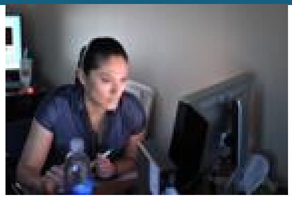
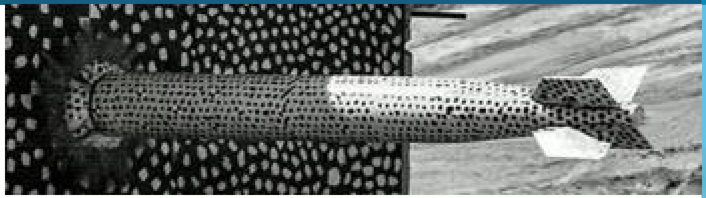
SAND2021-7895C

Physics-informed machine learning of flow and reactive transport in porous media





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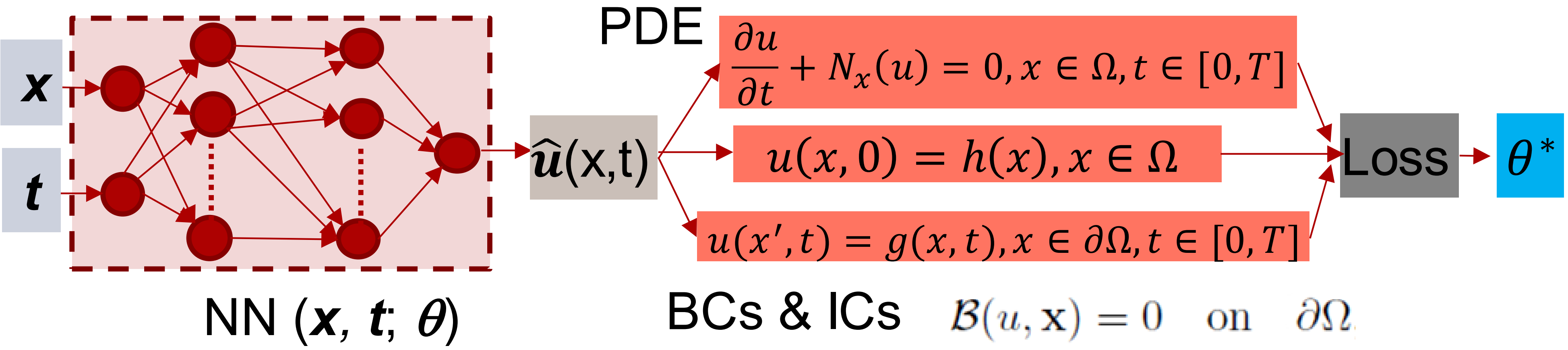
PINNs with Neural Networks for PDEs

- We are using a form of neural networks known as **Physics-Informed neural networks** (PINN) to solve **partial differential equations** (PDEs) involved in fluid flow and reactive transport.
- A main idea of PINNs is to **incorporate governing equations of physics** in the form of **partial differential equations** (PDEs) **into the loss** via automatic differentiation (AD)

$$f\left(\mathrm{x}; \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_d}; \frac{\partial^2 u}{\partial x_1 \partial x_1}, \ldots, \frac{\partial^2 u}{\partial x_1 \partial x_d}; \ldots; \lambda\right) = 0, \quad \mathrm{x} \in \Omega$$



$$\frac{\partial u}{\partial t} + N_x(u) = 0, x \in \Omega, t \in [0, T]$$

$$u(x, 0) = h(x), x \in \Omega$$

$$u(x', t) = g(x, t), x \in \partial\Omega, t \in [0, T]$$

$$\mathcal{B}(u, \mathrm{x}) = 0 \quad \text{on} \quad \partial\Omega$$

Loss = Sum of Data fit and physics regularization from PDEs, IC&BCs

Example of 2D Advection-Dispersion Reaction

3 different cases

1. Concentration data Only
2. Concentration data + Advection Dispersion PDE
3. Concentration data + head loss and conductivity + ADE + Darcy Eqn (For Darcy eqn, K field can be estimated inversely)

$$R\frac{\partial c}{\partial t} = -u\frac{\partial c}{\partial x} + D_x\frac{\partial^2 c}{\partial x^2} + D_y\frac{\partial^2 c}{\partial y^2} + \lambda c$$

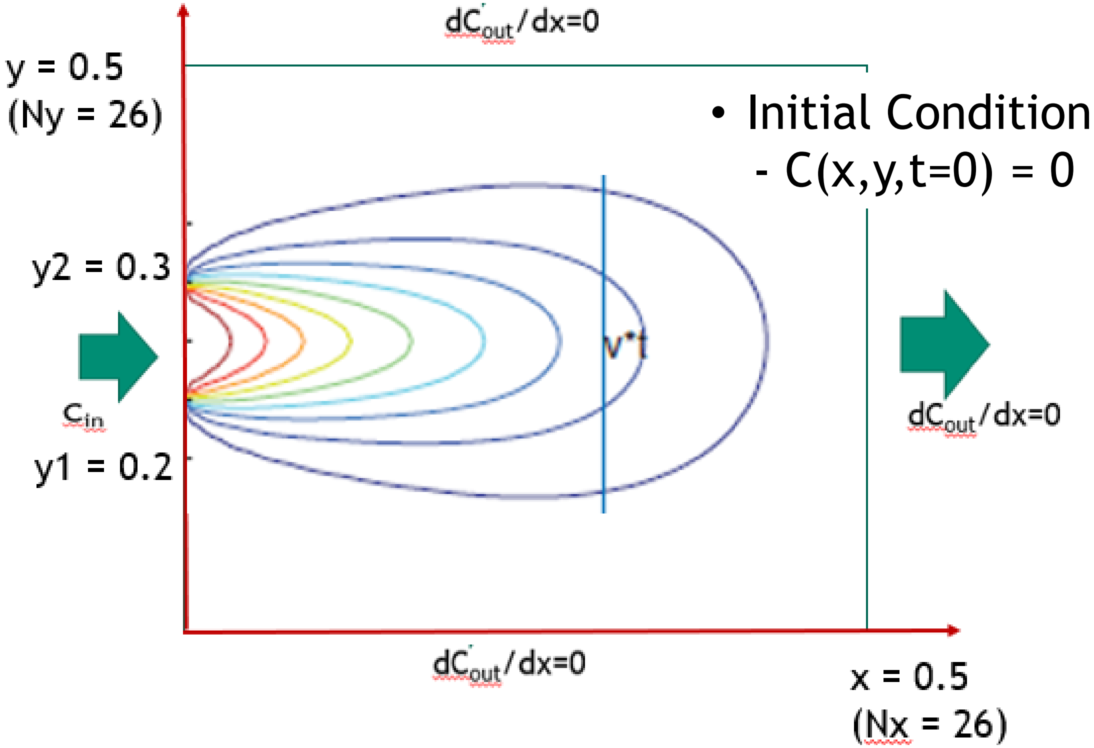
Analytical Solution:

