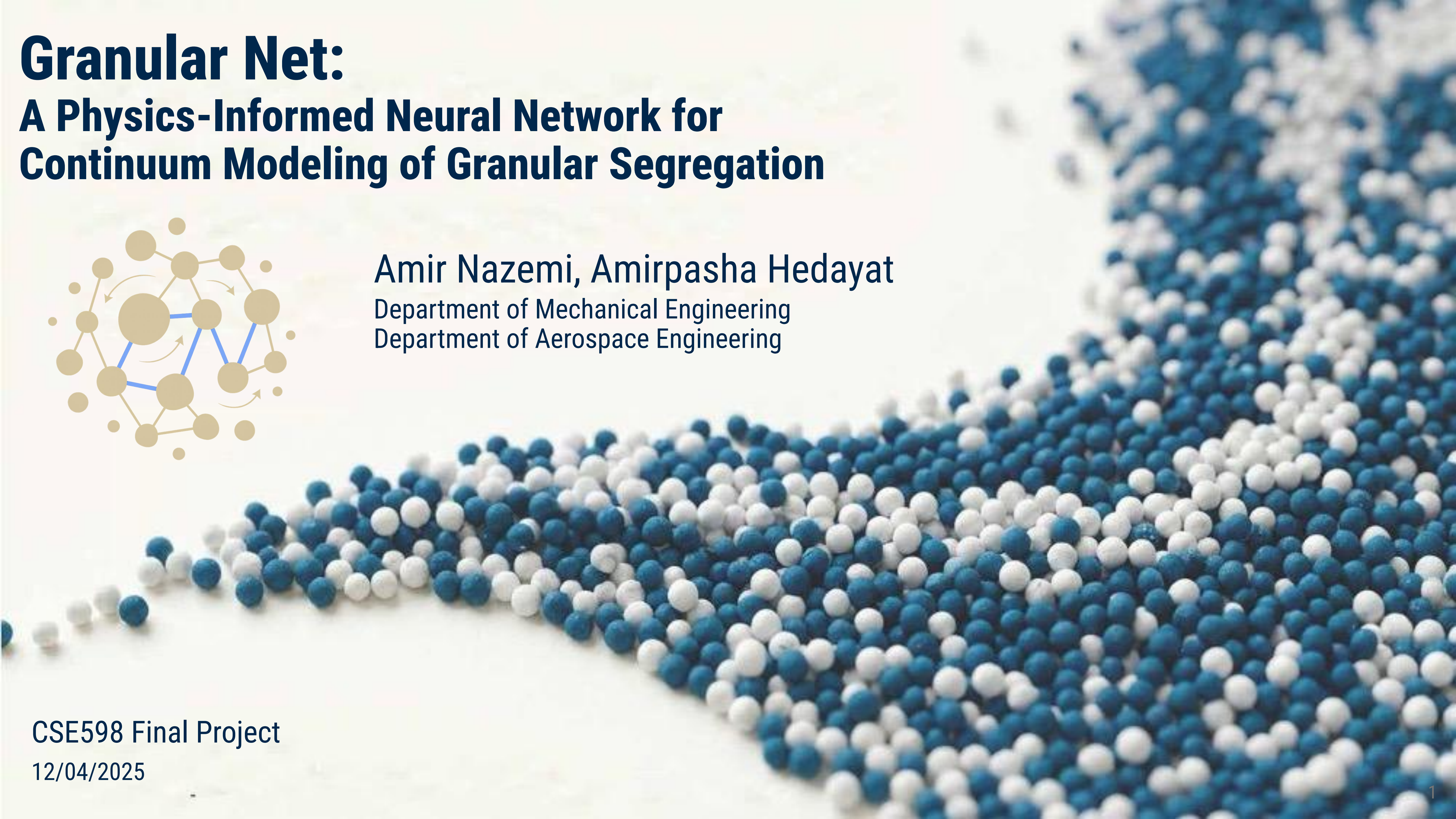

Granular Net:
A Physics-Informed Neural Network for Continuum Modeling of Granular Segregation

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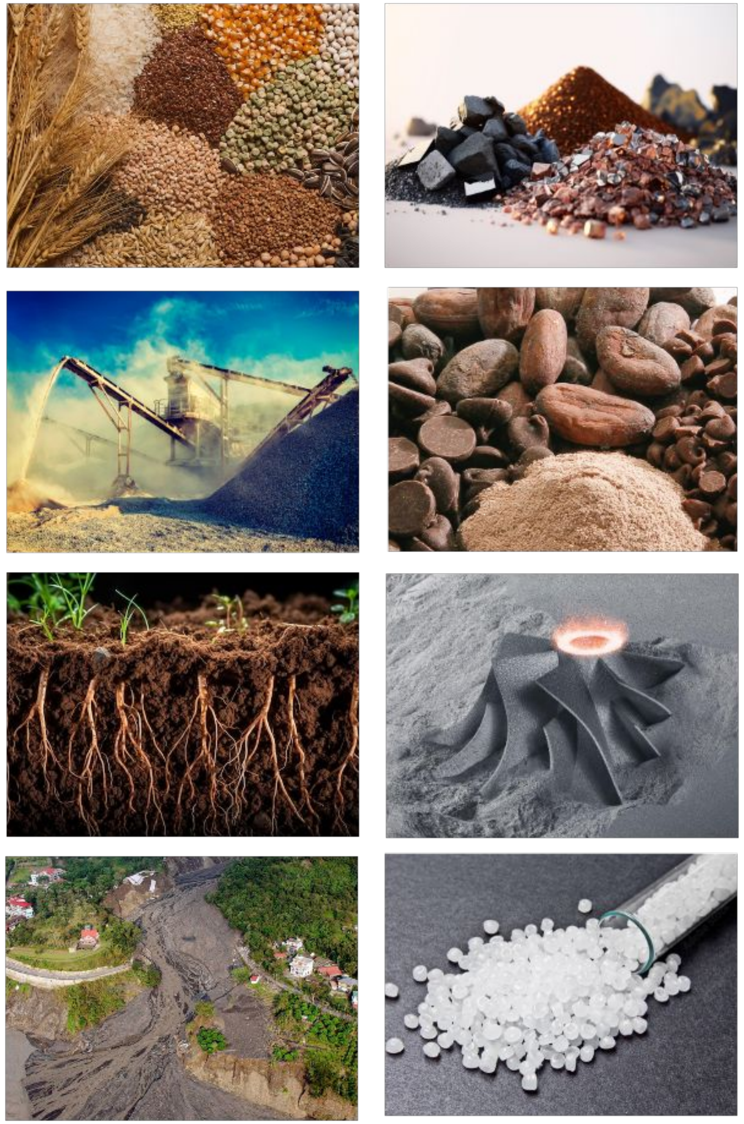
CSE598 Final Project
12/04/2025

Motivation

- Granular materials are complex and ubiquitous in different applications
  - food and agriculture
  - mining
  - pharmaceutical
  - polymer processing
  - manufacturing

- Defects in bulk materials handling and flow can result in catastrophic events, such as collapse of silos.
  - One of these defects is segregation in granular flows.



