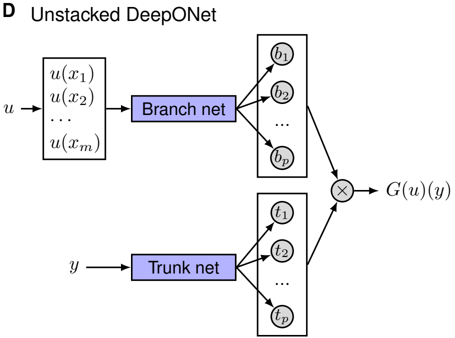
- Inputs: u at sensors $\{x_1, x_2, \ldots, x_m\} \in \mathbb{R}^m$, $y \in \mathbb{R}^d$
- Output: $G(u)(y) \in \mathbb{R}$

Lu et al., *Nature Mach Intell*, 2021

Deep operator network (DeepONet)

Lu et al., *Nature Mach Intell*, 2021

$$G(u)(y) \approx \sum_{k=1}^{p} \underbrace{b_k(u)}_{\text{branch}} \underbrace{t_k(y)}_{\text{trunk}}$$



Idea: $G(u)(y)$: a function of y conditioning on u

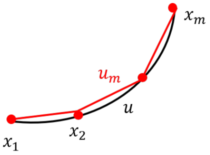
- $t_k(y)$: basis function of y
- $b_k(u)$: u-dependent coefficient, i.e., functional of u

Error analysis: the number of sensors

Consider $G : u(x) \mapsto \boldsymbol{s}(x)$ $(x \in [0,1])$ by ODE system

$$\frac{d}{dx}\boldsymbol{s}(x) = \boldsymbol{g}(\boldsymbol{s}(x), u(x), x), \quad \boldsymbol{s}(0) = \boldsymbol{s_0}$$

$\forall u \in V \Rightarrow u_m \in V_m$



Let $\kappa(m, V) := \sup_{u \in V} \max_{x \in [0,1]} |u(x) - u_m(x)|$

e.g., Gaussian process with kernel $e^{-\frac{\|x_1 - x_2\|^2}{2l^2}}$: $\kappa(m, V) \sim \frac{1}{m^2 l^2}$

Theorem (Lu et al., *Nature Mach Intell*, 2021)

Assume $\mathbf{g}$ *is Lipschitz continuous* (c)*.*
Then there exists a DeepONet $\mathcal{N}$*, such that*

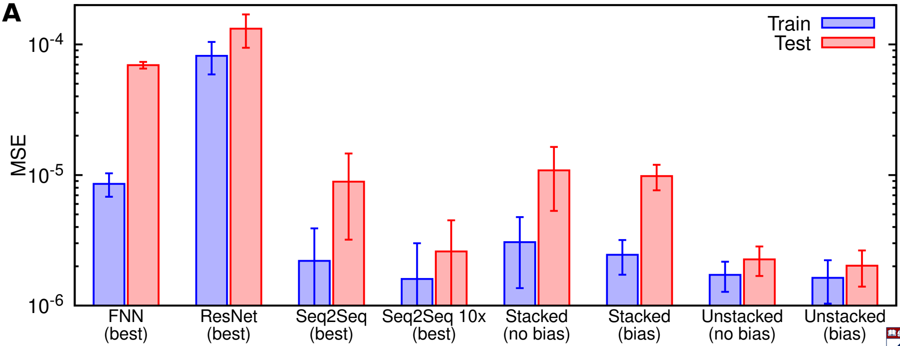
$$\sup_{u \in V} \max_{x \in [0,1]} \|G(u)(x) - \mathcal{N}([u(x_1), \ldots, u(x_m)], x)\|_2 < ce^c \kappa(m, V).$$

Explicit operator: A simple ODE case

$$\frac{ds(x)}{dx} = u(x), \quad x \in [0,1], \quad s(0) = 0$$

$$G : u(x) \mapsto s(y) = s(0) + \int_0^y u(\tau)d\tau$$

Very small generalization error!