$$c\left(x, y, z, t\right) = \frac{C_0}{8}\left\{\exp\left[\frac{\left(v-u'\right)x'}{2D_x}\right] erfc\left(\frac{x'-u't}{2\sqrt{D_x t}}\right) + \exp\left[\frac{\left(v+u'\right)x'}{2D_x}\right] erfc\left(\frac{x'+u't}{2\sqrt{D_x t}}\right)\right\}$$

$$\times\left[erfc\frac{y-y_2}{2\sqrt{D_y\tau_m}} - 4rfc\frac{y-y_1}{2\sqrt{D_y\tau_m}}\right]$$

$$u' = \sqrt{v^2+4\lambda D_x},\ \tau_m = x/v, \quad y_1 \le y \le y_2$$

Example of concentration field
(red-high, blue – low from analytical solution)



- Initial Condition:
  - C(x,y,t=0) = 0

$$\begin{cases} \boldsymbol{v}\left(\boldsymbol{x}\right) = -\frac{K(\boldsymbol{x})}{\phi}\nabla h\left(\boldsymbol{x}\right) \\ \nabla\cdot\boldsymbol{v}(\boldsymbol{x}) = 0, \quad \boldsymbol{x}\in\Omega \\ h\left(\boldsymbol{x}\right) = H_2, \quad x_1 = L_1 \\ -K\left(\boldsymbol{x}\right)\partial h\left(\boldsymbol{x}\right)/\partial x_1 = q, \quad x_1 = 0 \\ -K\left(\boldsymbol{x}\right)\partial h\left(\boldsymbol{x}\right)/\partial x_2 = 0, \quad x_2 = 0 \text{ or } x_2 = L_2 \end{cases}$$

- Boundary Conditions for Darcy Eqn:
  - Dirichlet BC at inlet/outlet:

    q(x=0,y,t) = u_{in}

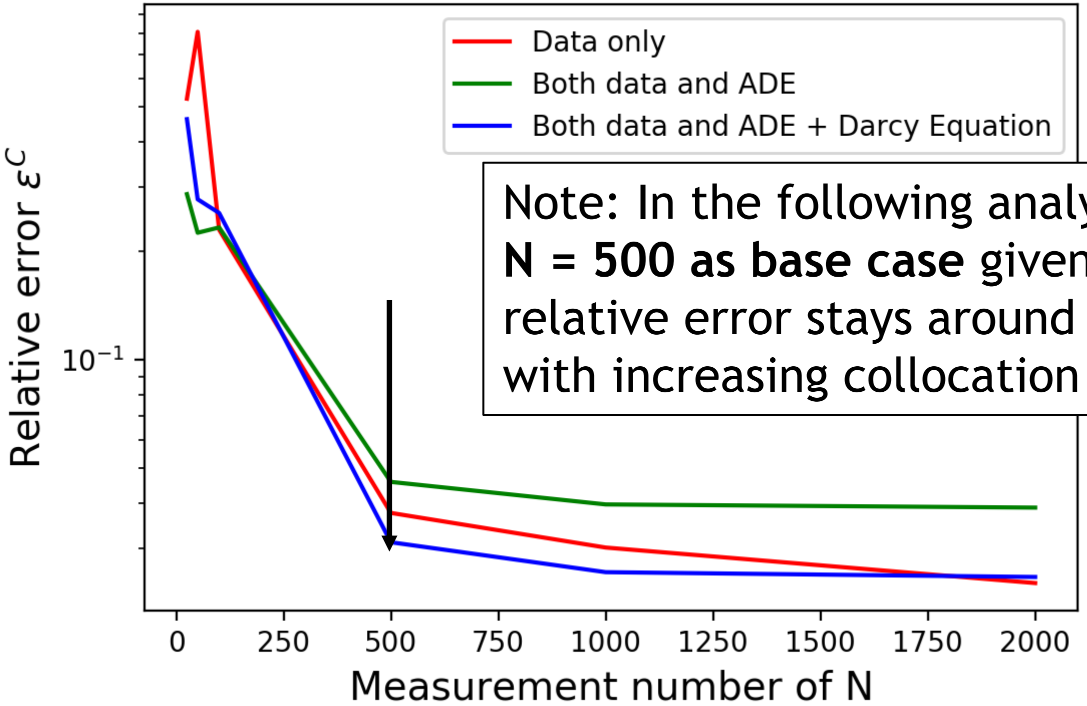
    H(x=1,y,t) = H_{out}

Key Model Parameters

- 10,000 Epochs
- 4 hidden layers with 40 nodes each
- The number of collocation points: 0.34%, 0.68%, 1.3%, 6.7%, 13.4%, 26.9%
- Loss: Mean-Squared Error (MSE)
- Weight factors for each loss component (Cases 2&3)
- As we increase collocation points (N), relative error of ML decreases

$$N = N_c = N_K = N_h = N_{fc} = N_f$$

Relative error of three different cases as a function of collocation points



Note: In the following analysis, we use **N = 500 as base case** given that the relative error stays around the same with increasing collocation points