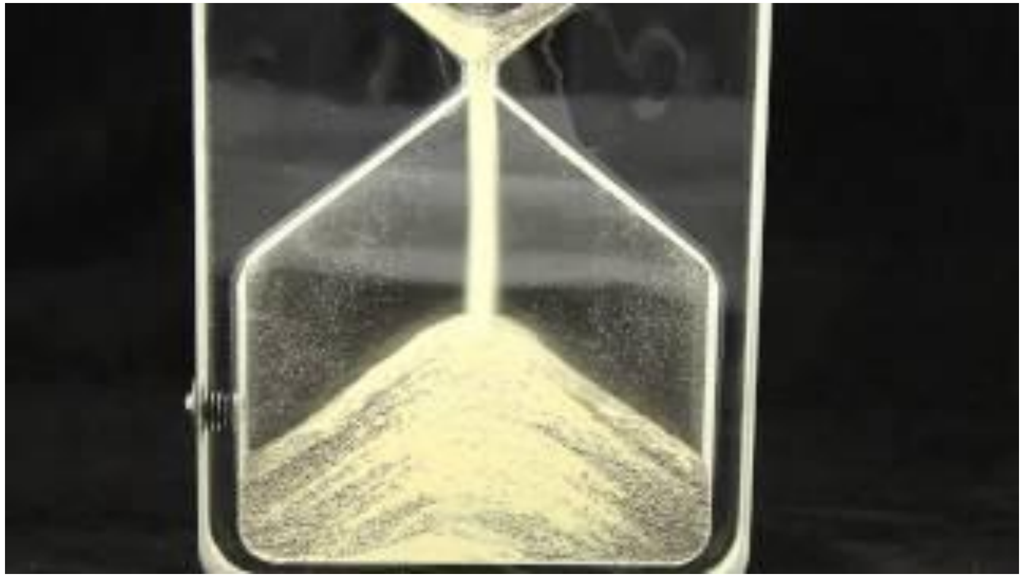
Background

Segregation

- The spontaneous demixing of species that differ in size, density, or shape during a flow.

Why we care about granular segregation?

- 2nd most manipulated industrial behind water.
- Over the 50% of the world's economy relies on granular materials.
- Leads to inconsistent product composition.



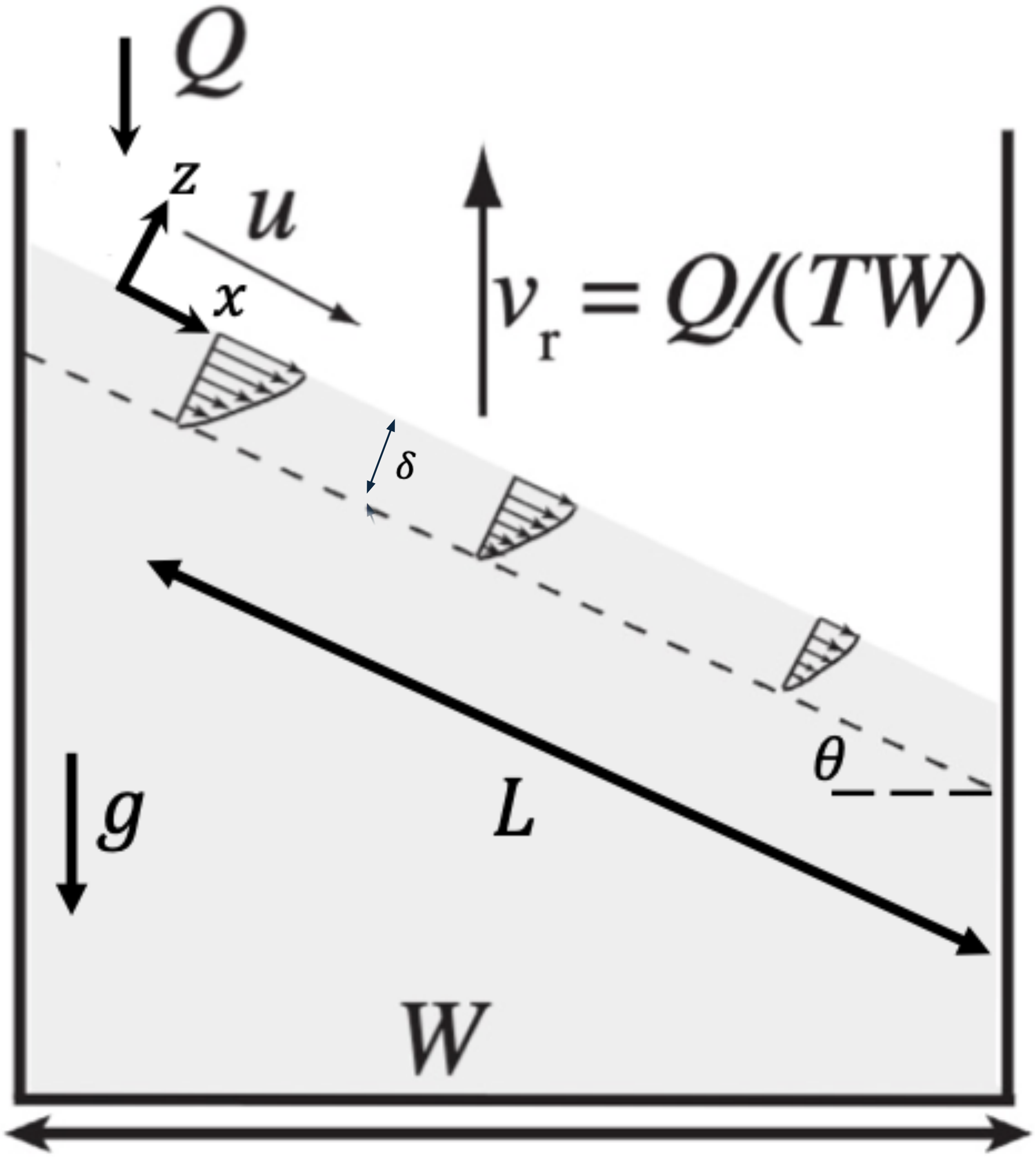
Problem Definition

Segregation can be described using an advection-segregation-diffusion transport equation.

$$\frac{\partial c_i}{\partial t} + \underbrace{\nabla \cdot (\mathbf{u}\, c_i)}_{\text{advection}} + \underbrace{\frac{\partial}{\partial z}(w_{s,i}\, c_i)}_{\text{segregation}} = \underbrace{\nabla \cdot (D\, \nabla c_i)}_{\text{diffusion}}$$

Assumptions:

- Diffusion in x-direction is neglected and its coefficient is approximated as a constant value.
- Segregation in x-direction is neglected.
- We mainly focus on the **steady filling** stage, which occurs when the heap extends to the downstream endwall and rises at a uniform velocity.



