Physics-Informed Neural Networks for Charge Transport in CdZnTe Detectors

Bachelor thesis presentation

- Josep Coll – Degree in data science and engineering – DTU

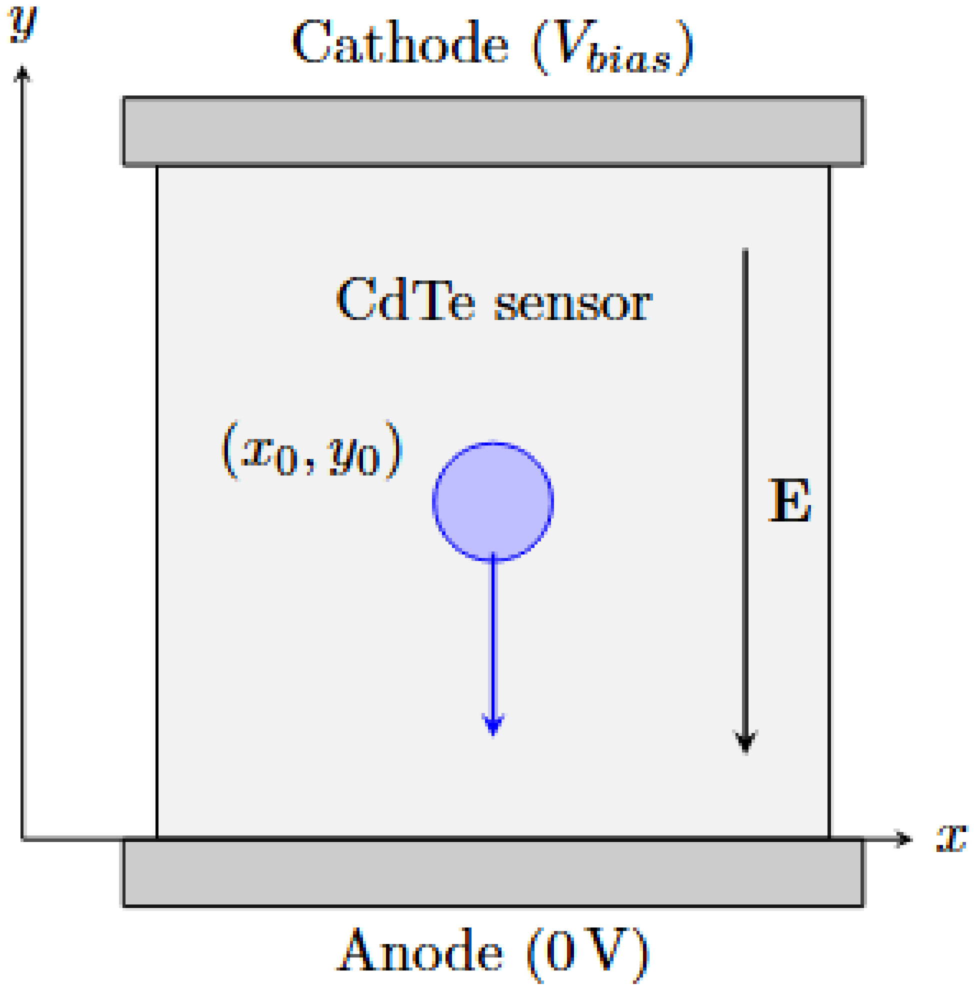
- Context: i-RASE project

Goal of the thesis

Build a physics-informed neural network that acts as a differentiable surrogate model for charge transport in a simplified CdZnTe detector.

Motivation: CdZnTe Detectors and Surrogates

- CdTe/CdZnTe detectors used in medical imaging and space instrumentation
- The electron cloud drift under the electric field, diffuses and is partially lost by trapping.
- TCAD drift-diffusion solvers are accurate but slow and not differentiable
- Need fast, differentiable models for planar CdZnTe charge transport



Physical Problem and Reduced PDE

- **Full detector model**
  – Electrostatics (Laplace/Poisson) → electric field E
  – Drift–diffusion transport of electrons and holes
  – Signal formation via Shockley–Ramo theorem
- **PDE variables and parameters**
  – n(t,x,y,) : normalised electron density
  – v : drift velocity
  – De : diffusion coefficient
  – τe : effective trapping time
- **Initial condition**
  – **Narrow Gaussian electron cloud centred at** (x0,y0) inside the sensor

$$\frac{\partial n}{\partial t} + \mathbf{v} \cdot \nabla n - D_e \nabla^2 n + \frac{n}{\tau_e} = 0$$

Methods – PINN Surrogate Model & Training

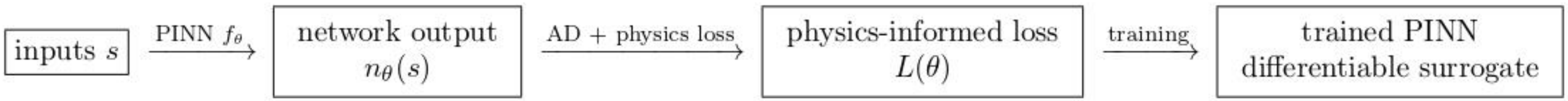
What is a Physics-Informed Neural Network?

It first takes inputs (time and space coordinates)