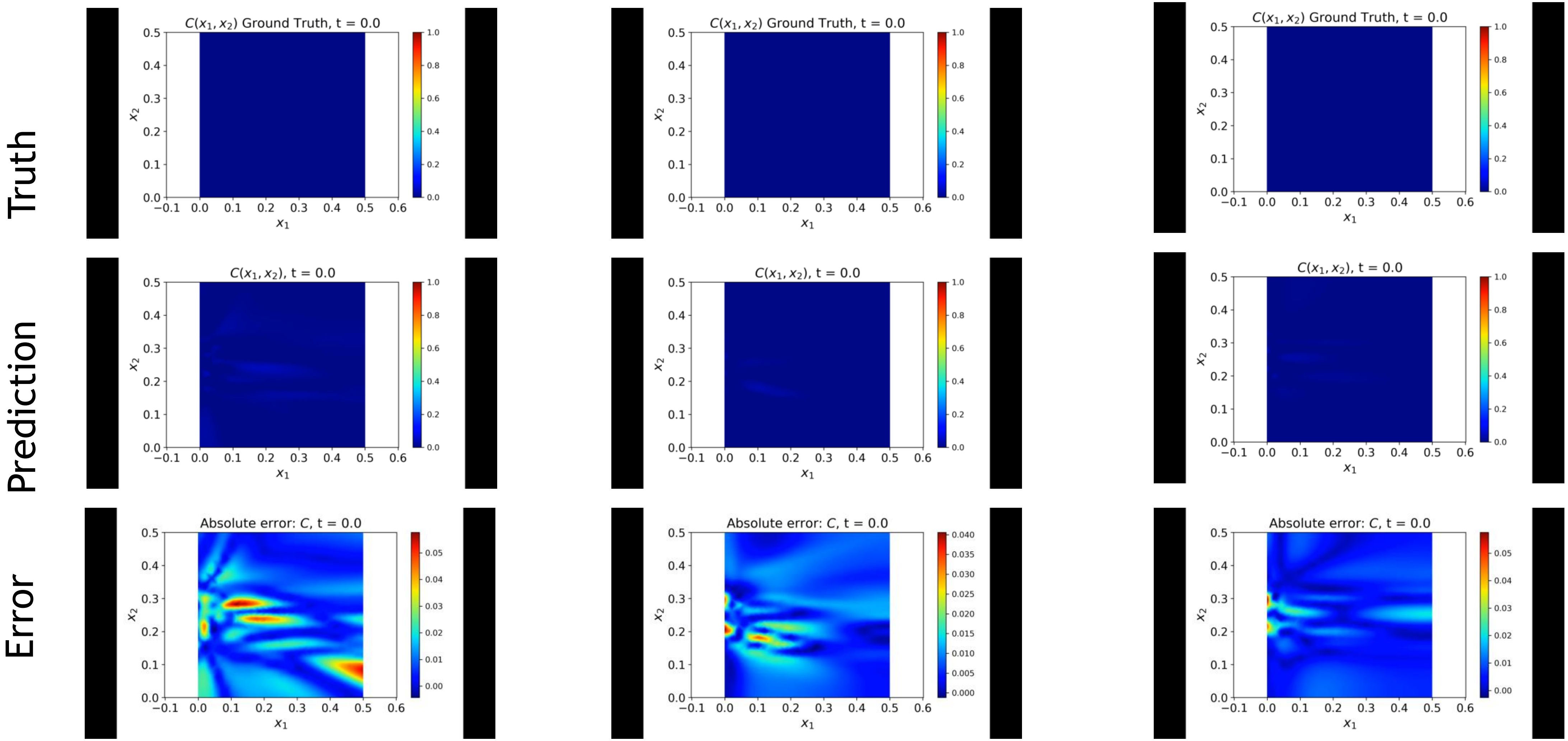
A total number of points:
26 (nx) * 26 (ny) *11 (nt)
= 7436 points

Results: Concentration field with λ = 0.5, N = 500

Case 1: Data-Driven

Case 2: Both data and ADE

Case 3: Both data and ADE + Darcy Equation



Comparison – λ = **0.5**, N = 500

Case 1: Data – driven Only

- Loss from only data

Case 2: Data + ADE

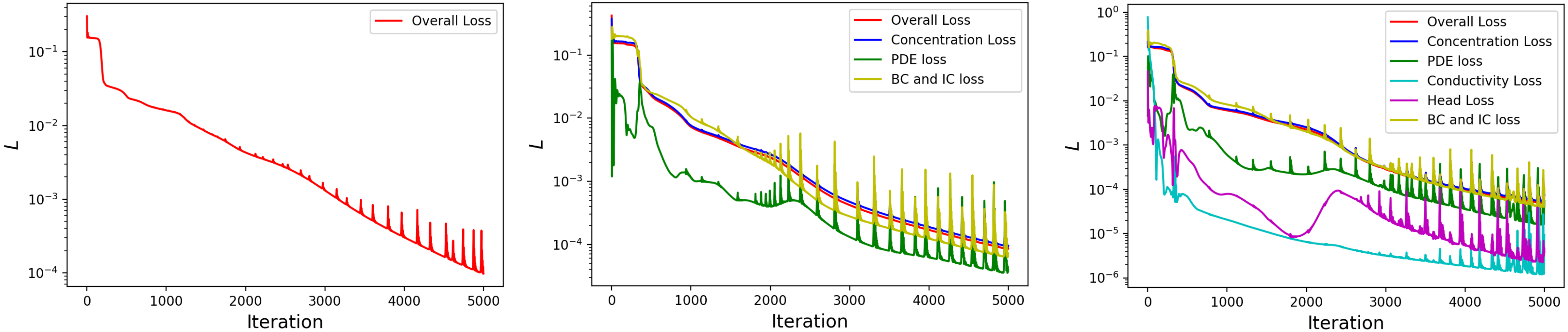
- Loss from data + ADE (& BCs+IC)

Case 3: Data + ADE + Darcy Eqn

- Loss from concentration & head (&K field) data and ADE
- For entire point, Case 3 performed better than other cases

MSE	Case 1	Case 2	Case 3
Collocation points	9.7611e-05	9.4096e-05	7.4566e-05
Entire space & time	2.7133e-03	2.0631e-03	2.2484e-03

Loss plot during training for three cases



Summary

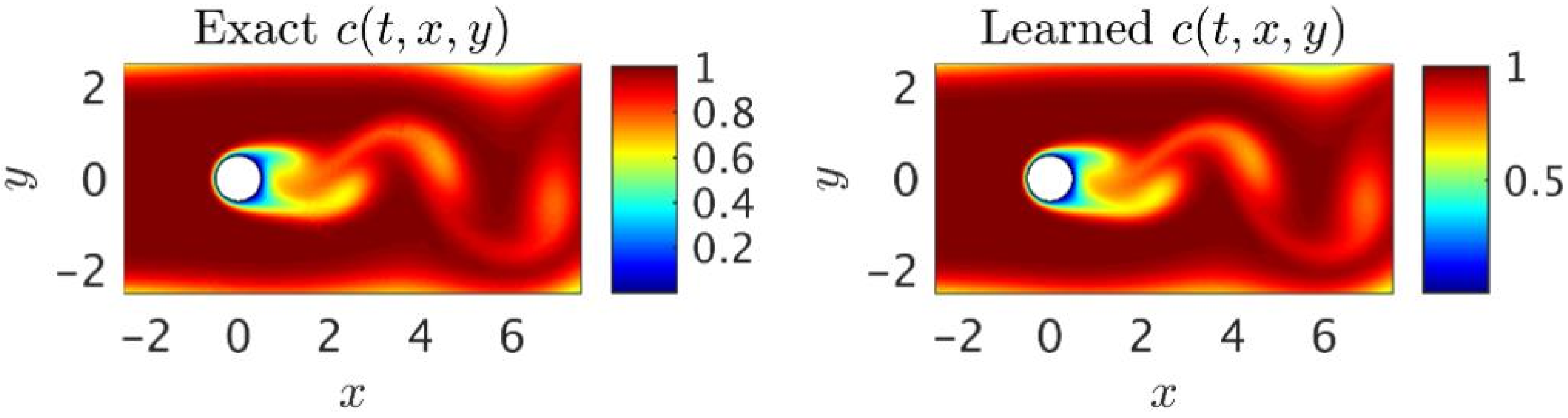
- Incorporation of physical equations and data can enhance ML prediction
- Physics-informed NNs can be formulated both in forward and inverse modeling frameworks
- PINNs can be very powerful with sensitivity analysis since AD can be easily utilized to compute all sensitivity terms automatically
- Current framework is in progress to achieve
    - More general datasets with a range of model parameter spaces (velocity, 2D random field)
    - Uncertainty quantification of advection-dispersion(or diffusion)-reaction systems

Backup

Motivations

- Recent advances in **deep learning neural networks** have allowed us to tackle scientific and engineering problems.
- We are using a form of neural networks known as **Physics-Informed neural networks** (PINN) to solve **partial differential equations** (PDEs) involved in fluid flow and reactive transport.
- The ultimate goal is to solve fluid dynamic problems at a **more efficient rate** than traditional mesh-based methods.