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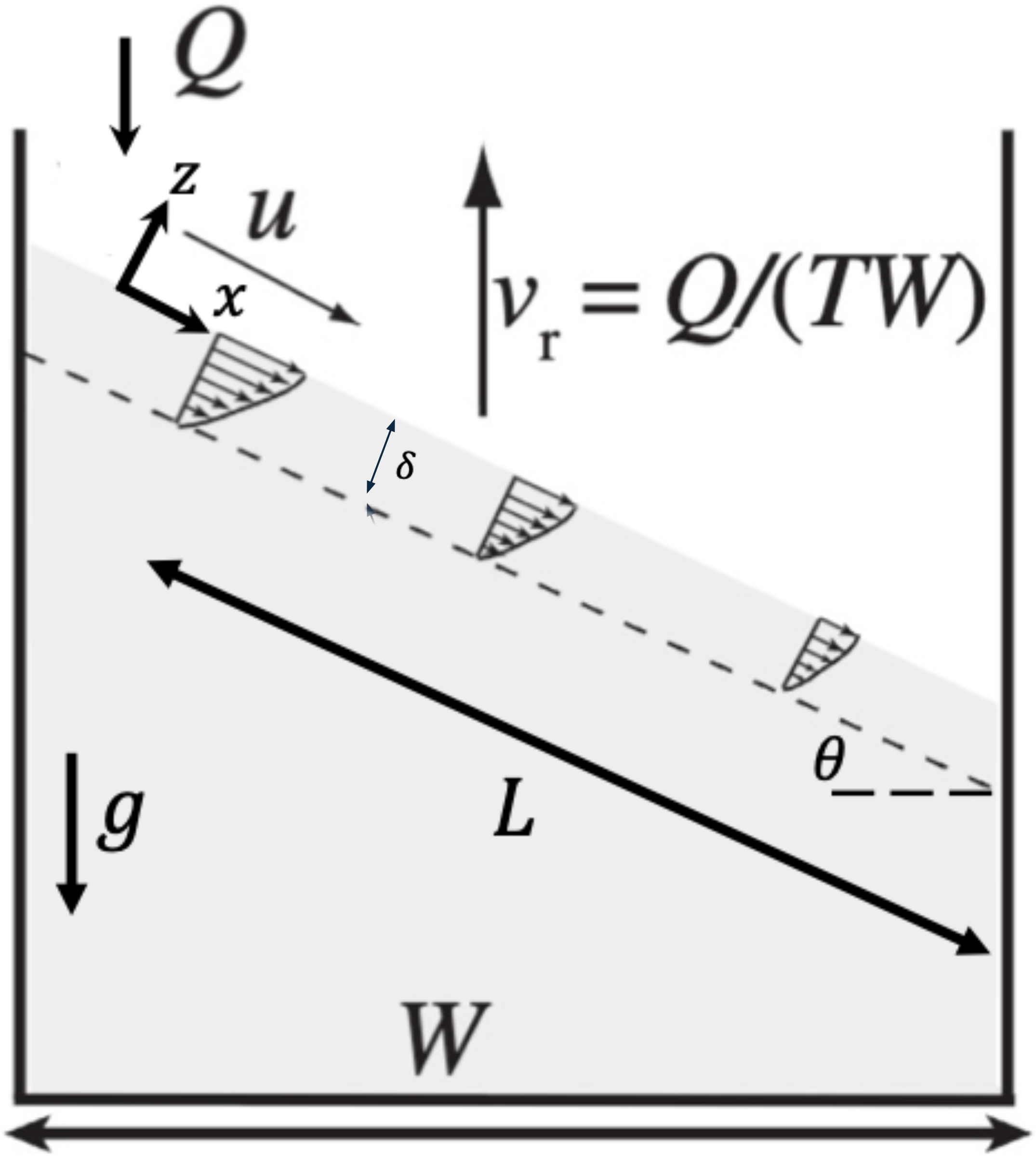
Boundary conditions:

- At the inlet boundary(x = 0), the particles are initially well mixed, so

$$c_s(0,z) = c_l(0,z) = 0.5$$

- At the top and bottom boundaries of the flowing layer (z = 0 and z =− δ), the segregation flux balances the diffusive flux.

$$\left(D\nabla c_i + w_{s,i}c_i\hat{\boldsymbol{z}}\right).\hat{\boldsymbol{n}} = 0$$



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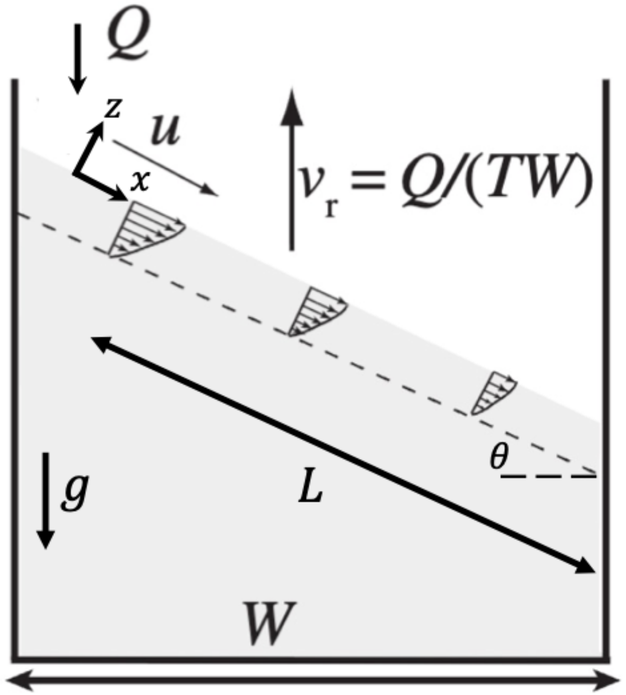
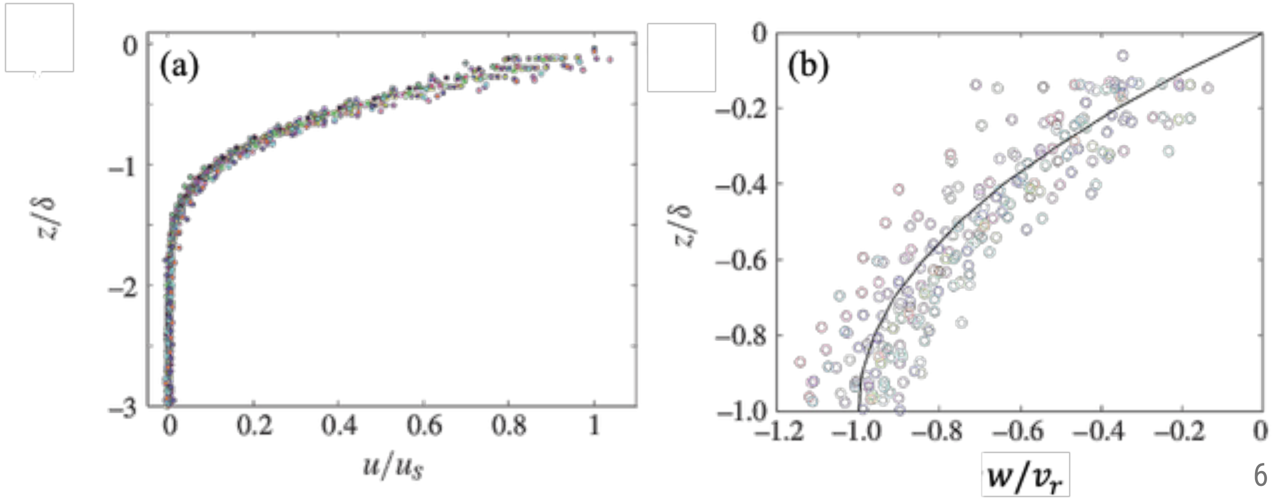


The normalized streamwise velocity profile and its normal component at different stream-wise locations collapses onto a single curve.