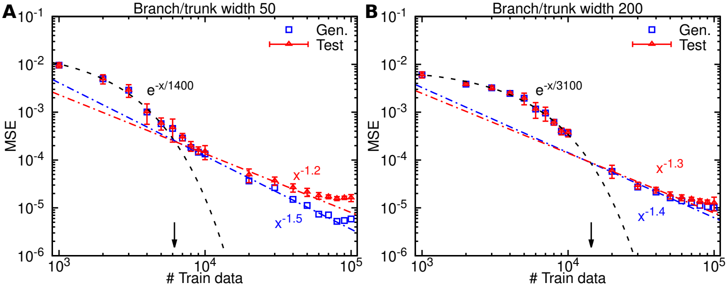


Lu et al., *Nature Mach Intell*, 2021

Implicit operator: Gravity pendulum with an external force

$$\frac{ds_1}{dt} = s_2, \qquad \frac{ds_2}{dt} = -k \sin s_1 + u(t)$$

$G : u(t) \mapsto \mathbf{s}(t)$



Test/generalization error:

- small dataset: exponential convergence
- large dataset: polynomial rates
- larger network has later transition point

Lu et al., *Nature Mach Intell*, 2021

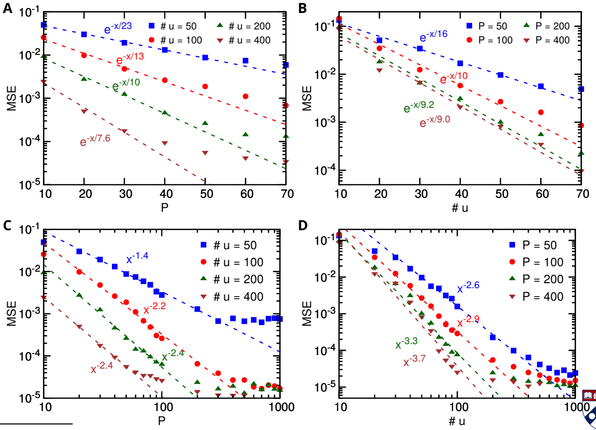
Implicit operator: Diffusion-reaction system

$$\frac{\partial s}{\partial t} = D\frac{\partial^2 s}{\partial x^2} + ks^2 + u(x), \quad x \in [0,1], t \in [0,1]$$

$\#$ Training points $= \#u \times P$

Small dataset: Exponential convergence

Large dataset: Polynomial convergence



Lu et al., *Nature Mach Intell*, 2021

Stochastic ODE

Consider the population growth model

$$dy(t;\omega) = k(t;\omega)y(t;\omega)dt, \quad y(0) = 1$$

Stochastic process $k(t;\omega) \sim \mathcal{GP}(0, \sigma^2 \exp(-\|t_1 - t_2\|^2/2l^2))$

$$G : k(t;\omega) \mapsto y(t;\omega)$$

Ideas:

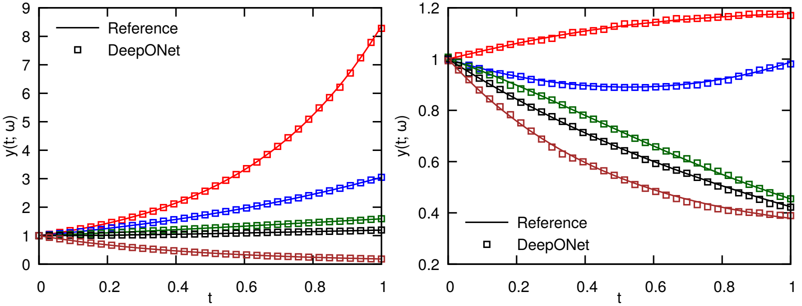
- Karhunen-Loève (KL) expansion: $k(t;\omega) \approx \sum_{i=1}^{N} \sqrt{\lambda_i} e_i(t) \xi_i(\omega)$
- branch net inputs: $[\sqrt{\lambda_1} e_1(t), \sqrt{\lambda_2} e_2(t), \ldots, \sqrt{\lambda_N} e_N(t)] \in \mathbb{R}^{N \times m}$, where $\sqrt{\lambda_i} e_i(t) = \sqrt{\lambda_i}[(e_i(t_1), e_i(t_2)), \ldots, e_i(t_m)] \in \mathbb{R}^m$
- trunk net inputs: $[t, \xi_1, \xi_2, \ldots, \xi_N] \in \mathbb{R}^{N+1}$