Example of hydrodymaics velocity field in the presence of an obstacle

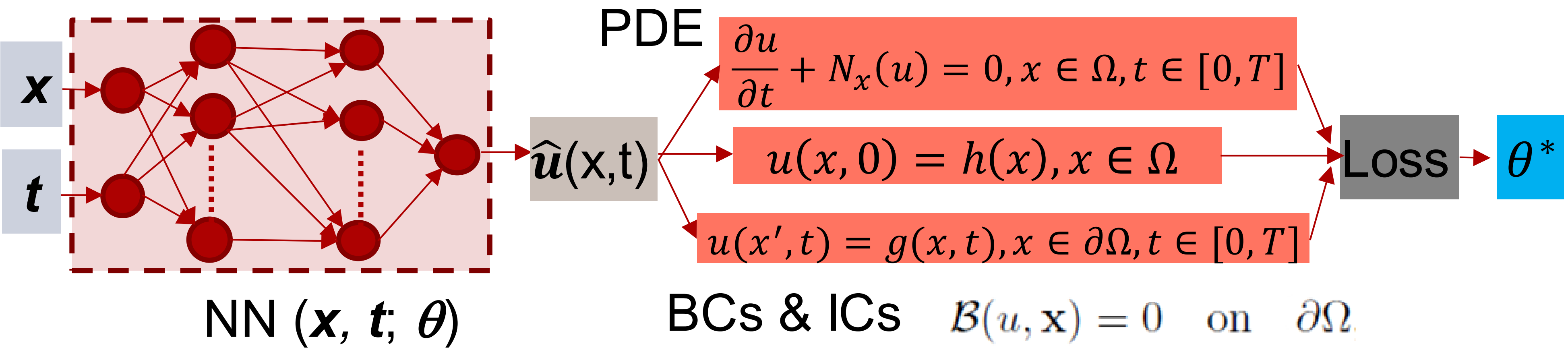


(Maziar Raissi et al, Hidden Fluid Mechanics)

Neural Network Architecture

- A main idea of PINNs is to **incorporate governing equations of physics** in the form of **partial differential equations** (PDEs) **into the loss** via automatic differentiation (AD)

$$f\left(\mathrm{x}; \frac{\partial u}{\partial x_1}, \ldots, \frac{\partial u}{\partial x_d}; \frac{\partial^2 u}{\partial x_1 \partial x_1}, \ldots, \frac{\partial^2 u}{\partial x_1 \partial x_d}; \ldots; \boldsymbol{\lambda}\right) = 0, \quad \mathrm{x} \in \Omega$$



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$$\mathcal{B}(u, \mathrm{x}) = 0 \quad \text{on} \quad \partial\Omega$$

Loss = Sum of Data fit and physics regularization from PDEs, IC&BCs

Differential Equations

- Advection Dispersion Equation (ADE)
  - PDE used to introduce physics into ML

$$R\frac{\partial C}{\partial t} = -u\frac{\partial C}{\partial x} + D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2} + \lambda c$$

IC: C(x,y,t=0) = 0

$$\left.\begin{array}{ll} C\left(\boldsymbol{x}\right) = C_0\left(x_2\right), & x_1 = 0 \\ \partial C\left(\boldsymbol{x}\right)/\partial x_1 = 0, & x_1 = L_1 \\ \partial C\left(\boldsymbol{x}\right)/\partial x_2 = 0, & x_2 = 0 \quad \text{or} \quad x_2 = L_2 \end{array}\right\} \text{Boundary Conditions}$$

Where:

R = retardation factor

C = concentration

u = fluid velocity

D_x, D_y = dispersion coefficient

λ = first order decay constant

* Note that *u* and D can be a full tensor if fully heterogeneous fields are considered.

- Darcy Flow Equation (DE)
  - Calculate velocity using head loss and conductivity

$$\left\{\begin{array}{l} \boldsymbol{v}\left(\boldsymbol{x}\right) = -\frac{K(\boldsymbol{x})}{\phi}\nabla h\left(\boldsymbol{x}\right) \\ \nabla\cdot\boldsymbol{v}(\boldsymbol{x}) = 0, \quad \boldsymbol{x}\in\Omega \\ h\left(\boldsymbol{x}\right) = H_2, \quad x_1 = L_1 \\ -K\left(\boldsymbol{x}\right)\partial h\left(\boldsymbol{x}\right)/\partial x_1 = q, \quad x_1 = 0 \\ -K\left(\boldsymbol{x}\right)\partial h\left(\boldsymbol{x}\right)/\partial x_2 = 0, \quad x_2 = 0 \text{ or } x_2 = L_2 \end{array}\right.$$

Boundary Conditions

Where:

Φ = effective porosity of the medium

h = hydraulic head

K = conductivity

Updated for transient part from He et al (AWR, 2020)