$$u = \frac{kq}{\delta(1-e^{-k})}\left(1-\frac{x}{L}\right)e^{kz/\delta},$$

$$w = \frac{q}{L(1-e^{-k})}\left(e^{kz/\delta}-1\right),$$



Problem Definition

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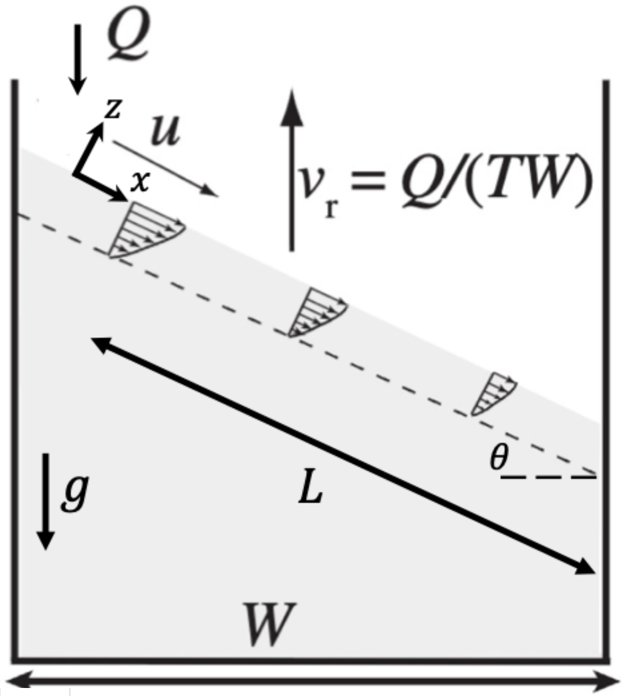
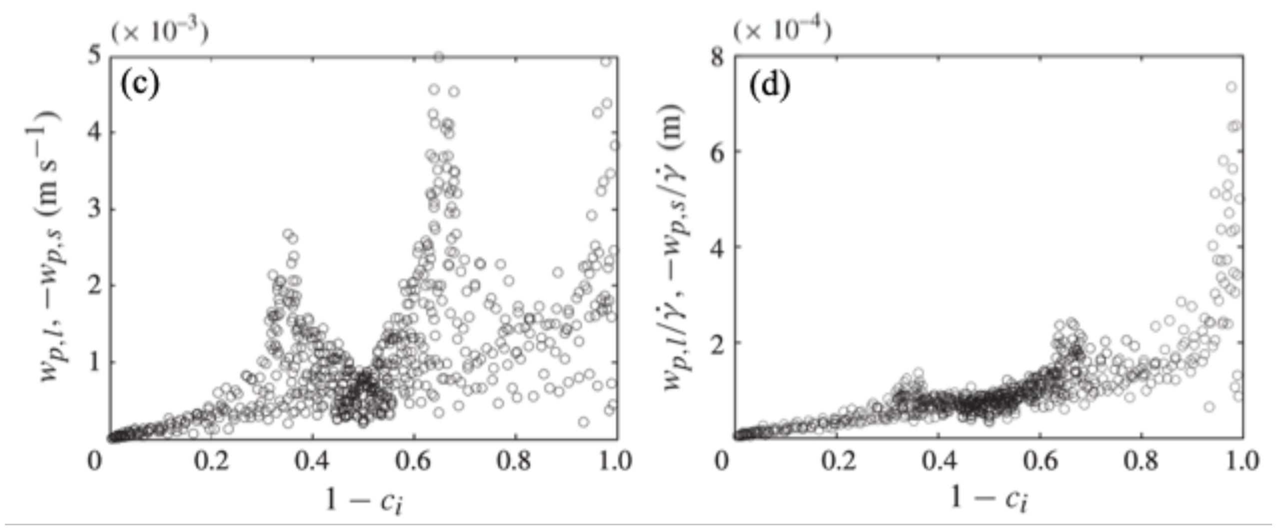


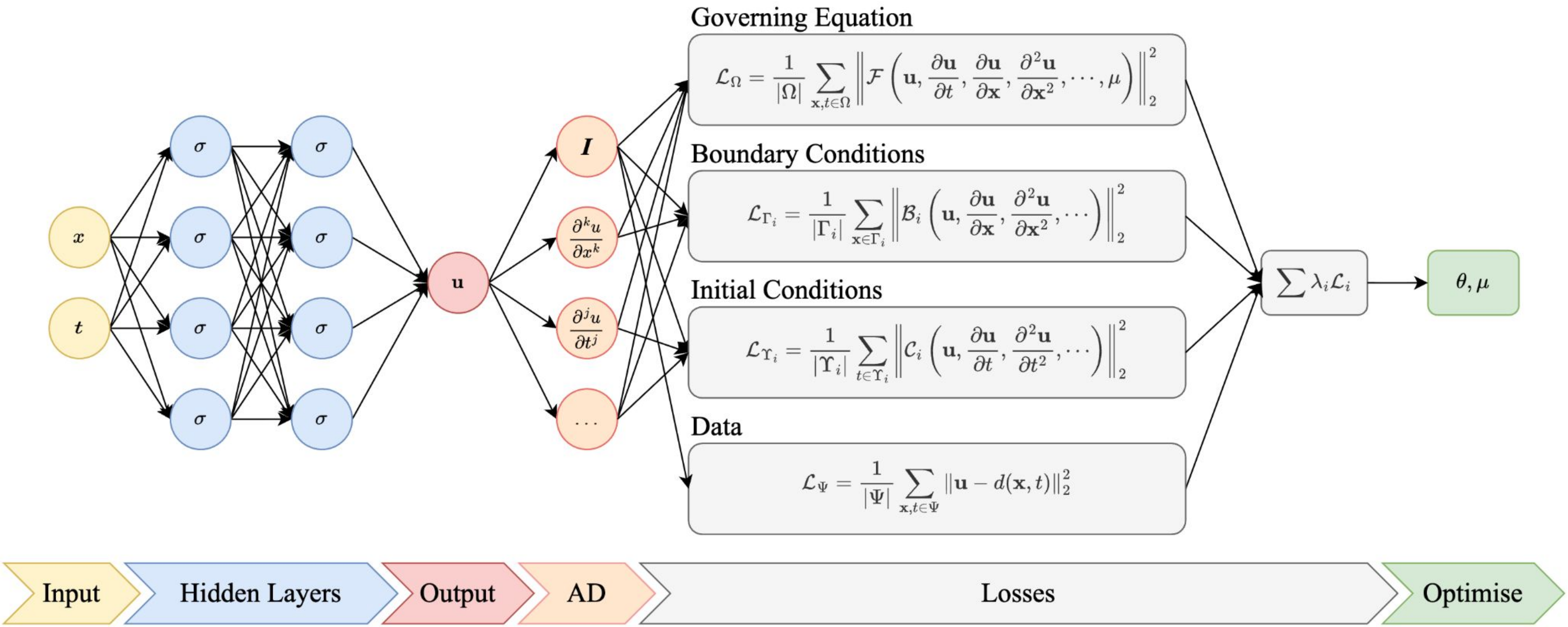
The segregation velocity depends on the particle size ratio, strain rate, and normal stress (neglected due to thin flowing layer).

$$w_{s,l} = S\dot{\gamma}(1 - c_l),$$

$$w_{s,s} = -S\dot{\gamma}(1 - c_s),$$



Proposed Methods: physics-informed neural network (recap)

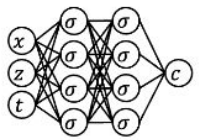


Credit: Bischof and Kraus (2025)

Proposed Method

Inputs (x, z, t) →

MLP



$f_\theta : (x, z, t) \rightarrow c_\theta$

→ Autodiff: $\partial_t c_\theta$, ∇c_θ , $\nabla^2 c_\theta$ →

PDE residual:

$$\frac{1}{|P|}\sum_{p\in P}|\partial_t c_\theta + u\partial_x c_\theta + w\partial_z c_\theta + \partial_z(\boldsymbol{w_s} c_\theta) - \nabla.(D\nabla c_\theta)|^2$$

Top and bottom B.C. residual:

$$\frac{1}{|B|}\sum_{b\in B}|(\boldsymbol{w_s} c_\theta)\hat{z} - D\nabla c_\theta|^2$$

Inlet B.C. residual:

$$\frac{1}{|B_{in}|}\sum_{b_{in}\in B_{in}}|c_\theta - 0.5|^2$$

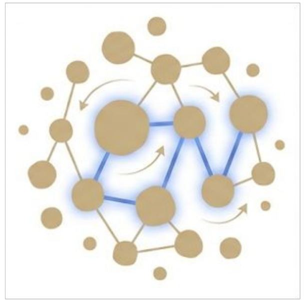
I.C. residual:

$$\frac{1}{|I|}\sum_{i\in I}|c_\theta - 0.5|^2$$

(if available) Data residual:

$$\frac{1}{|D|}\sum_{d\in D}|c_\theta - c_{\exp}|^2$$

→ Loss = $\sum \lambda_i\,.\,(\text{residual})_i$ → Optimizer: update $\theta, (\boldsymbol{\alpha}, \boldsymbol{\phi})$



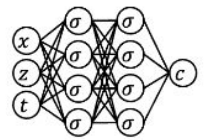
Granular Net

A PINN architecture capable of both "**forward**" and "**inverse**" modeling of the segregation mechanism in granular material.