Lu et al., *Nature Mach Intell*, 2021

Stochastic ODE

- Choose $N = 5$ to conserve 99.9% stochastic energy
- Train with 10000 different $k(t;\omega)$ with l randomly sampled in $[1, 2]$, and for each $k(t;\omega)$ we use only one realization
- Test MSE is $8.0 \times 10^{-5} \pm 3.4 \times 10^{-5}$

Example: 10 different random samples of $y(t;\omega)$ for $k(t;\omega)$ with $l = 1.5$



Lu et al., *Nature Mach Intell*, 2021

Stochastic PDE

Consider the elliptic problem with multiplicative noise

$$-\text{div}(e^{b(x;\omega)}\nabla u(x;\omega)) = f(x), \quad x \in (0,1)$$

with zero boundary conditions, $f(x) = 10$.
Stochastic process $b(x;\omega) \sim \mathcal{GP}(0, \sigma^2 \exp(-\|x_1 - x_2\|^2/2l^2))$

$$G : b(x;\omega) \mapsto u(x;\omega)$$

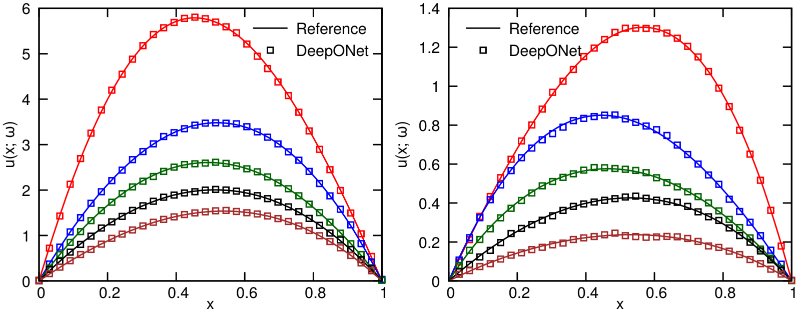
Ideas:

- Karhunen-Loève (KL) expansion: $b(x;\omega) \approx \sum_{i=1}^{N} \sqrt{\lambda_i} e_i(x)\xi_i(\omega)$
- branch net inputs: $[\sqrt{\lambda_1}e_1(x), \sqrt{\lambda_2}e_2(x), \ldots, \sqrt{\lambda_N}e_N(x)] \in \mathbb{R}^{N\times m}$, where $\sqrt{\lambda_i}e_i(x) = \sqrt{\lambda_i}[e_i(x_1), e_i(x_2), \ldots, e_i(x_m)] \in \mathbb{R}^m$
- trunk net inputs: $[x, \xi_1, \xi_2, \ldots, \xi_N] \in \mathbb{R}^{N+1}$

Lu et al., *Nature Mach Intell*, 2021

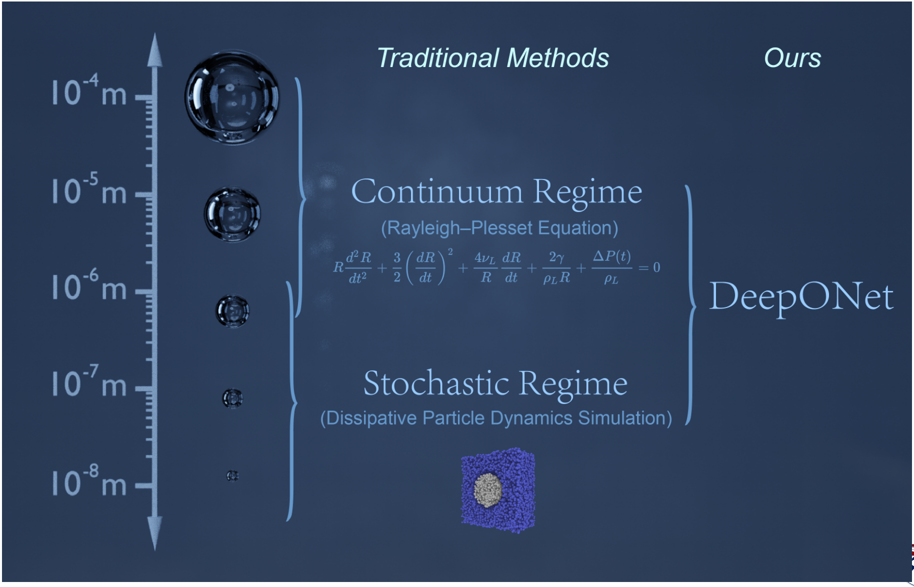
Stochastic PDE

Example: 10 different random samples of $u(x;\omega)$ for $b(x;\omega)$ with $l = 1.5$