2D Advection-Dispersion Reaction

Single Dataset: 3 Cases

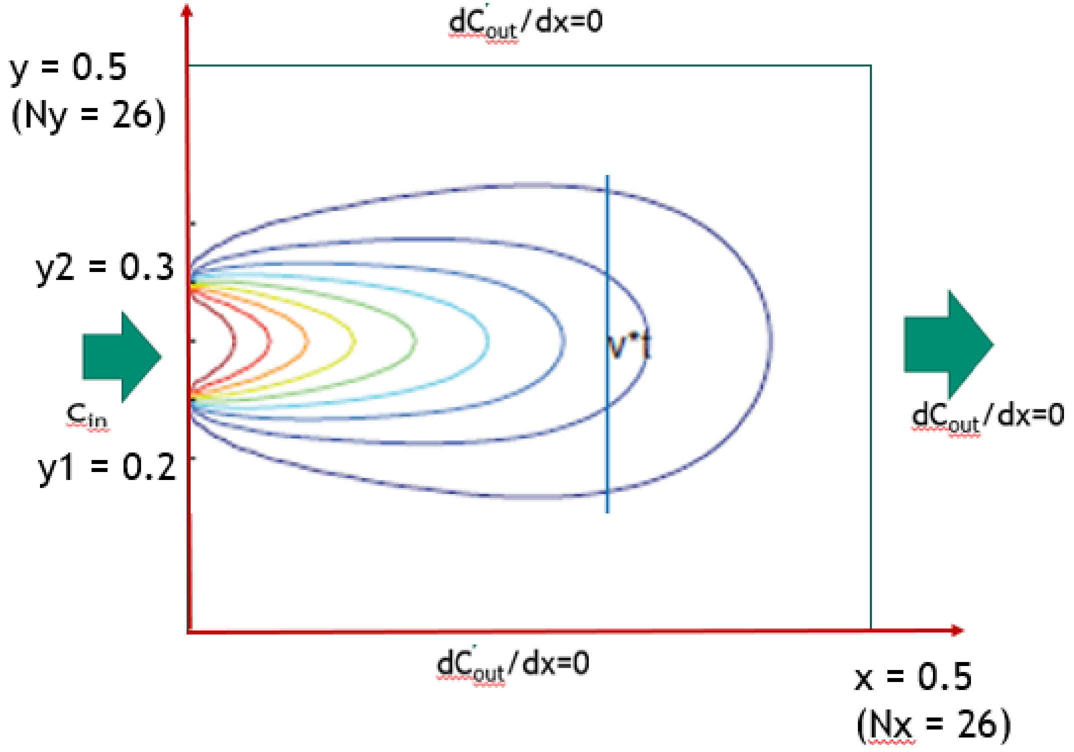
1. Concentration data Only
2. Concentration data + Advection Dispersion PDE
3. Concentration data + head loss and conductivity + ADE + Darcy Eqn (For Darcy eqn, K field can be estimated inversely)

Analytical Solution:

$$c(x, y, t) = \frac{C_0}{4}\left\{\exp\left[\frac{(v-u')x'}{2D_x}\right] erfc\left(\frac{x'-u't}{2\sqrt{D_x t}}\right) + \exp\left[\frac{(v+u')x'}{2D_x}\right] erfc\left(\frac{x'+u't}{2\sqrt{D_x t}}\right)\right\} \times \left[erfc\frac{y-y_2}{2\sqrt{D_y \tau_m}} - erfc\frac{y-y_1}{2\sqrt{D_y \tau_m}}\right]$$

$$u' = \sqrt{v^2 + 4\lambda D_x},\ \tau_m = x/v, \quad y_1 \le y \le y_2$$

Example of concentration field (red-high, blue – low from analytical solution)



- Boundary Conditions for Darcy Eqn:
  - Dirichlet BC at inlet/outlet:
    $q(x=0,y,t) = u_{in}$
    $H(x=1,y,t) = H_{out}$

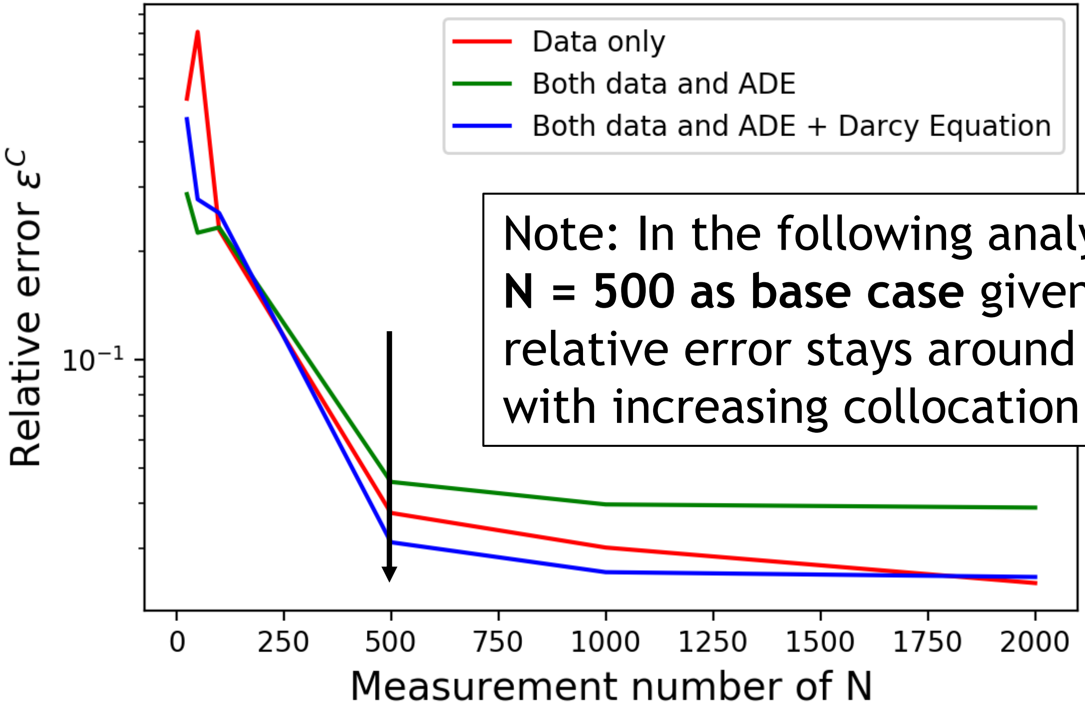
- Initial Condition:
  - $C(x,y,t=0) = 0$

Key Model Parameters

- 10,000 Epochs
- 4 hidden layers with 40 nodes each
- The number of collocation points: 0.34%, 0.68%, 1.3%, 6.7%, 13.4%, 26.9%
- Loss: Mean-Squared Error (MSE)
- As we increase collocation points (*N*), relative error of ML decreases

$$N = N_c = N_K = N_h = N_{fc} = N_f$$

Relative error of three different cases as a function of collocation points



Note: In the following analysis, we use **N = 500 as base case** given that the relative error stays around the same with increasing collocation points