Uses automatic differentiation to compute derivatives

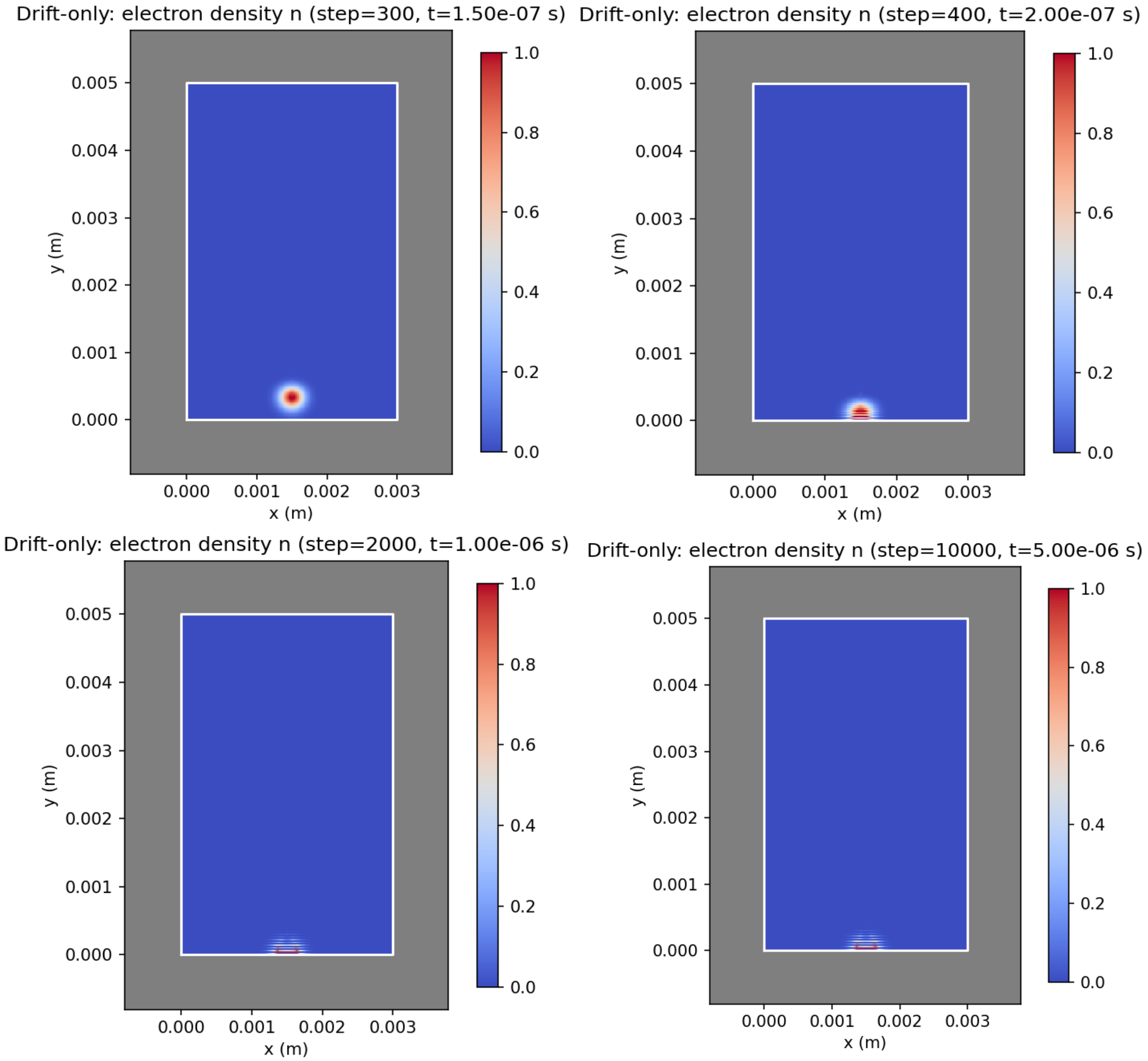
Loss includes PDE, initial condition and boundary terms

Output is a differentiable surrogate of the solution



Baseline Drift-Only Simulator

- Simple drift-only finite-difference solver on a 2D grid (explicit time stepping)
- Absorbing anode at y = 0 with an extended outer padding region
- **Role 1 – Sanity check:** validates geometry, drift direction and units
- **Role 2 – Diagnostic:** reveals numerical artefacts (spurious reflected packets at the anode)



From 3-variable PINN to 5-input Conditional PINN

First step: 3-input PINN n_hat(t,x,y)for one fixed (x0,y0)

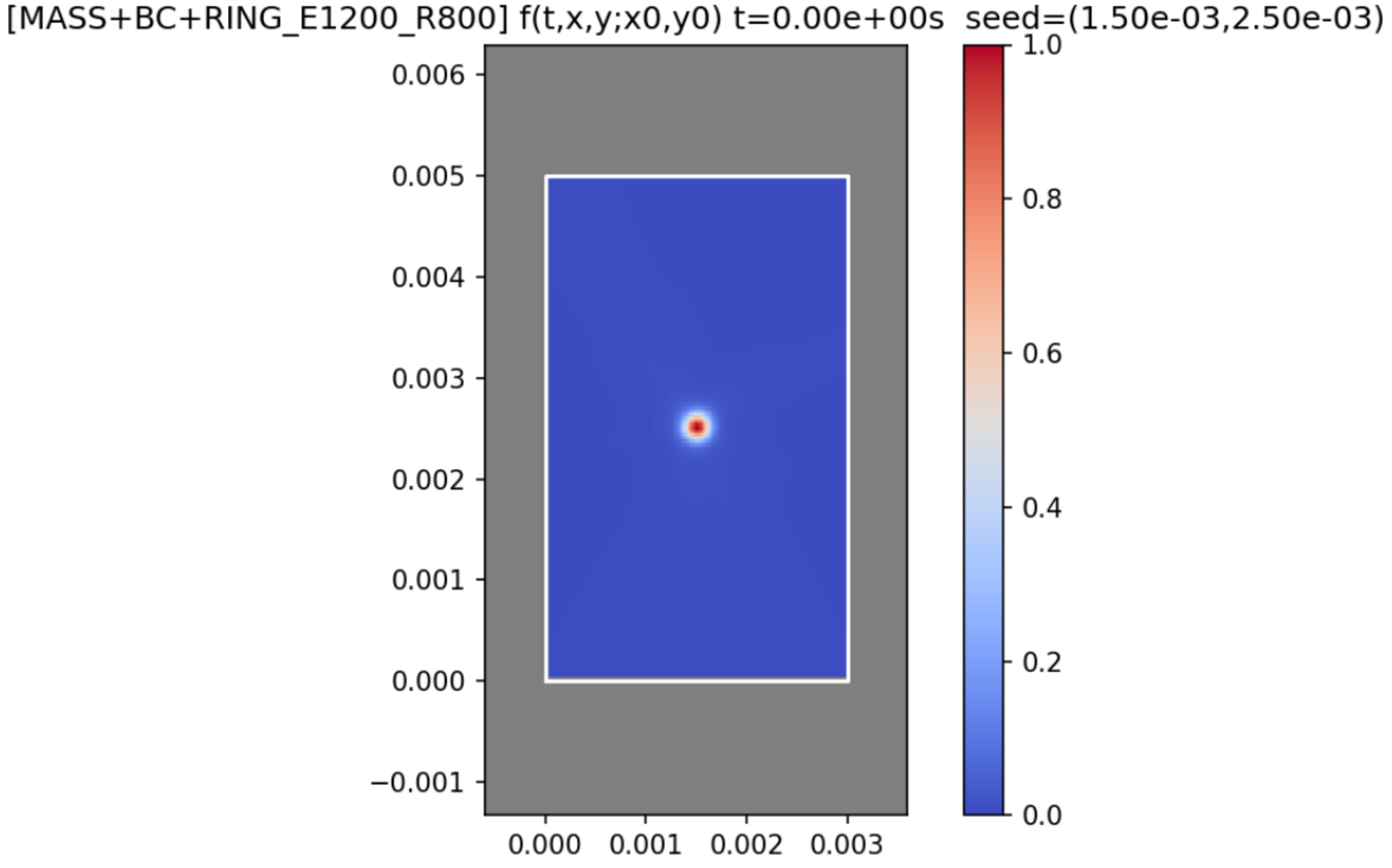
Limitation: need a new model for every interaction point

Final model: 5-input conditional PINN n_hat(t,x,y;x0,y0)

One network reused for many interaction positions

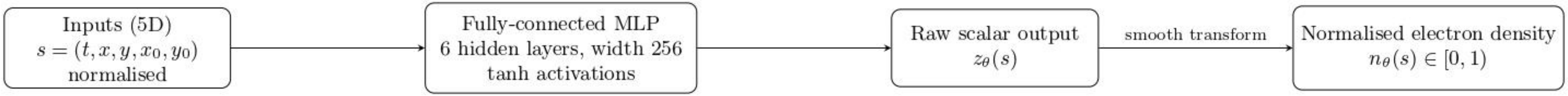
Where does the PINN Lives in the Code

- PINN implemented in JAX/Equinox
- Inner white box = physical CdZnTe detector
- Grey padding = extended training domain around the sensor
- Different loss terms applied inside the sensor and in the padding