Lu et al., *Nature Mach Intell*, 2021

DeepONet for bubble growth dynamics



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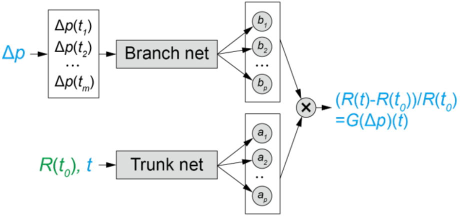
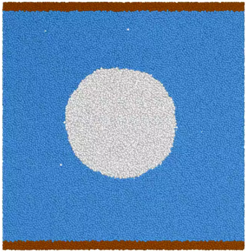
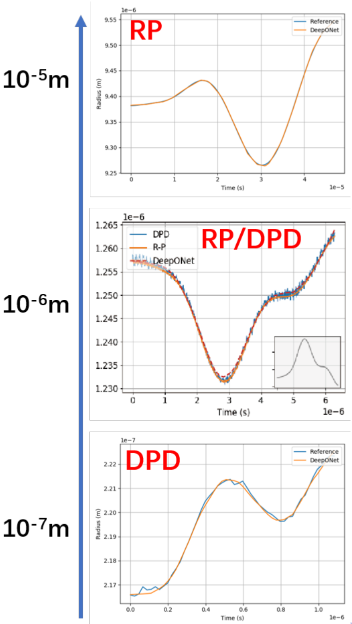
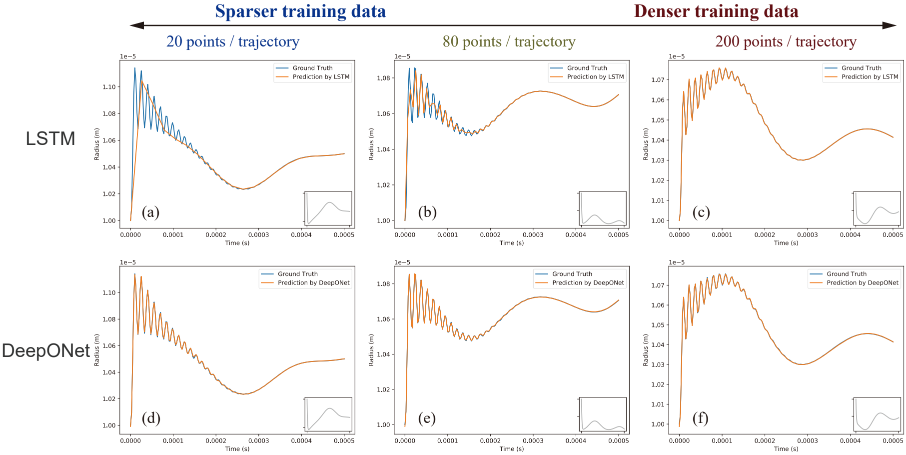