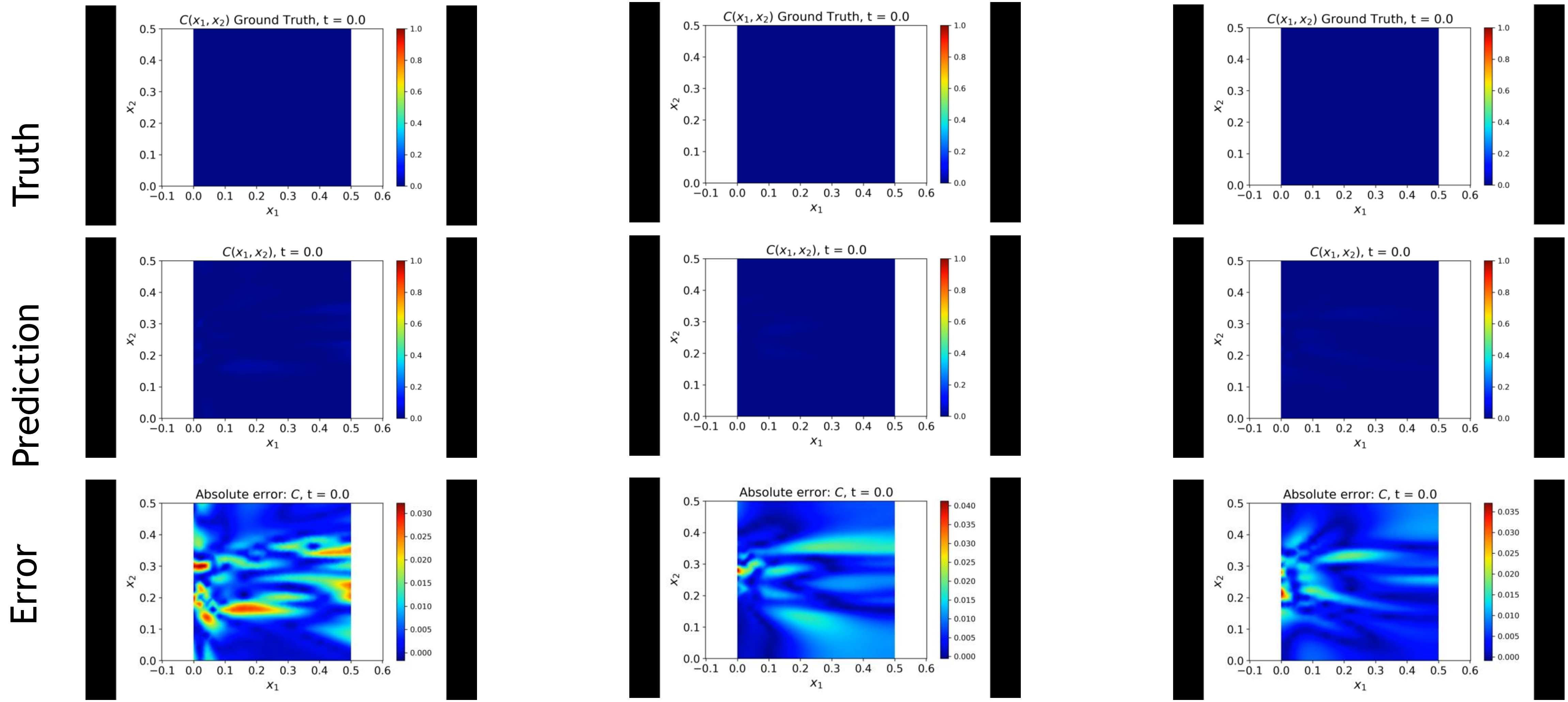
A total number of points:
26 (nx) * 26 (ny) *11 (nt)
= 7436 points