Proposed Method

Inputs
(x, z, t) →

MLP



$f_\theta : (x, z, t) \rightarrow c_\theta$

→ Autodiff:
$\partial_t c_\theta \,, \nabla c_\theta \,, \nabla^2 c_\theta$ →

PDE residual:

$$\frac{1}{|P|}\sum_{p\in P}\left|\partial_t c_\theta + u\partial_x c_\theta + w\partial_z c_\theta + \partial_z(\boldsymbol{w_s} c_\theta) - \nabla.(D\nabla c_\theta)\right|^2$$

Top and bottom B.C. residual:

$$\frac{1}{|B|}\sum_{b\in B}\left|(\boldsymbol{w_s} c_\theta)\hat{z} - D\nabla c_\theta\right|^2$$

Inlet B.C. residual:

$$\frac{1}{|B_{in}|}\sum_{b_{in}\in B_{in}}\left|c_\theta - 0.5\right|^2$$

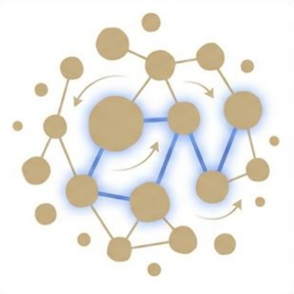
I.C. residual:

$$\frac{1}{|I|}\sum_{i\in I}\left|c_\theta - 0.5\right|^2$$

(if available) Data residual:

$$\frac{1}{|D|}\sum_{d\in D}\left|c_\theta - c_{\exp}\right|^2$$

→ Loss $= \sum \lambda_i \,.\, (\text{residual})_i$ → Optimizer: update $\theta, (\boldsymbol{\alpha}, \boldsymbol{\phi})$



Granular Net

Phase 1: **Forward PINN**

Assuming a known segregation velocity function:

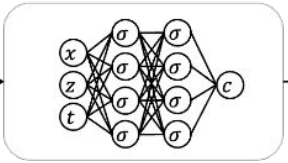
$w_s = \Lambda(1-\tilde{x})g(\tilde{z})(1-c)$

with $\Lambda = 0.39$.

Proposed Method

Inputs (x, z, t) →

MLP



$f_\theta : (x, z, t) \to c_\theta$

→ Autodiff: $\partial_t c_\theta \, , \nabla c_\theta \, , \nabla^2 c_\theta$ →

PDE residual:

$$\frac{1}{|P|}\sum_{p\in P}\left|\partial_t c_\theta + u\partial_x c_\theta + w\partial_z c_\theta + \partial_z(\boldsymbol{w_s} c_\theta) - \nabla.(D\nabla c_\theta)\right|^2$$

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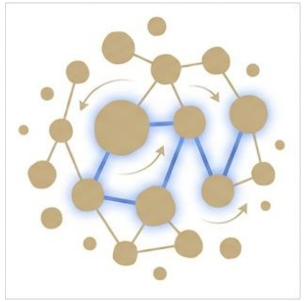
(if available) Data residual:

$$\frac{1}{|D|}\sum_{d\in D}\left|c_\theta - c_{\text{exp}}\right|^2$$

→ Loss $= \sum \lambda_i \, . \, (\text{residual})_i$ → Optimizer: update $\theta, (\boldsymbol{\alpha}, \boldsymbol{\phi})$



Granular Net

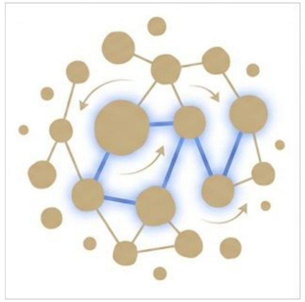
Phase 2.1: **Inverse PINN**

We take two different formulations:

$$\begin{cases} w_s = \Lambda(1-\tilde{x})g(\tilde{z})(1-c) \\ w_s = \Gamma(1-\tilde{x})g(\tilde{z})(1-c)\,[A + B(1-c)] \end{cases}$$

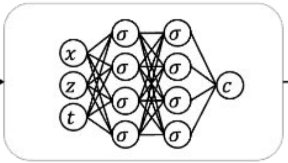
with unknown parameters stored in $\boldsymbol{\alpha}$.

Proposed Method



Granular Net

Inputs (x, z, t) → MLP



$f_\theta : (x, z, t) \to c_\theta$

→ Autodiff: $\partial_t c_\theta$, ∇c_θ , $\nabla^2 c_\theta$ →

PDE residual:

$$\frac{1}{|P|}\sum_{p\in P}\left|\partial_t c_\theta + u\partial_x c_\theta + w\partial_z c_\theta + \partial_z(\boldsymbol{w_s} c_\theta) - \nabla.(D\nabla c_\theta)\right|^2$$

Top and bottom B.C. residual:

$$\frac{1}{|B|}\sum_{b\in B}\left|(\boldsymbol{w_s} c_\theta)\hat{z} - D\nabla c_\theta\right|^2$$

Inlet B.C. residual:

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(if available) Data residual:

$$\frac{1}{|D|}\sum_{d\in D}\left|c_\theta - c_{\exp}\right|^2$$

→ Loss $= \sum \lambda_i \,.\, (\text{residual})_i$ → Optimizer: update $\theta, (\boldsymbol{\alpha}, \boldsymbol{\phi})$

Phase 2.2: **Inverse PINN**

We take a neural representation of the segregation velocity:

$$w_s = v_{\text{seg},\phi}(\tilde{x}, \tilde{z}, \tilde{t}, \dot{\gamma}, c)$$

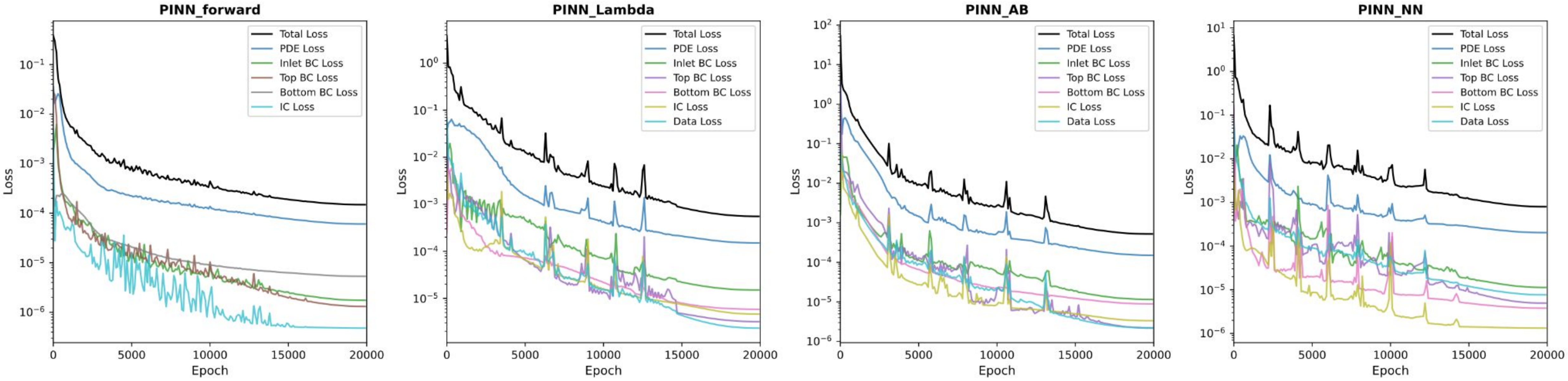
with learnable network weights $\boldsymbol{\phi}$.