Lin et al., *J Chem Phys*, 2021

DeepONet vs. LSTM



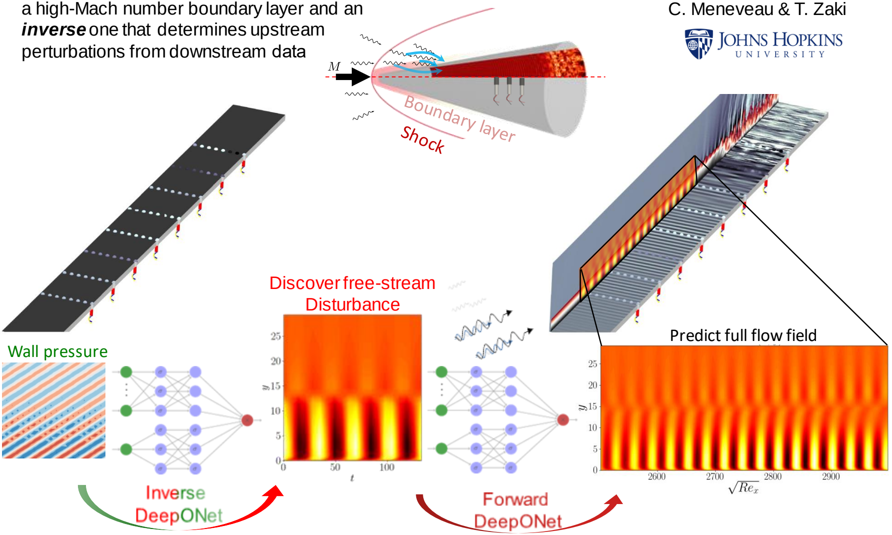
Lin et al., *J Chem Phys*, 2021

Data assimilation in high-Mach boundary layers

We trained a ***forward*** DeepONet that predicts the evolution of instability waves in a high-Mach number boundary layer and an ***inverse*** one that determines upstream perturbations from downstream data

In collaboration with
P. Clark Di Leoni, Y. Hao,
C. Meneveau & T. Zaki

JOHNS HOPKINS UNIVERSITY



Clark Di Leoni et al., arXiv:2105.08697

Multiphysics & Multiscale problems

Electroconvection problem

- Stokes equation

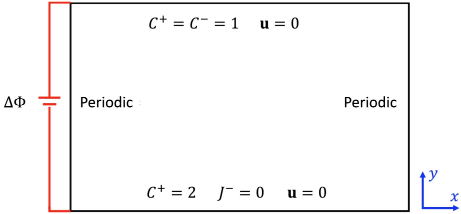
$$\frac{\partial \mathbf{u}}{\partial t} = -\nabla p + \nabla^2 \mathbf{u} - \frac{\kappa}{2\epsilon^2}\rho_e \nabla \phi$$
$$\nabla \cdot \mathbf{u} = 0$$

- Electric potential

$$-2\epsilon^2 \nabla^2 \phi = \rho_e = z(c^+ - c^-)$$

- Ion transport equation

$$\frac{\partial c^\pm}{\partial t} = -\nabla \cdot \mathbf{J}^\pm$$
$$\mathbf{J}^\pm = c^\pm \mathbf{u} - \nabla c^\pm \mp c^\pm \nabla \phi$$

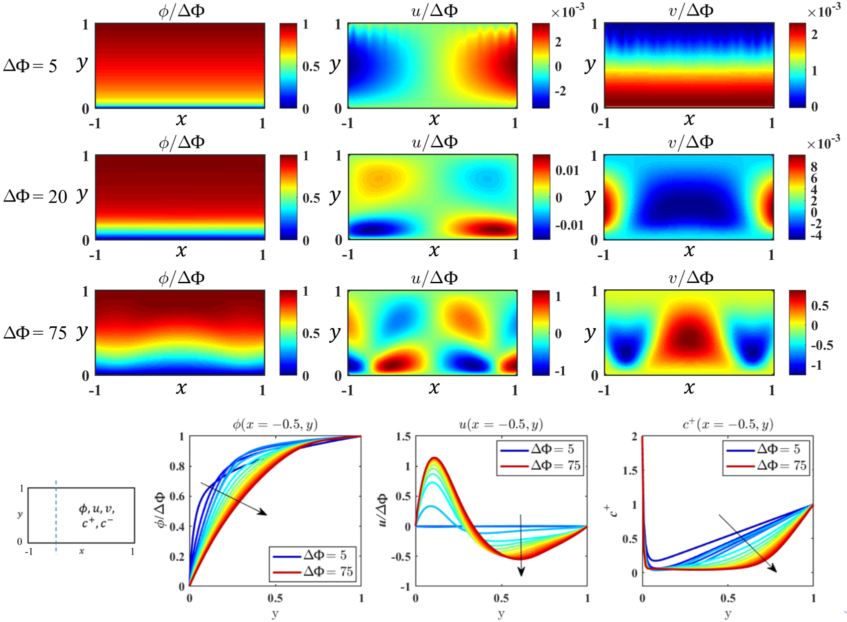


$$\Delta\phi \in [5, 75]$$

- $\mathbf{u}$: velocity
- p: pressure
- ϕ: electric potential
- ρ_e: free charge density
- $c^\pm$: cation/anion concentrations
- $\mathbf{J}^\pm$: flux

