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

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Introduction

Granular materials (e.g., grains, pellets, powders) frequently segregate during flow due to mechanisms such as kinetic sieving, producing non-uniform mixtures that complicate industrial handling.

Traditional continuum models rely on advection– segregation–diffusion PDEs, but their predictive accuracy is limited by uncertainties in segregation velocity closures, diffusion models, and geometry-dependent kinematics.

This project explores Physics-Informed Neural Networks (PINNs) as a framework that:

- Embeds the segregation PDE directly into the network loss,
- Performs forward simulation of concentration fields, and
- Enables inverse discovery of material parameters or full segregation-velocity models,

aiming to improve generalization across flow conditions.

Problem Definition

We model granular segregation in a quasi-2D bounded heap: a 50–50 binary mixture flows down a sloped free surface. The governing equation is an advection–segregation–diffusion transport PDE:

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

where c is concentration, D is diffusion coefficient, $\dot{\gamma}$ is local shear rate, and mean components (u and w) and segregation velocities are:

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

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

The boundary condition on top and bottom layers is balance of segregation and diffusive fluxes:

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

Key challenge: The segregation velocity closure w_s depends on material properties and flow conditions, making accurate prediction difficult across different geometries and materials.

Methodology

We develop **Granular Net**, a two-phase PINN framework:

Phase 1: Forward PINN

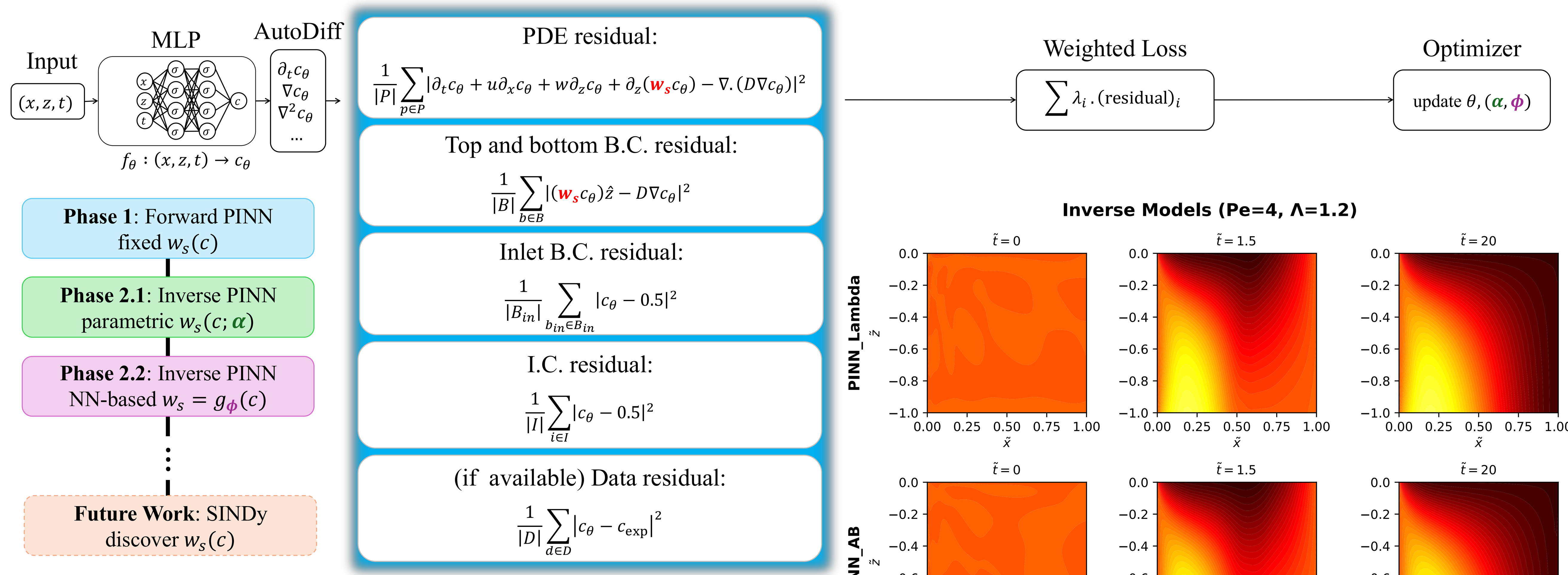
Solves the PDE with known segregation velocity parameters

- Architecture: 4-layer MLP (64 neurons/layer) with tanh activations
- Loss function enforces PDE residual, boundary conditions, and initial conditions
- Mesh-free, continuous solution representation

Phase 2: Inverse PINNs

Three variants for discovering unknown constitutive relationships:

- **PINN_Lambda:** Learns the segregation parameter Λ from sparse experimental data while maintaining the known functional form: $w_{s,i} = \Lambda(1-\tilde{x})g(\tilde{z})(1-c_i)$
- **PINN_AB:** Learns two parameters (A, B) in an extended segregation velocity form:
$$w_{s,i} = \Gamma(1-\tilde{x})g(\tilde{z})(1-c_i)[A + B(1-c_i)]$$
- **PINN_NN:** Learns a fully flexible neural network closure
$$w_{s,i} = v_{\mathrm{seg},\phi}(\tilde{x}, \tilde{z}, \tilde{t}, \dot{\gamma}, c_i)$$
that replaces the analytical form entirely.