Results: training convergence

Phase 1: **Forward PINN**

Phase 2.1: **Inverse PINN**

Phase 2.2: **Inverse PINN**

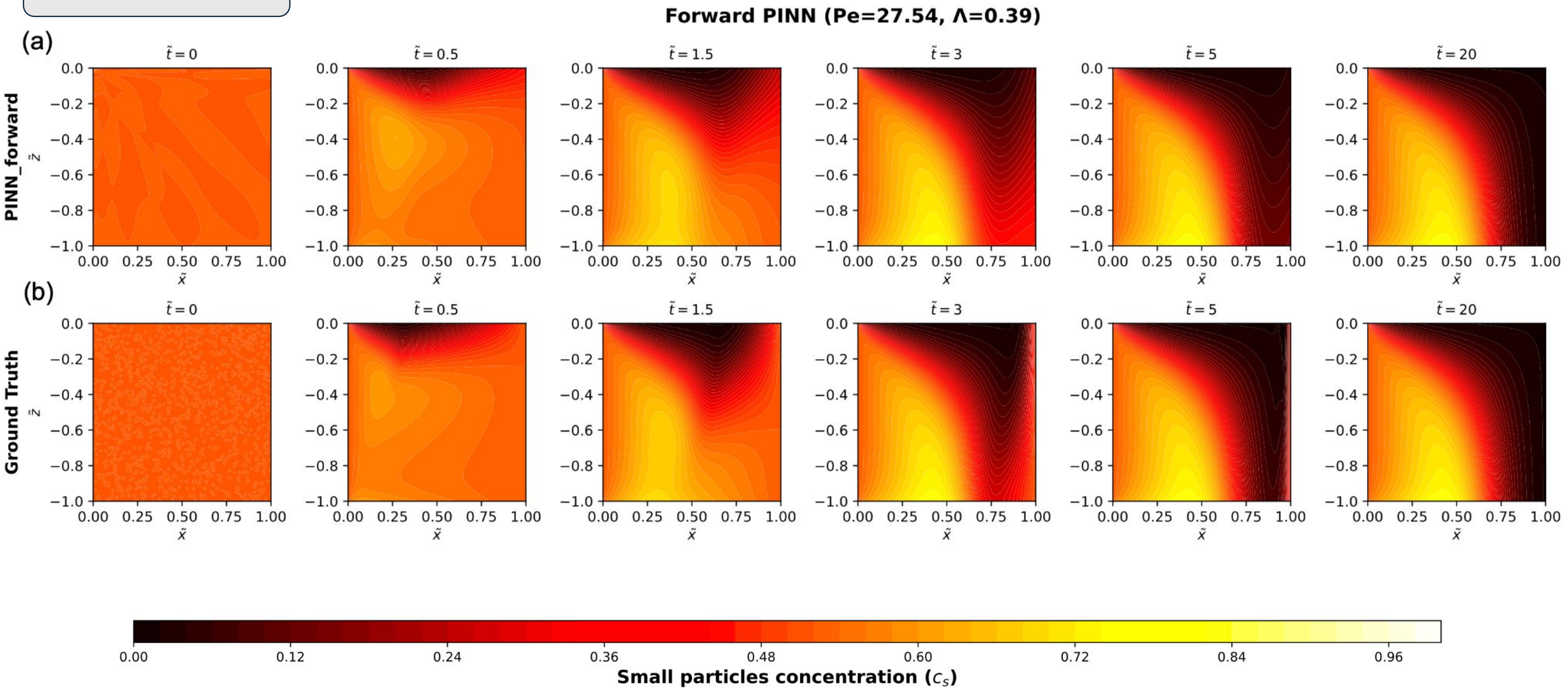


Model	**Final Loss**
Forward PINN	1.49×10^{-4}
PINN_Lambda	5.54×10^{-4}
PINN_AB	5.22×10^{-4}
PINN_NN	8.01×10^{-4}

Results: concentration fields

Phase 1: **Forward PINN**

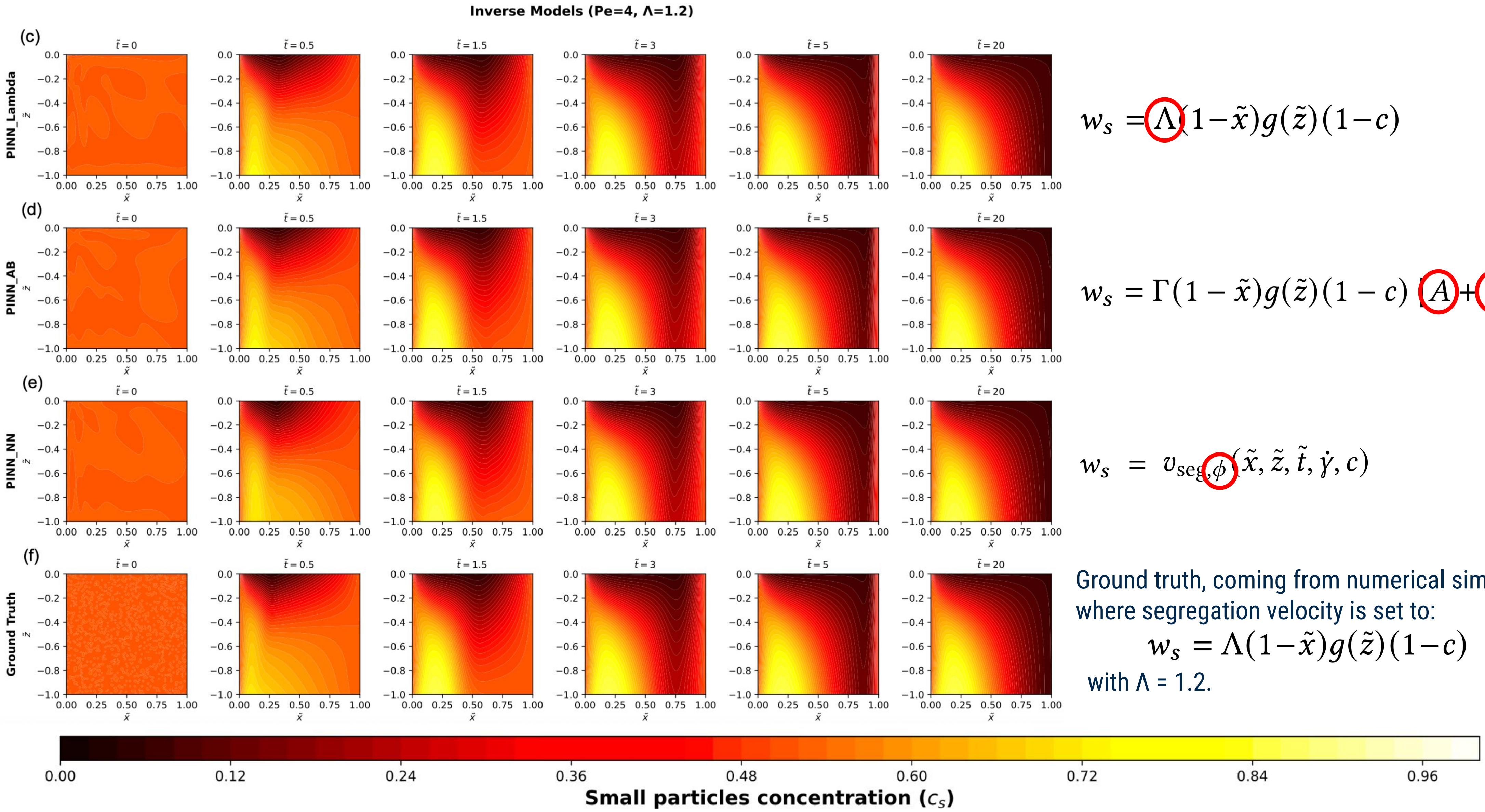
$$w_s = \Lambda(1-\tilde{x})g(\tilde{z})(1-c)$$



Results: concentration fields

Phase 2.1: Inverse PINN

Phase 2.2: Inverse PINN



$$w_s = \Lambda(1-\tilde{x})g(\tilde{z})(1-c)$$

$$w_s = \Gamma(1-\tilde{x})g(\tilde{z})(1-c)\,[A + B(1-c)]$$

$$w_s = v_{\mathrm{seg},\phi}(\tilde{x}, \tilde{z}, \tilde{t}, \dot{\gamma}, c)$$