PINN Architecture: 5 Input Coordinates

- Fully-connected multilayer perceptron (MLP)
- 5 inputs (t, x, y, x_0, y_0), all normalised to [0, 1]
- 6 hidden layers, width 256, with **tanh** activations
- Single scalar output → smooth transform → density n_hat ∈ (0, 1)
- Normalisation + smooth output improve conditioning of derivatives



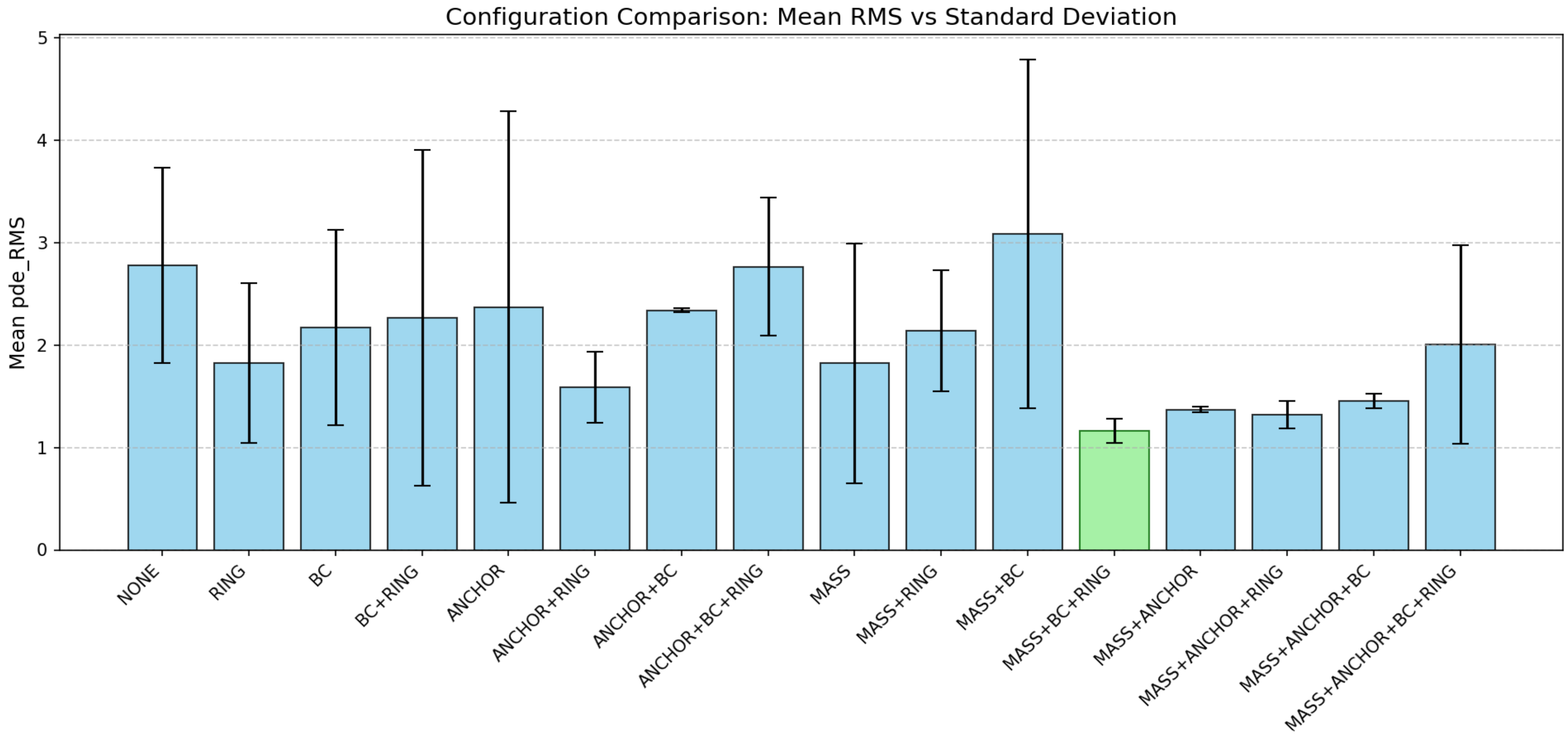
From PDE to Loss Terms

$$\mathrm{R}_\theta = \partial_t n_\theta + \mathbf{v} \cdot \nabla n_\theta - D_e \nabla^2 n_\theta + \frac{1}{\tau_e} n_\theta$$

Loss components:	L_{IC} : initial-condition loss at t=0 (Gaussian packet at (x0,y0)).
	L_{PDE} : mean-squared PDE residual in the interior.
	L_{BC} : loss enforcing the anode boundary condition at y=0.
	L_{ring} : loss enforcing near-zero density in the outer ring of the extended domain.
	L_{mass} : global mass-decay loss enforcing the expected exp(−t/τe) behaviour.

Ablation Study on Loss Terms

- Optional terms: Lmass, Lanchor, LBC, Lring.
- LIC and LPDE always active.
- 2^4 = 16 configurations, 2 runs each, 100 epochs.
- Metric: best diagnostic PDE residual RMS.
- **Best:** MASS+BC+RING (no anchor) → lowest mean residual, stable across seeds.