All inverse models jointly optimize the concentration field and closure parameters/laws while enforcing physical consistency through the PDE residual.

Results

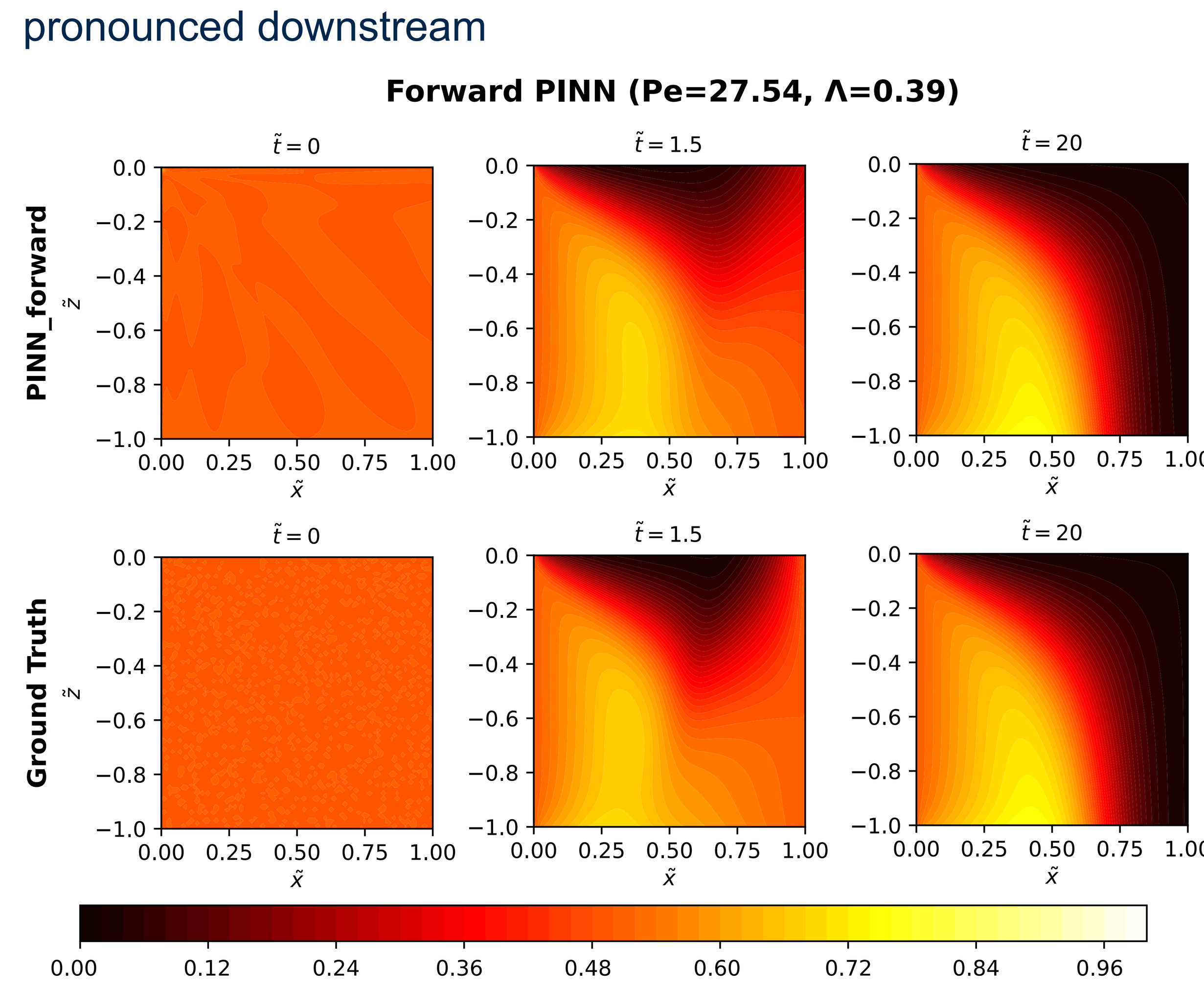
Training Convergence:

All four models (Forward, PINN_Lambda, PINN_AB, PINN_NN) converge successfully:

- Forward PINN: Final loss $= 1.49 \times 10^{-4}$
- Inverse models: Final losses $= \sim 6.50 \times 10^{-4}$
- PDE residuals remain low ($\sim 10^{-4}$), confirming physical consistency