Results: Concentration field with λ = 0, N = 500

Case 1: Data-Driven

Case 2: Both data and ADE

Case 3: Both data and ADE + Darcy Equation



Results: Concentration field with λ = 0.1, N = 500

Case 1: Data-Driven

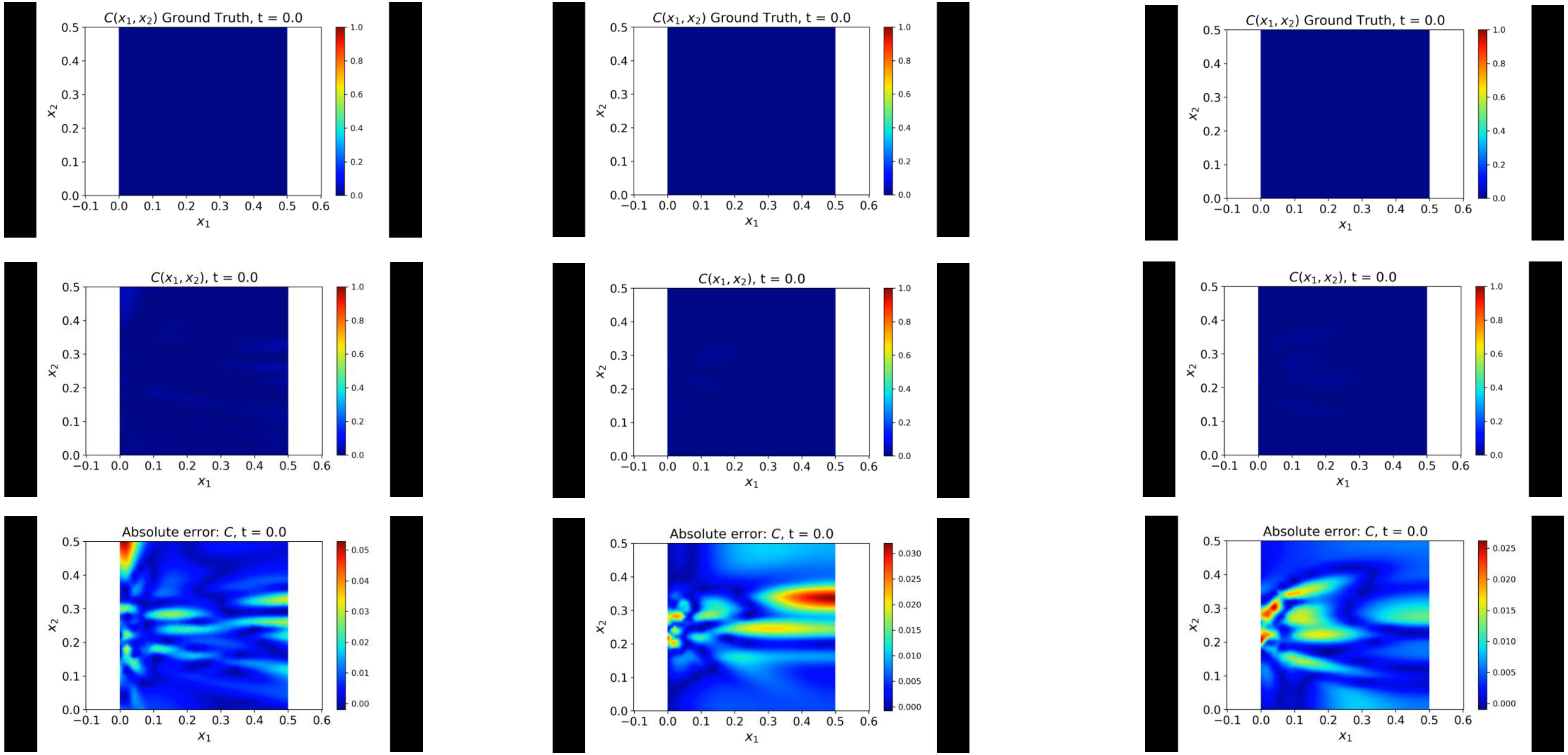
Case 2: Both data and ADE

Case 3: Both data and ADE + Darcy Equation

Truth

Prediction

Error



Results: Concentration field with $\lambda = 0.5$, $N = 500$

Case 1: Data-Driven

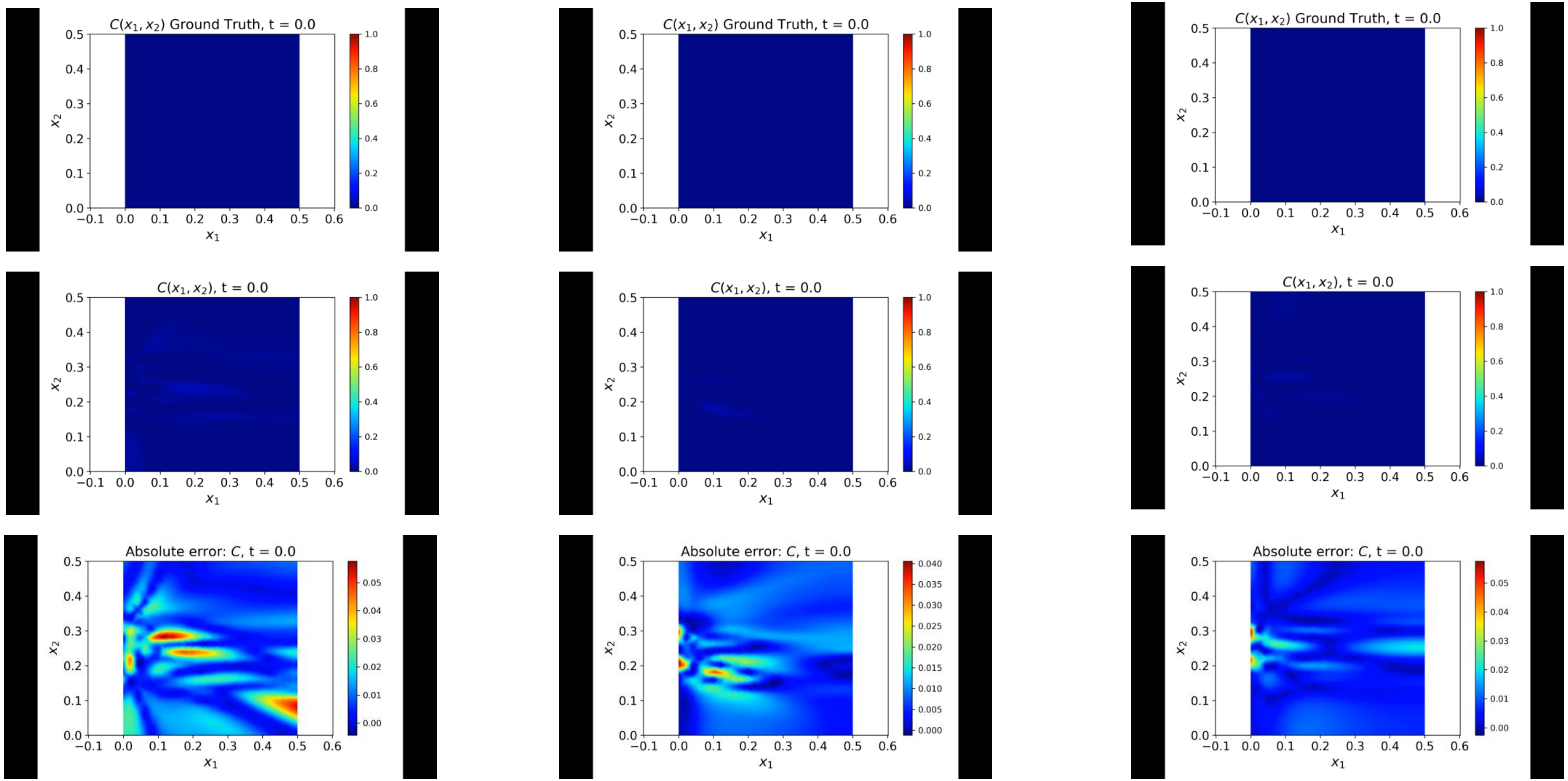
Case 2: Both data and ADE

Case 3: Both data and ADE + Darcy Equation

Truth

Prediction

Error



Comparison – λ = 0, N = 500

Case 1: Data – driven Only

- Loss from only data

Case 2: Data + ADE

- Loss from data + ADE (& BCs+IC)

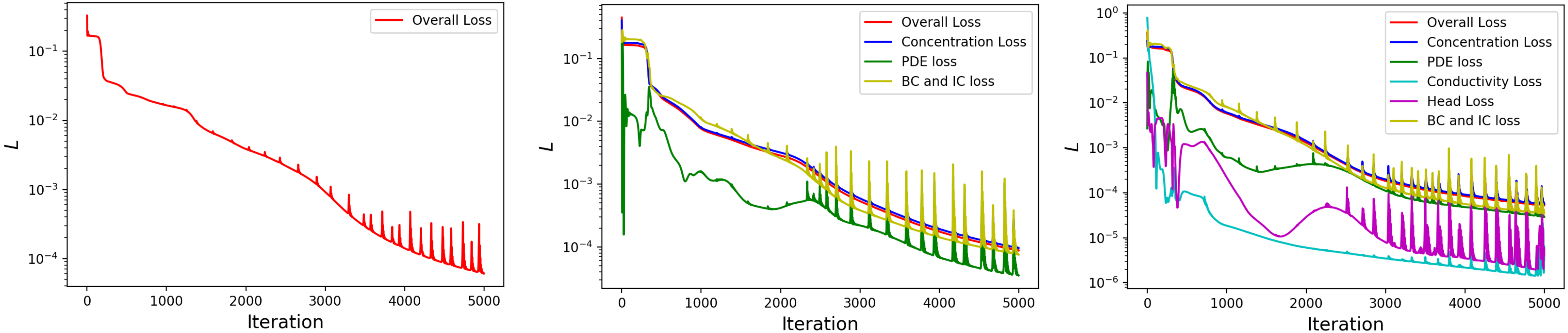
Case 3: Data + ADE + Darcy Eqn

- Loss from concentration & head (&K field) data and ADE

MSE	Case 1	Case 2	Case 3
Collocation points	6.0945e-05	9.5795e-05	5.6173e-05
Entire space & time	3.5409e-03	2.6118e-03	2.2517e-03