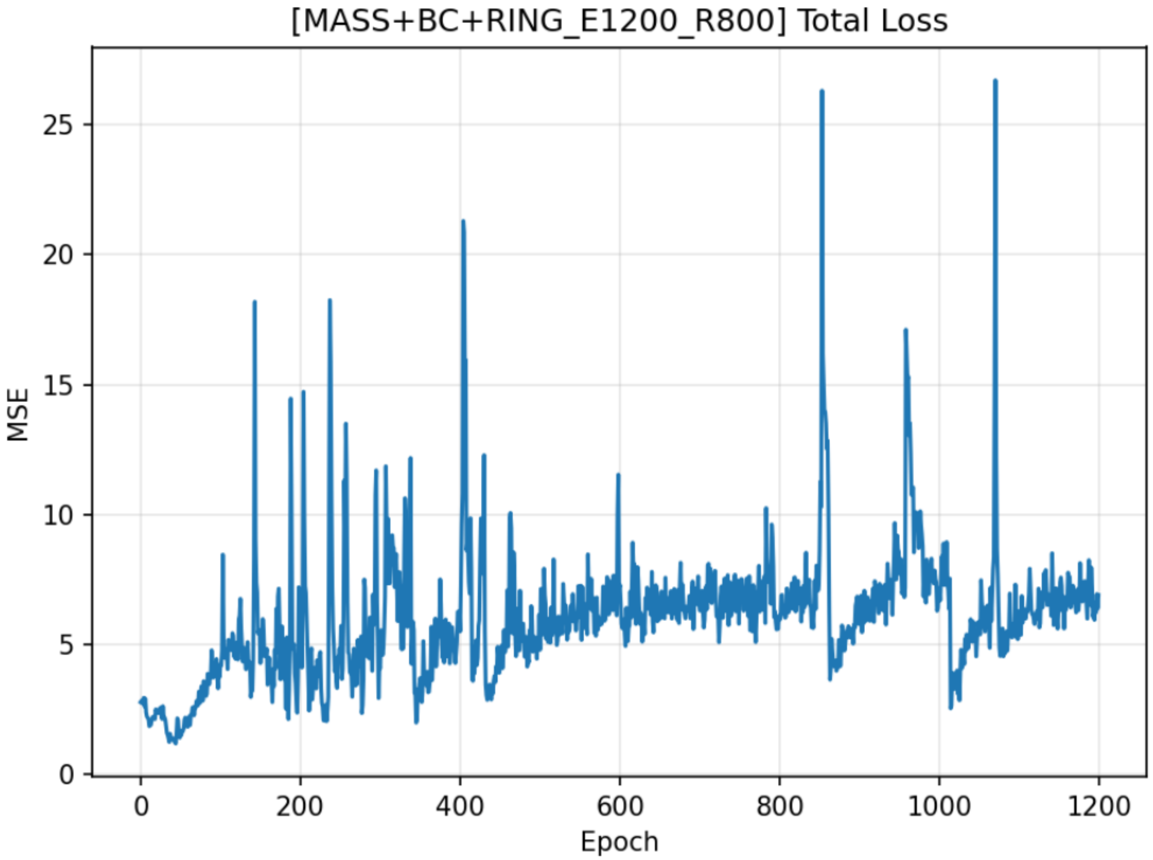
Hyperparameter Tuning

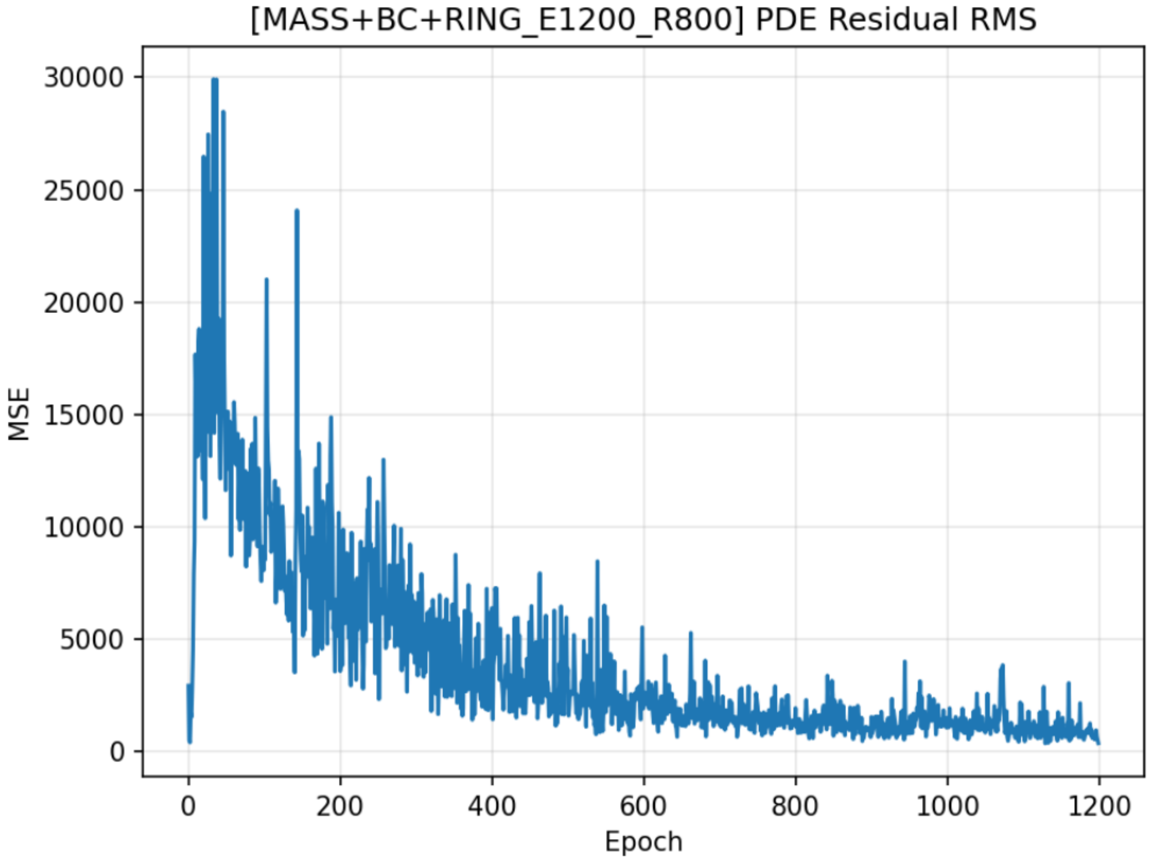
- Tune hidden width and learning rate
- Widths: 256 and 320; learning rates: 1e-4, 3e-4, 5e-4
- 400-epoch runs, best PDE residual RMS as metric
- Best choice: width 256, learning rate 3e-4

Width	Learning rate	Best PDE RMS
256	1.0×10^{-4}	1.0×10^{2}
320	1.0×10^{-4}	1.1×10^{2}
256	3.0×10^{-4}	1.5×10^{-2}
320	3.0×10^{-4}	1.8×10^{-2}
256	5.0×10^{-4}	1.6×10^{-2}
320	5.0×10^{-4}	5.0×10^{2}