Ground truth, coming from numerical simulation, where segregation velocity is set to:

$$w_s = \Lambda(1-\tilde{x})g(\tilde{z})(1-c)$$

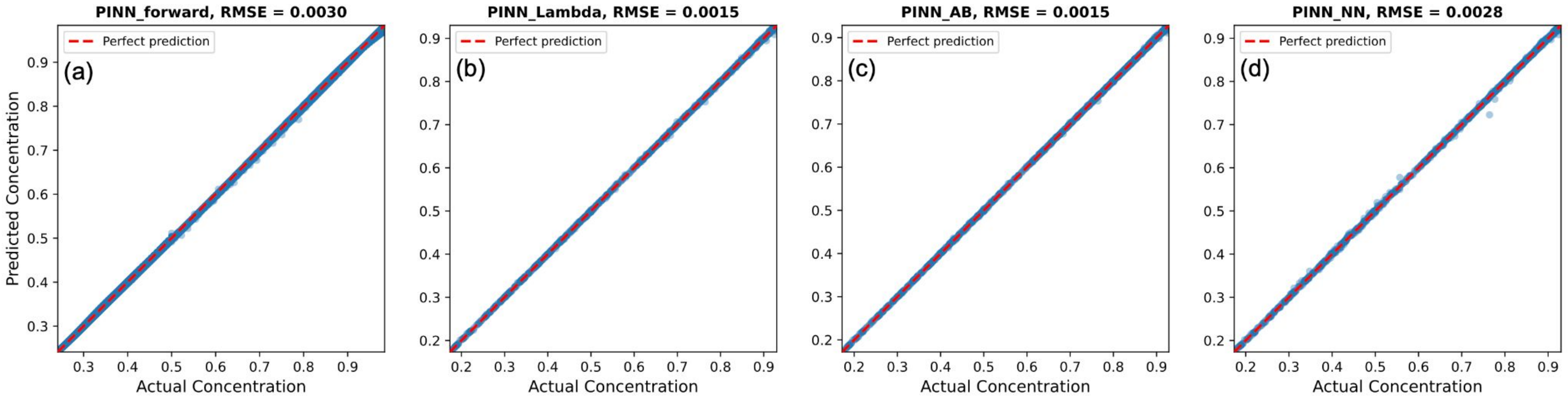
with Λ = 1.2.

Results: prediction accuracy

Phase 1: **Forward PINN**

Phase 2.1: **Inverse PINN**

Phase 2.2: **Inverse PINN**

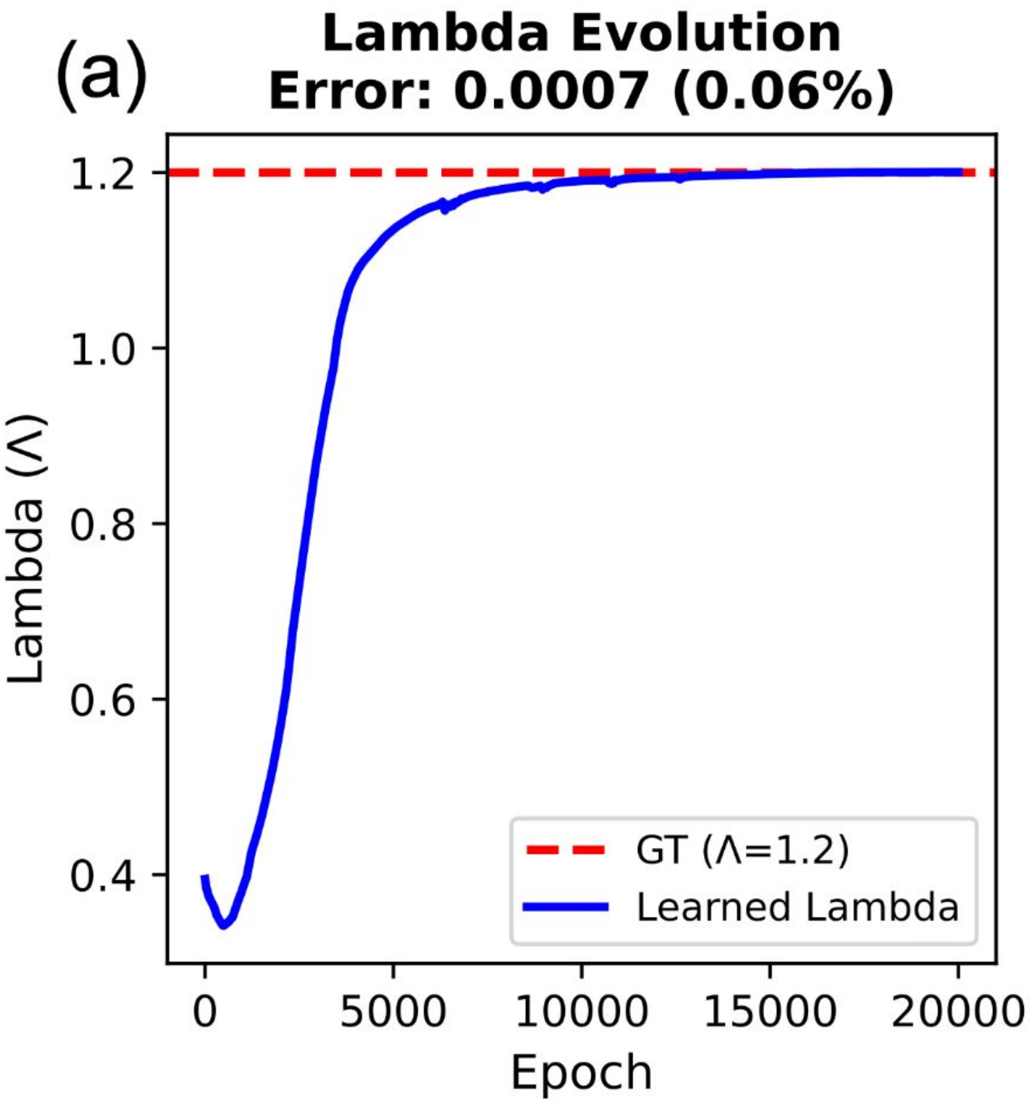


Model	Final Loss	RMSE
Forward PINN	1.49×10^{-4}	0.0030
PINN_Lambda	5.54×10^{-4}	0.0015
PINN_AB	5.22×10^{-4}	0.0015
PINN_NN	8.01×10^{-4}	0.0028