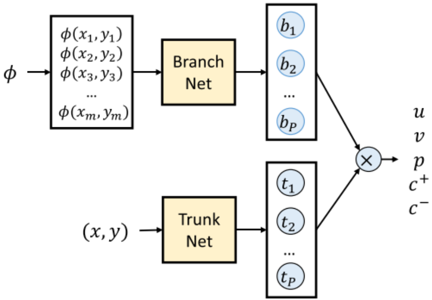
Cai et al., *J Comput Phys*, 2021

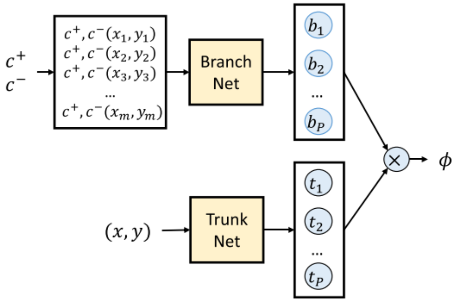
Data examples (steady state)



Physics decomposition via 6 DeepONets

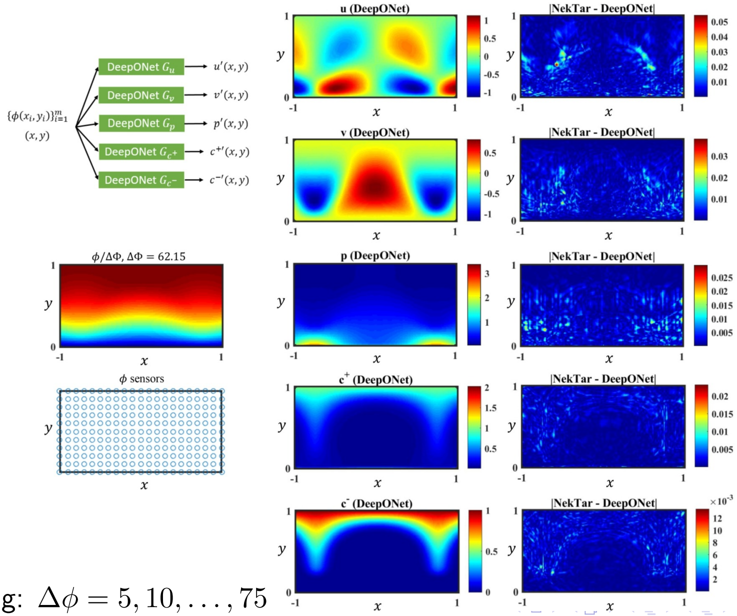
DeepONets	Input function	Output function
G_ϕ	$c^+(x,y), c^-(x,y)$	$\phi(x,y)$
G_u	$\phi(x,y)$	$u(x,y)$
G_v	$\phi(x,y)$	$v(x,y)$
G_p	$\phi(x,y)$	$p(x,y)$
G_{c^+}	$\phi(x,y)$	$c^+(x,y)$
G_{c^-}	$\phi(x,y)$	$c^-(x,y)$