Results – PINN Behaviour & Diagnostics

Training Dynamics: Total Loss and PDE Residual RMS



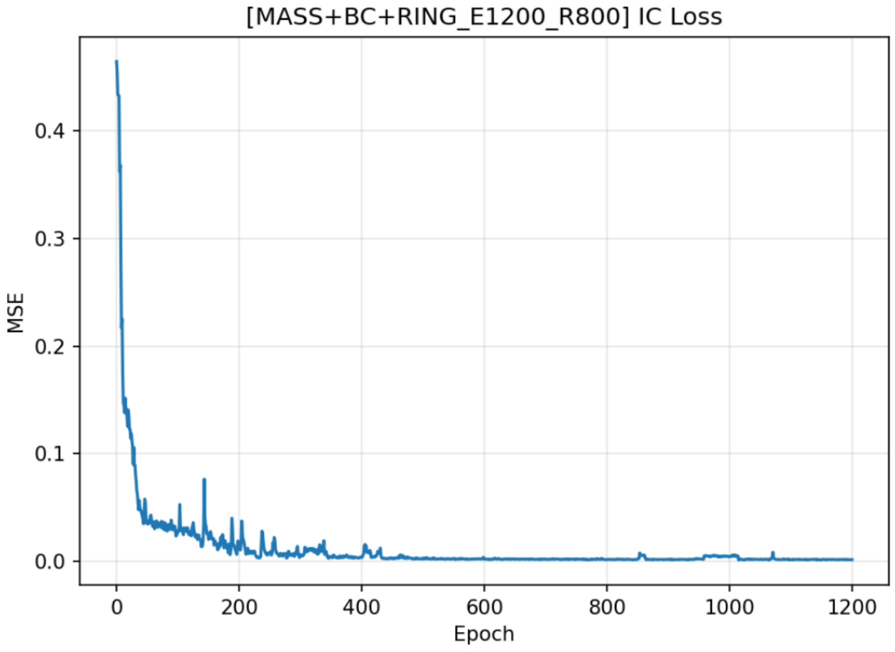


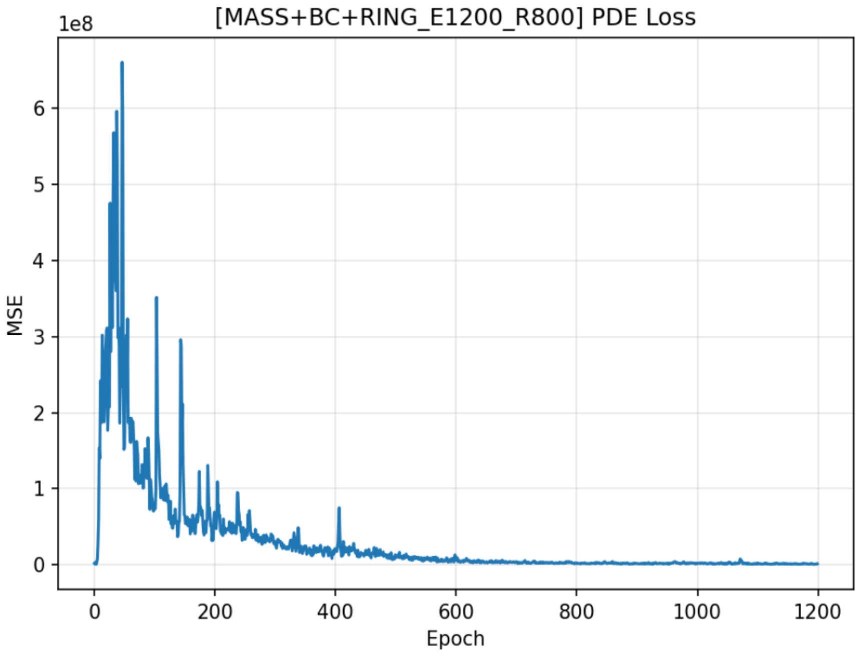
Why the Total Loss is Spiky

- Curriculum: ramp-up of λPDE(t) and λmass(t)
- Normalisation: ratios LIC/sICL, LPDE/sPDE balance the scales
- Random resampling of collocation points → extra noise in Ltotal
- Result: spiky total loss but smooth, meaningful PDE residual RMS

$$\boxed{\mathrm{L}_{\mathrm{total}}(t_{\mathrm{ep}}) = \lambda_{\mathrm{IC}}\frac{L_{\mathrm{IC}}}{s_{\mathrm{IC}}} + \lambda_{\mathrm{PDE}}(t_{\mathrm{ep}})\frac{L_{\mathrm{PDE}}}{s_{\mathrm{PDE}}} + \lambda_{\mathrm{BC}}L_{\mathrm{BC}} + \lambda_{\mathrm{ring}}L_{\mathrm{ring}} + \lambda_{\mathrm{mass}}(t_{\mathrm{ep}})L_{\mathrm{mass}}}$$

Individual Loss Components



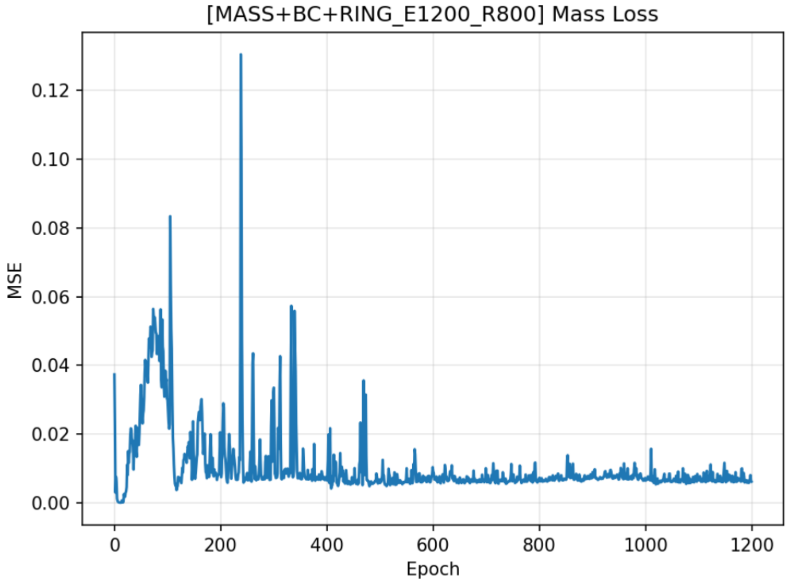


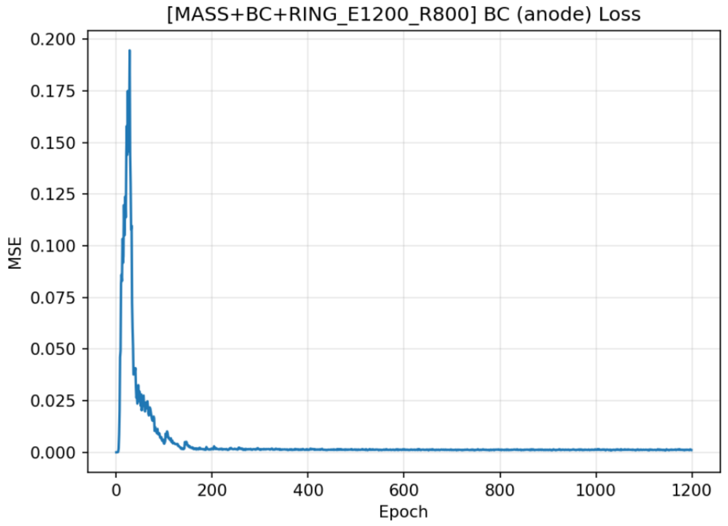
L_{IC}: fast decay, small plateau

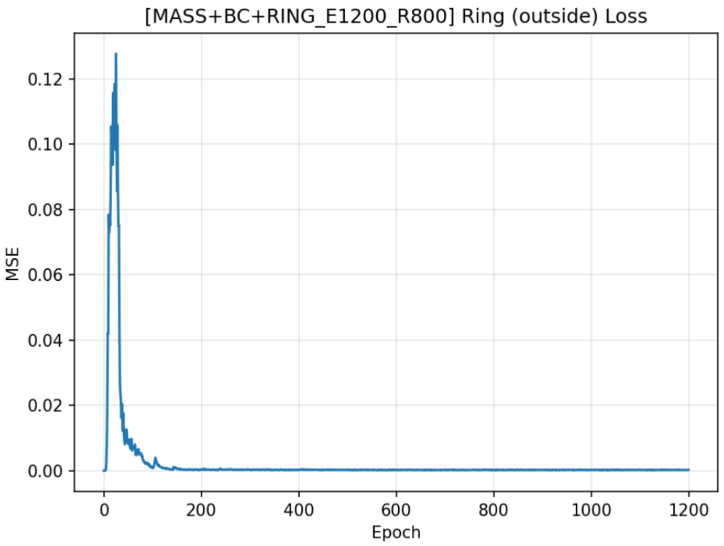
L_{PDE}: large at start, then decreases by >1 order of magnitude