- For entire point, Case 3 performed better than other cases

Loss plot during training for three cases



Comparison – λ = 0.1, N = 500

Case 1: Data – driven Only

- Loss from only data

Case 2: Data + ADE

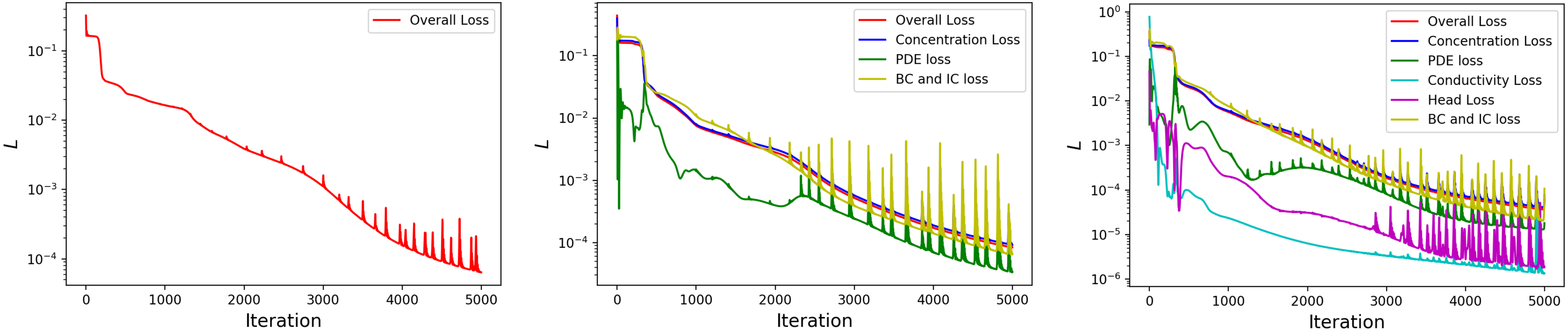
- Loss from data + ADE (& BCs+IC)

Case 3: Data + ADE + Darcy Eqn

- Loss from concentration & head (&K field) data and ADE
- For entire point, Case 3 performed better than other cases

MSE	Case 1	Case 2	Case 3
Collocation points	6.3934e-05	9.1593e-05	7.8149e-05
Entire space & time	3.4033e-03	2.9904e-03	1.6247e-03

Loss plot during training for three cases



Comparison – λ = 0.5, N = 500

Case 1: Data – driven Only

- Loss from only data

Case 2: Data + ADE

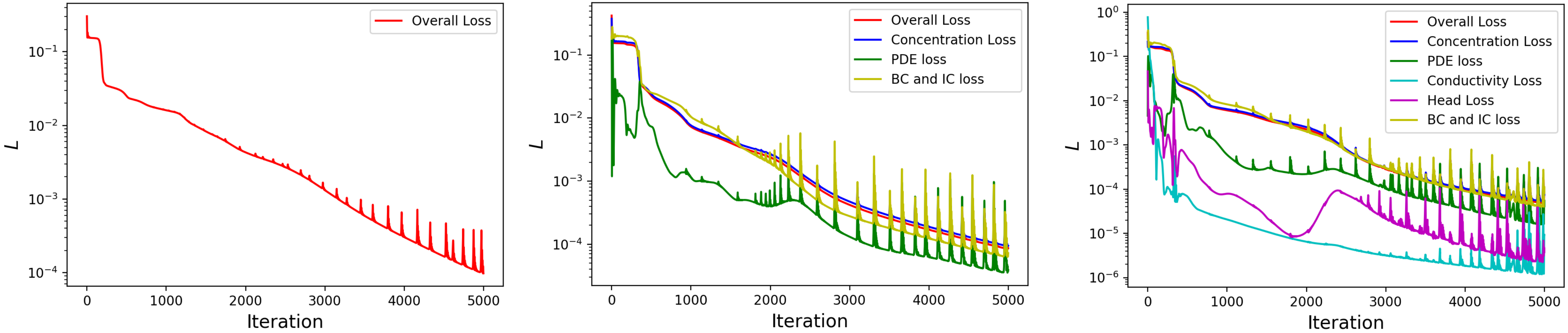
- Loss from data + ADE (& BCs+IC)

Case 3: Data + ADE + Darcy Eqn

- Loss from concentration & head (&K field) data and ADE
- For entire point, Case 3 performed better than other cases

MSE	Case 1	Case 2	Case 3
Collocation points	9.7611e-05	9.4096e-05	7.4566e-05
Entire space & time	2.7133e-03	2.0631e-03	2.2484e-03

Loss plot during training for three cases



Comparison – λ = 0.5, N = 1000

Case 1: Data – driven Only

- Loss from only data

Case 2: Data + ADE

- Loss from data + ADE (& BCs+IC)

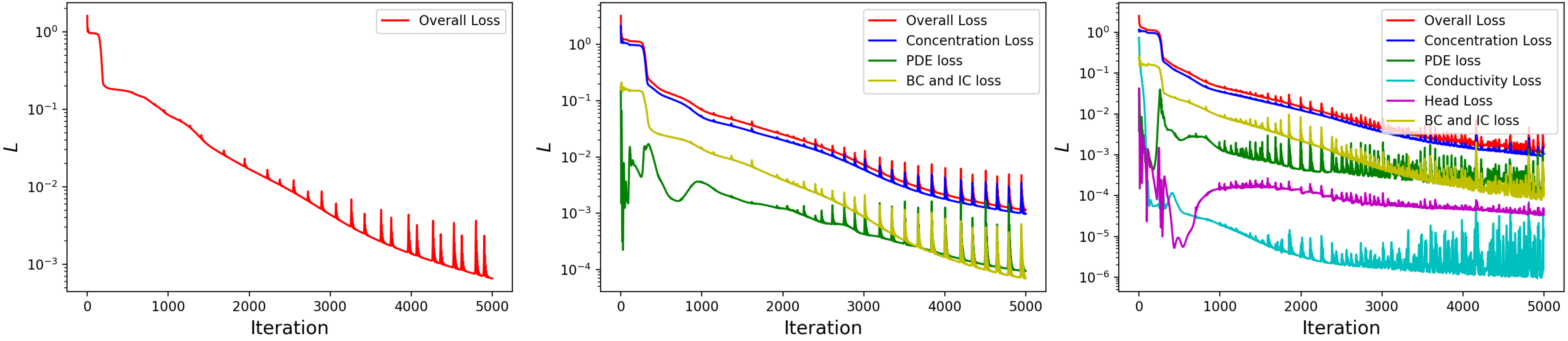
Case 3: Data + ADE + Darcy Eqn

- Loss from concentration & head (&K field) data and ADE

MSE	Case 1	Case 2	Case 3
Collocation points	6.5471e-4	9.7633e-4	1.0500e-3
Entire space & time	4.8075e-05	1.0856e-4	1.0787e-4

- For entire point, Case 1 performed better than other cases

Loss plot during training for three cases



Results: Case 3: Data (concentration, head) + ADE + Darcy Equation

- Input: Data (head, conductivity)
- Output: Velocity Fields generated using Darcy Equation
- Ground truth: velocity u_x = 0.5 and u_y =0