Cai et al., *J Comput Phys*, 2021

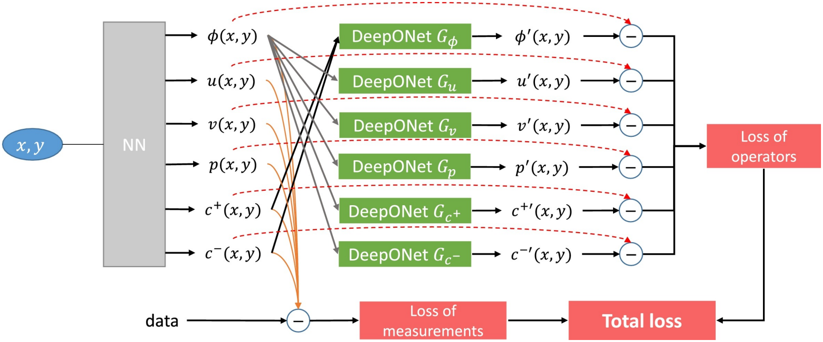
Physics decomposition via 6 DeepONets



Training: $\Delta\phi = 5, 10, \ldots, 75$

DeepM&Mnet: DeepONets coupling

Parallel DeepONets



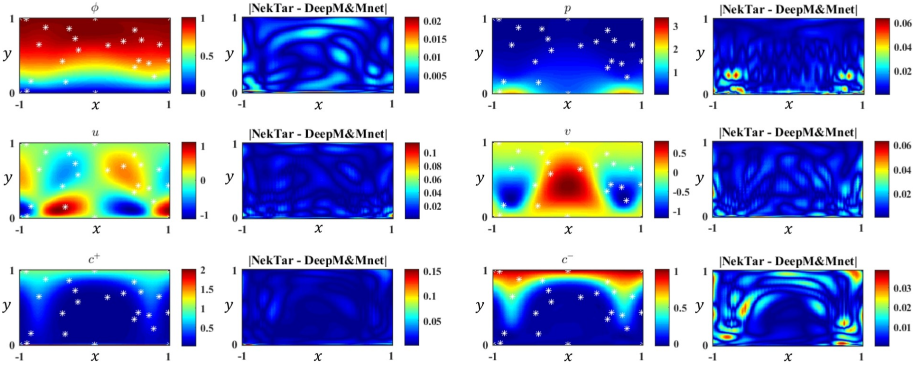
Loss function:

$$\mathcal{L} = \lambda_d \mathcal{L}_{data} + \lambda_o \mathcal{L}_{op} + \lambda_r \mathcal{L}_2(\theta)$$

$$\mathcal{L}_{op} = \sum_{V \in \{\phi, u, v, p, c^+, c^-\}} \frac{1}{N_{op}} \sum_{i=1}^{N_{op}} \left(V(x^i, y^i) - V'(x^i, y^i) \right)^2$$

Testing example

$\Delta \phi = 62.15$



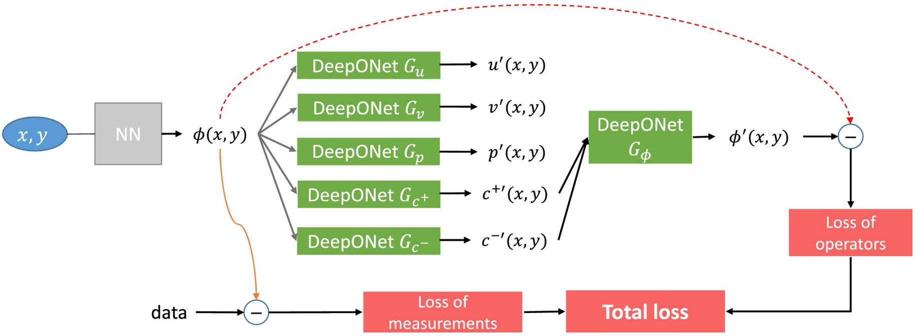
Relative error $\sim 1\%$

ϕ: 0.54%, u: 1.26%, v: 0.54%, p: 0.93%, c^+: 0.67%, c^-: 0.48%

Cai et al., *J Comput Phys*, 2021

DeepM&Mnet: DeepONets coupling

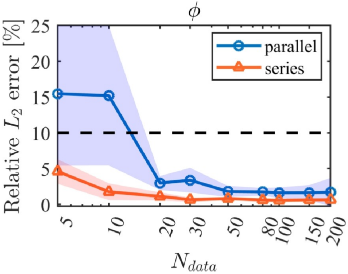
Serial DeepONets



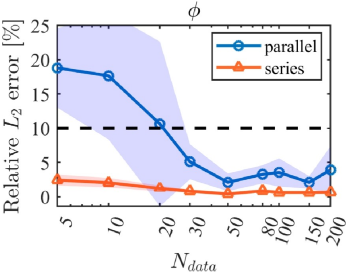
Cai et al., *J Comput Phys*, 2021

DeepM&Mnet: Parallel vs. Serial

Only have data of ϕ:



(a) NN size: 6×100



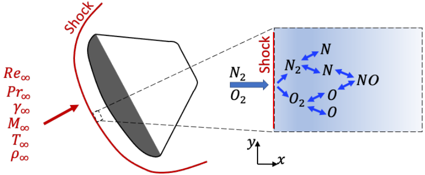
(b) NN size: 3×50

- Serial: Better accuracy
  - especially when the data is small
- Parallel: More flexible