L_{mass}: transient then plateau consistent with exponential decay

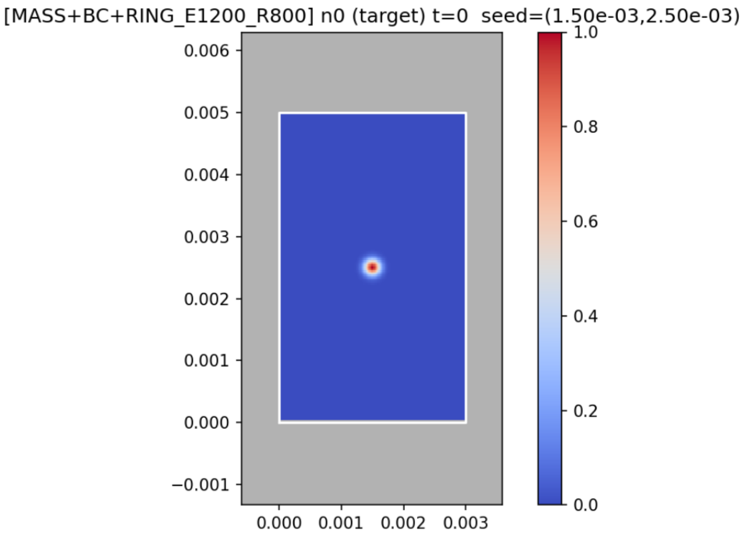
L_{BC} and L_{ring}: rapid drop, remain very small

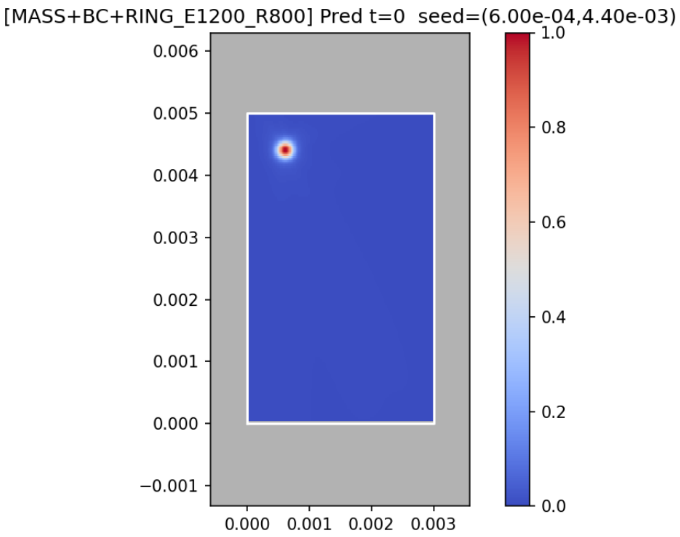






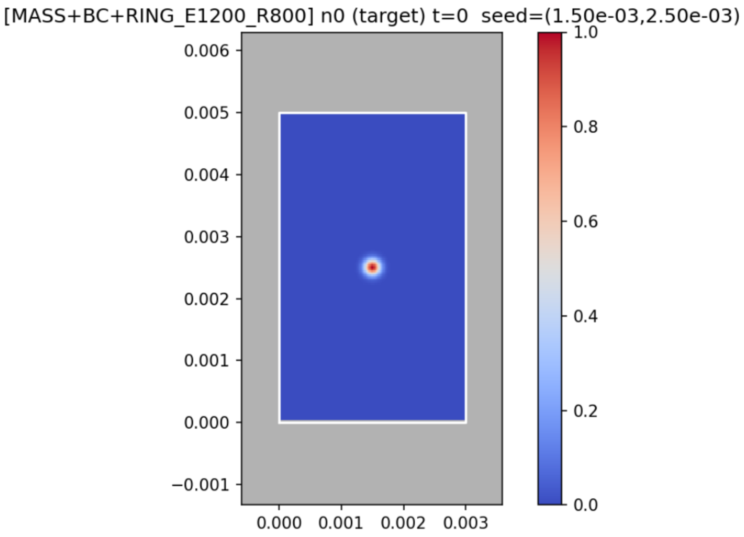
Initial Condition at t = 0: Analytic vs PINN