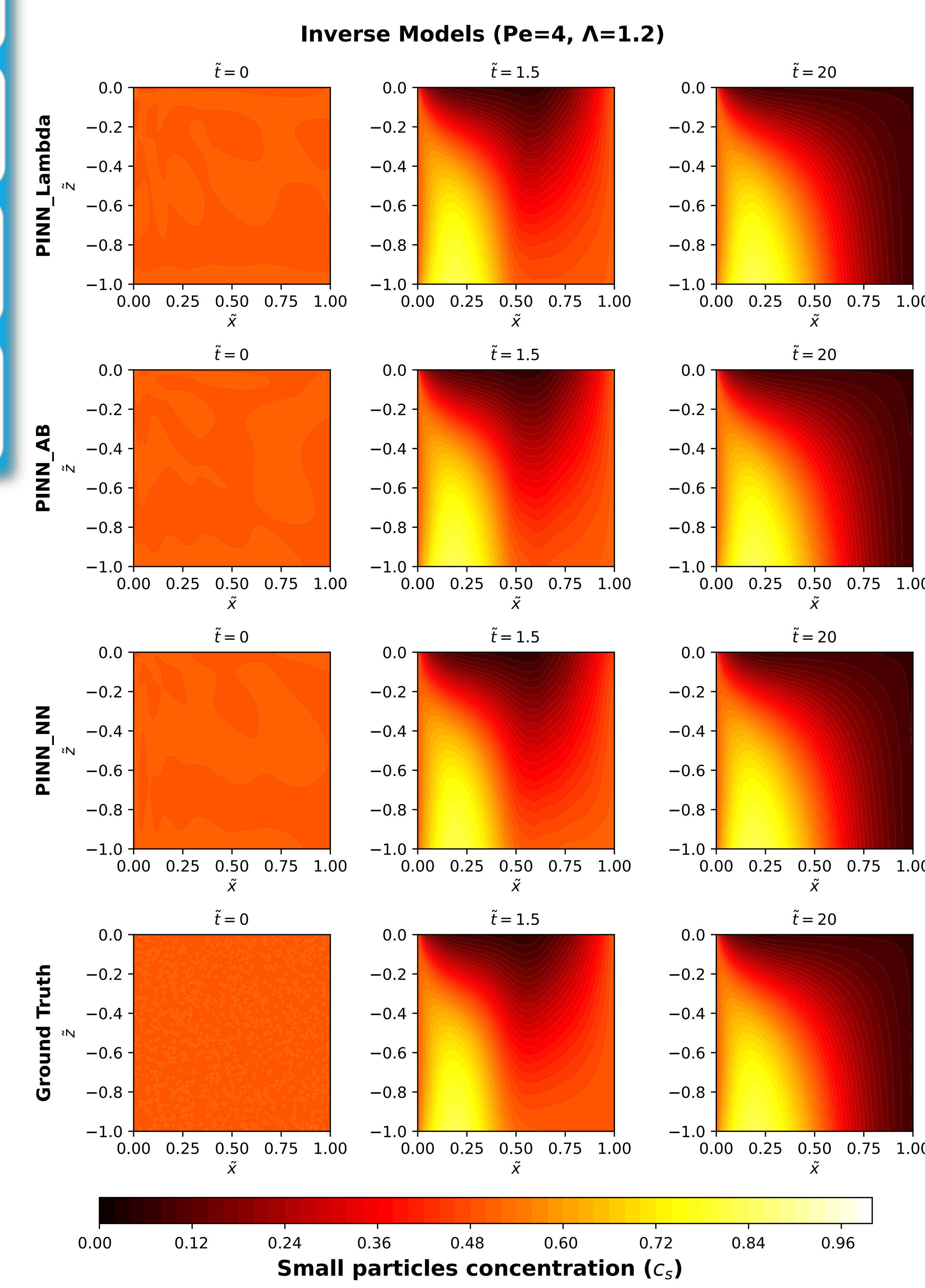
Concentration Field Prediction:

- Forward PINN accurately captures segregation patterns: small particles accumulate at bottom-left, large particles dominate at upper-right
- All inverse models produce concentration fields visually indistinguishable from ground truth
- Segregation develops gradually over time, becoming more pronounced downstream



Quantitative Accuracy:

Model	RMSE	MAE
Forward PINN	0.0030	0.0022
PINN_Lambda	0.0015	0.0009
PINN_AB	0.0015	0.0010
PINN_NN	0.0028	0.0015



Parameter Discovery

- PINN_Lambda recovers $\Lambda = 1.2007$ (ground truth: 1.2), error $= 0.06\%$
- PINN_AB learns $A = 0.5254$ and $B = 0.0536$ (ground truth: 0.5479 and 0.00), error $= 4.1\%$
- Neural network closure captures general trends of segregation velocity function

Key Contributions

Key Contributions:

- **Forward Simulation:** Demonstrated that PINNs can accurately solve the advection–segregation–diffusion equation without labeled training data (unsupervised).
- **Parameter Identification:** Successfully recovered constitutive parameters from sparse experimental data with errors < 5%, while maintaining physical consistency through PDE constraints.
- **Closure Discovery:** Showed that neural network closures can be learned directly from data, automatically capturing complex dependencies of segregation velocity on spatial coordinates, shear rate, and concentration without assuming analytical forms.

Future Directions

- Combining with Neural Operators to improve generalizability
- Uncertainty quantification through Bayesian approaches
- Symbolic regression for interpretability (e.g. SINDy)