Cai et al., *J Comput Phys*, 2021

DeepM&Mnet: Multiphysics & Multiscale problems

Hypersonics with chemical reaction: fluid flow & chemical reaction



$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_j) = 0$$

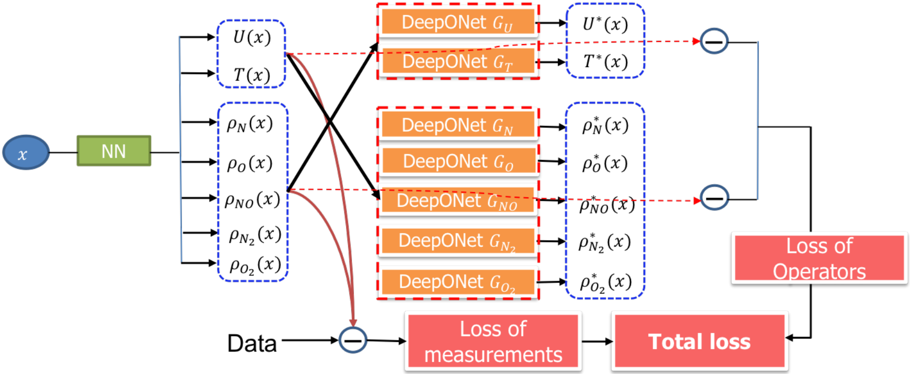
$$\frac{\partial \rho^s}{\partial t} + \frac{\partial}{\partial x_j}(\rho^s u_j) = \dot{w}^s, \quad s = 1, \ldots, 5$$

$$\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j + p\delta_{ij}) = \frac{\partial \sigma_{ij}}{\partial x_j}, \quad i = 1, 2$$

$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x_j}[(E+p)u_j] = -\frac{\partial q_j}{\partial x_j} + \frac{\partial}{\partial x_k}(u_j \sigma_{jk})$$

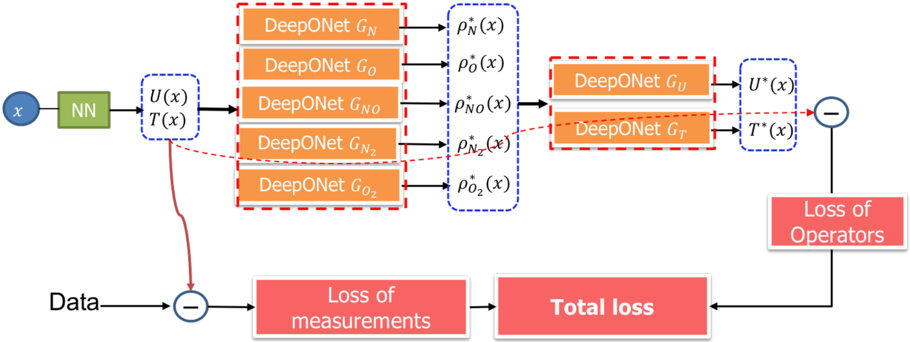
Mao et al., arXiv:2011.03349

Parallel DeepM&Mnet



Mao et al., arXiv:2011.03349

Serial DeepM&Mnet



Mao et al., arXiv:2011.03349

DeepONet for learning operators

DeepONet (**Lu** et al., *Nature Mach Intell*, 2021)

- **Algorithms & Applications**
  - 16 ODEs/PDEs (nonlinear, fractional & stochastic)
  - Multiphysics & Multiscale problems
    - ★ Bubble growth dynamics from nm to mm (Lin et al., *J Chem Phys*, 2021)
    - ★ Linear instability waves in high-speed boundary layers (Clark Di Leoni et al., arXiv:2105.08697)
    - ★ Electroconvection (Cai et al., *J Comput Phys*, 2021)
    - ★ Hypersonics (Mao et al., arXiv:2011.03349)
- **Observation**: Good performance
  - Small generalization error
  - Exponential/polynomial error convergence
- **Theory**
  - Convergence rate for advection-diffusion equations (Deng et al., arXiv:2102.10621)