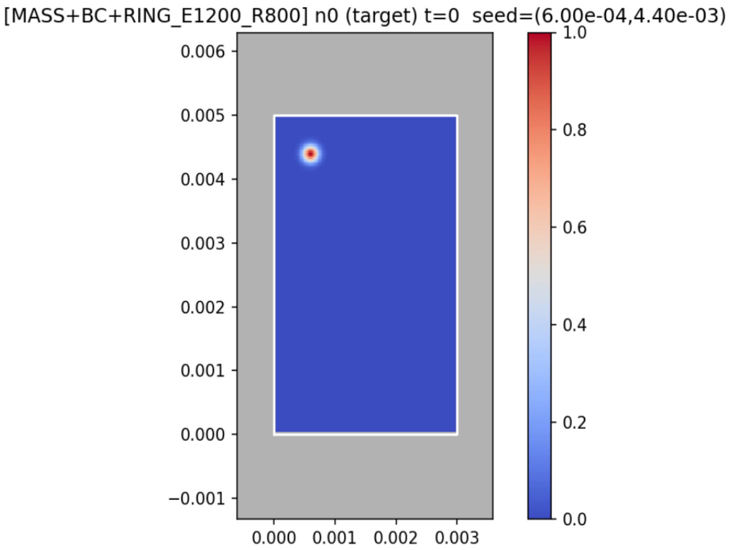




Seed 1, $\|n_\theta - n_0\|_{\text{RMS}} \approx 5.1 \times 10^{-3}$

Seed 2, $\|n_\theta - n_0\|_{\text{RMS}} \approx 5.5 \times 10^{-3}$



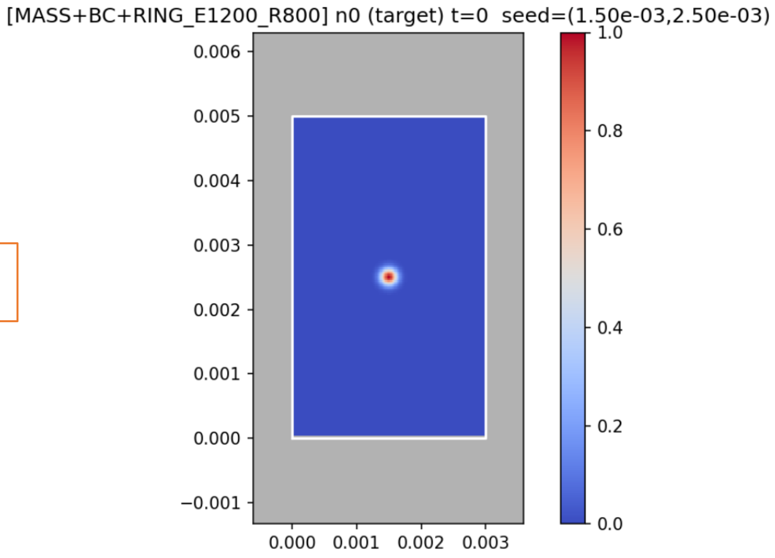


Initial Condition at t = 0: Error and Mass Metrics

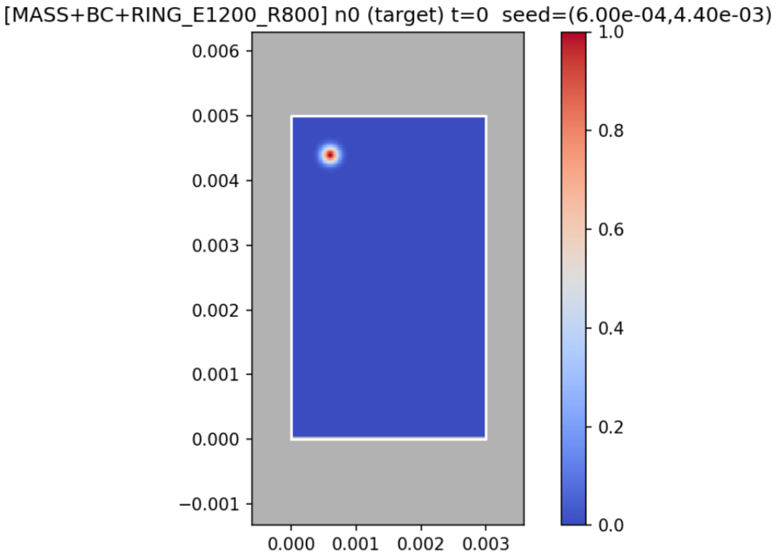
- Seed-wise MSE values are of order 10−5, i.e. RMS deviations of ≈5×10^{-3} on a [0,1] density scale.
- The predicted total mass Qθ(0) lies in the range 5.2–5.7×10^{-8}, while the analytic target is Q0=2.37×10^{-8}: the PINN overestimates the mass by a roughly constant factor ≈2.3 across seeds.
- The COM displacement is very small for the central seed (0.06 mm) but increases to 0.5–1.0 mm for more extreme seeds, indicating reduced localisation accuracy near the edges and close to the anode.

Seed	(x_0, y_0) [mm]	MSE	$Q_\theta(0)$	Q_0	$\lVert\Delta r_{\mathrm{COM}}\rVert$ [mm]
1	(1.5, 2.5)	2.61×10^{-5}	5.60×10^{-8}	2.37×10^{-8}	0.06
2	(0.6, 4.4)	3.01×10^{-5}	5.66×10^{-8}	2.37×10^{-8}	1.00
3	(2.4, 3.6)	2.82×10^{-5}	5.65×10^{-8}	2.37×10^{-8}	0.65
4	(1.0, 1.2)	2.49×10^{-5}	5.19×10^{-8}	2.37×10^{-8}	0.53