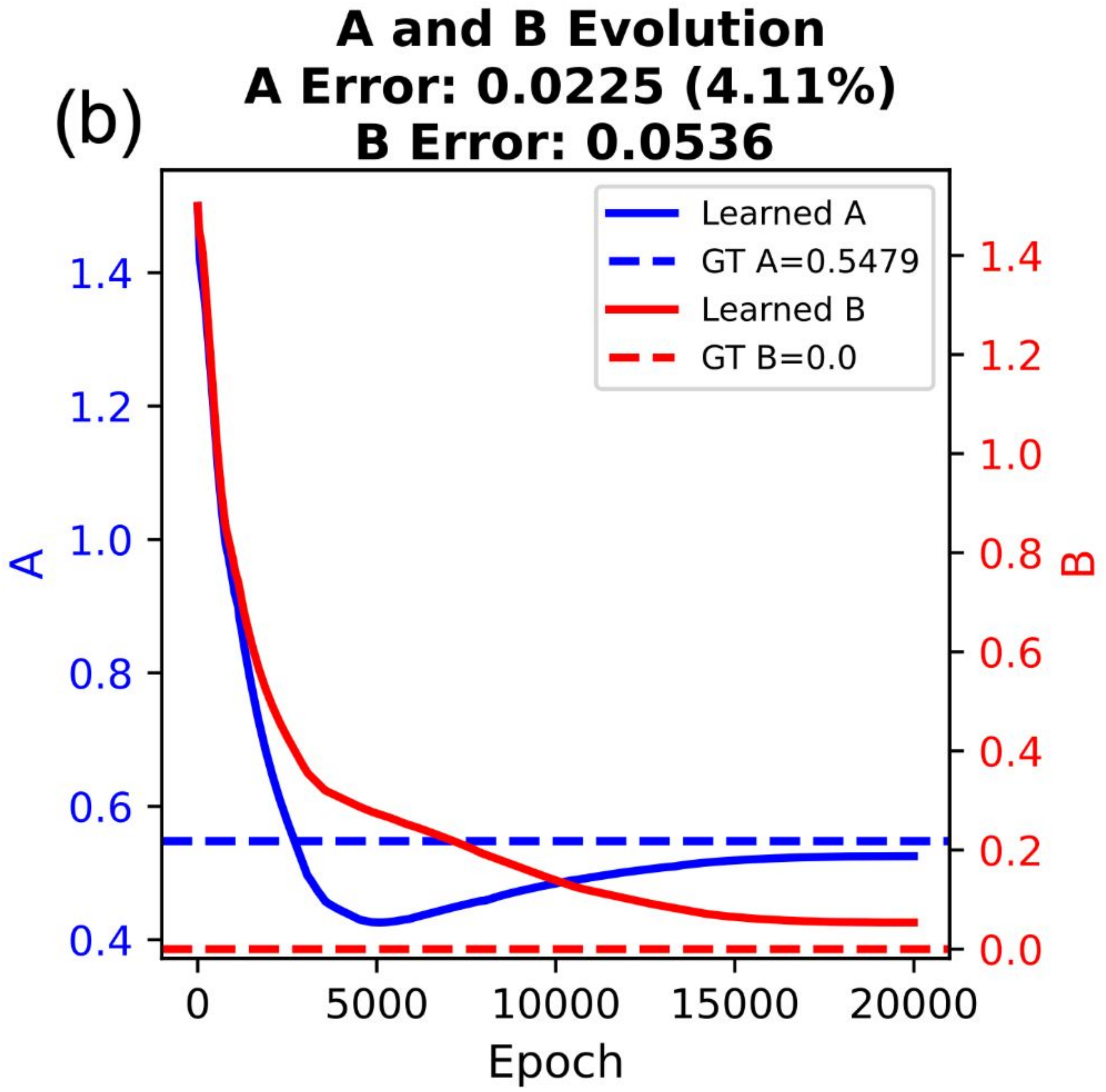
Results: parameter discovery

Phase 2.1: **Inverse PINN**

(a)

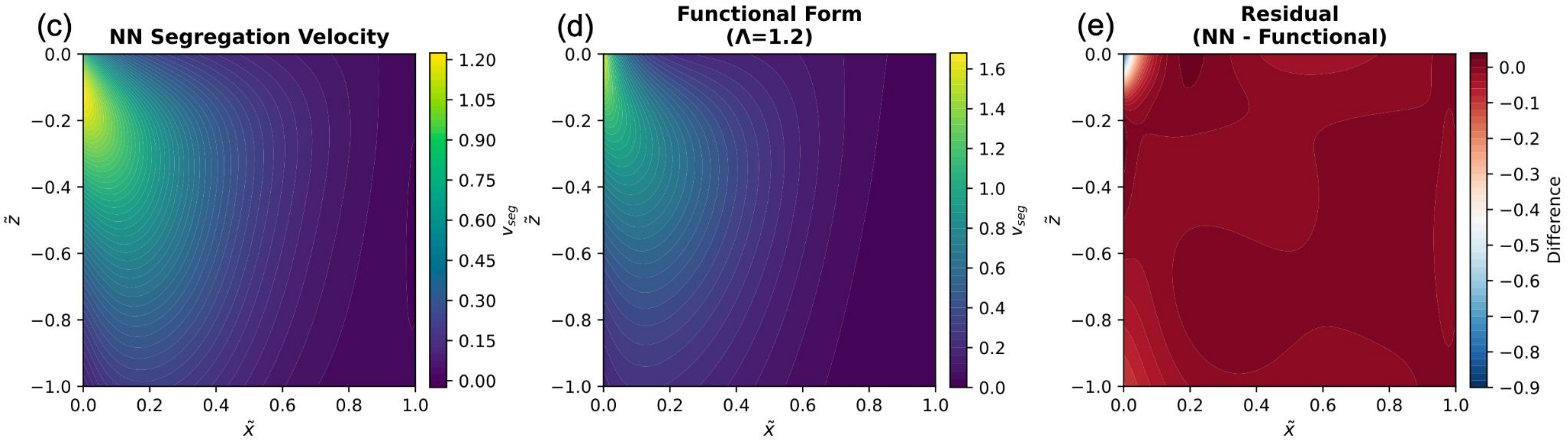


(b)



Results: parameter discovery

Phase 2.2: **Inverse PINN**

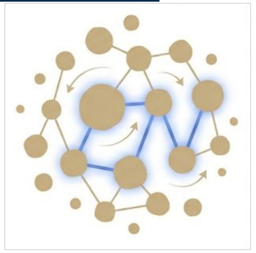


predicted

ground truth

error

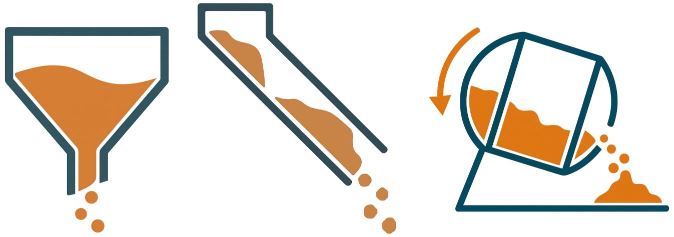
Conclusion


Granular Net

Summary of contribution

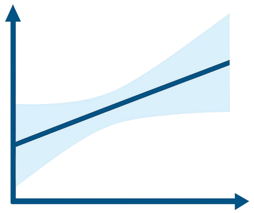
- **A capable forward solver**: PINNs provide a mesh-free, accurate method for solving the segregation problem without labeled data.
- **A material-related parameter identifier**: The inverse PINN framework can recover unknown physical parameters (like A) from sparse data with high fidelity.
- **A surrogate model for segregation velocity discovery**: Neural network closures allow the model to learn complex constitutive relationships directly, moving beyond the limitations of fixed analytical forms.

Future work



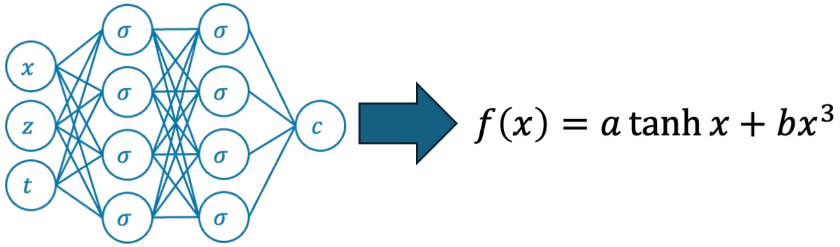
Generalization & Robustness

FNO & DeepONet



Uncertainty Quantification

Bayesian NN



Interpretability & Symbolic Discovery

SINDy


ANY QUESTIONS?
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Conclusion

Summary of contribution

- **A capable forward solver**: PINNs provide a mesh-free, accurate method for solving the segregation problem without labeled data.
- **A material-related parameter identifier**: The inverse PINN framework can recover unknown physical parameters (like A) from sparse data with high fidelity.
- **A surrogate model for segregation velocity discovery**: Neural network closures allow the model to learn complex constitutive relationships directly, moving beyond the limitations of fixed analytical forms.

Future work

- **Generalization & robustness**: Enable the models to generalize across different experimental configurations, operating conditions, and material properties.
- **Uncertainty quantification**: Incorporating Bayesian or ensemble methods to provide not just point estimates but also credible uncertainty bounds on learned parameters and closures.
- **Interpretability and symbolic discovery**: Coupling PINNs with symbolic regression techniques (e.g., SINDy) to translate the learned neural network closures into simple, interpretable mathematical equations, aiding scientific understanding.