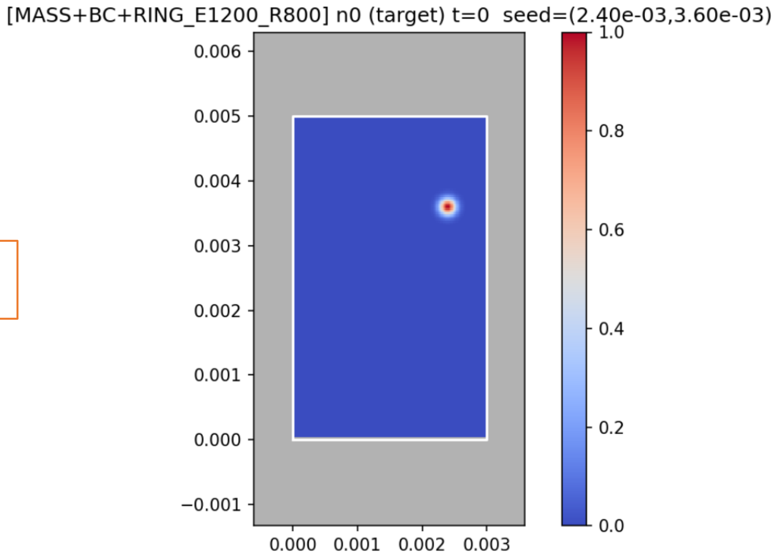
Seed 1



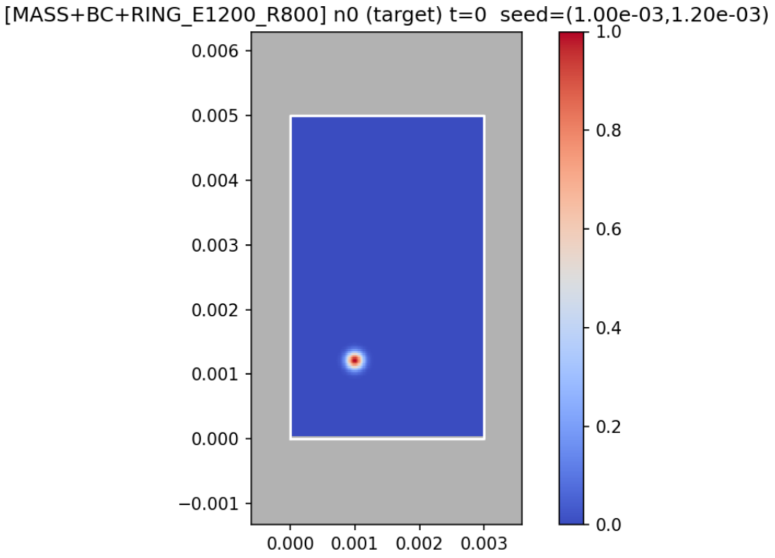
Seed 2



Seed 3

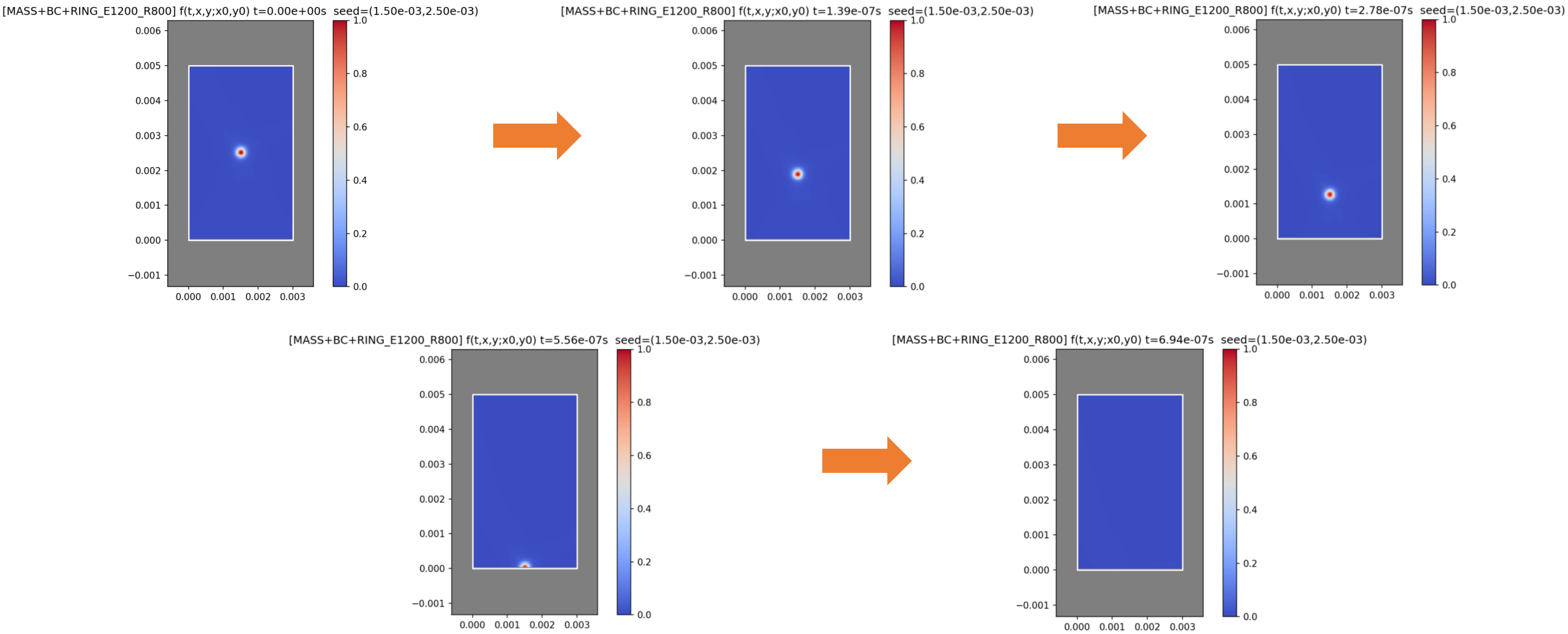


Seed 4

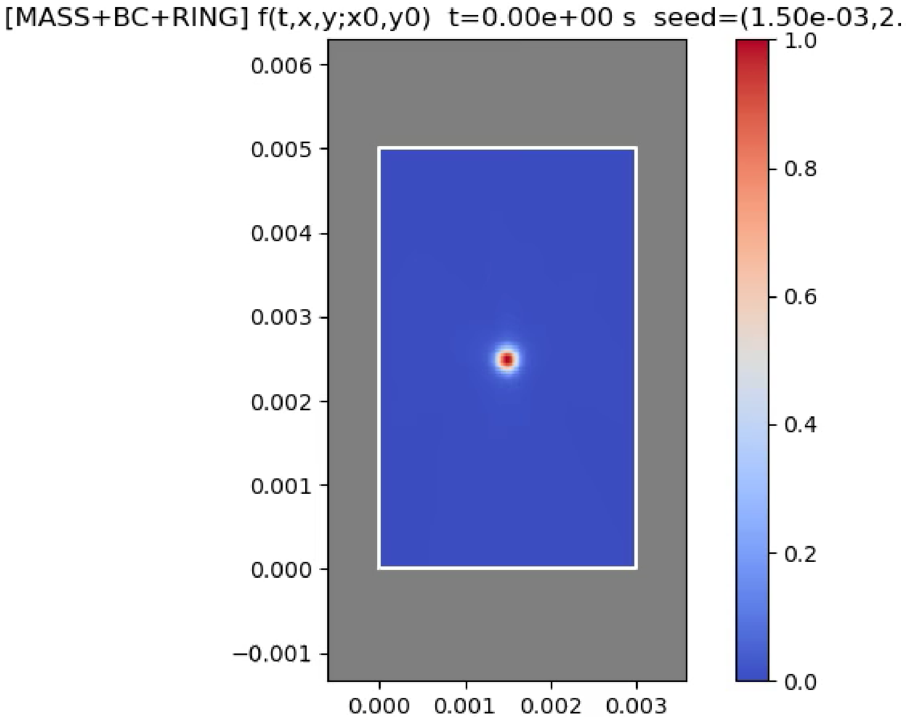


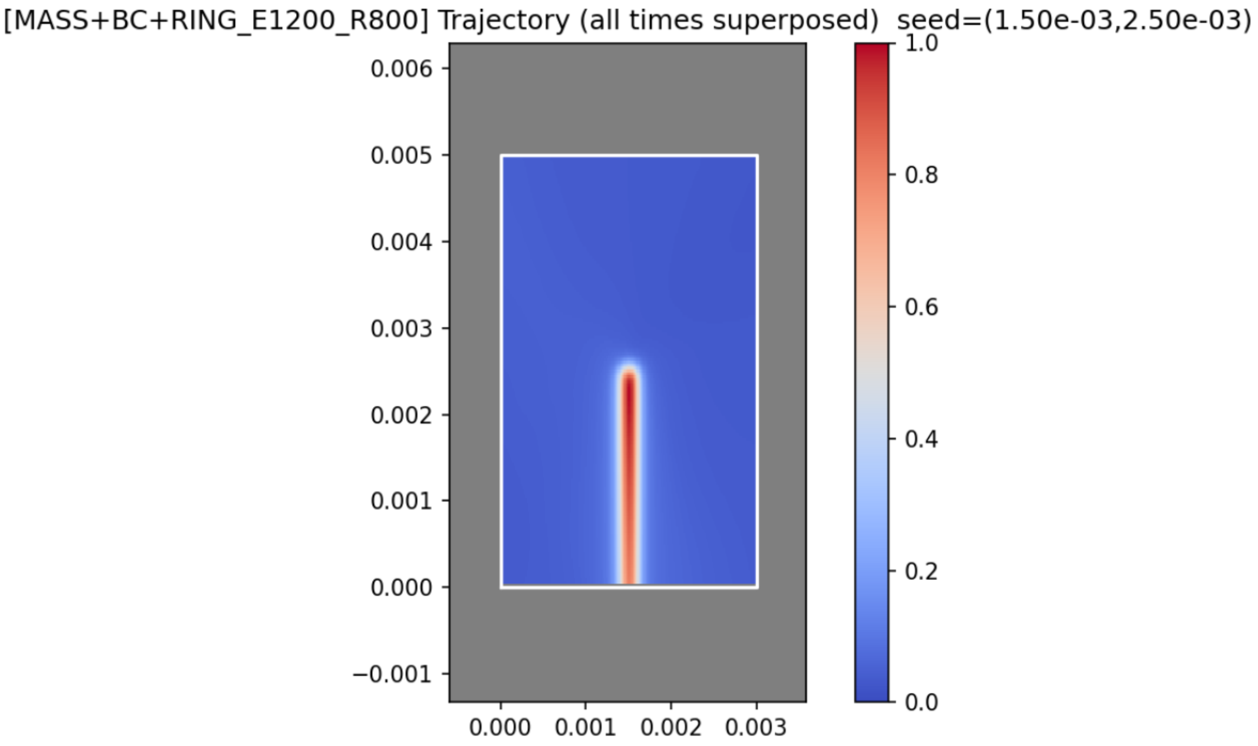
Spatio-Temporal Evolution of the Electron

- Central interaction point inside the detector.
- Electron drifts downwards along the electric field.
- Electron spreads out over time due to diffusion.
- Extended domain; the white box marks the physical detector.



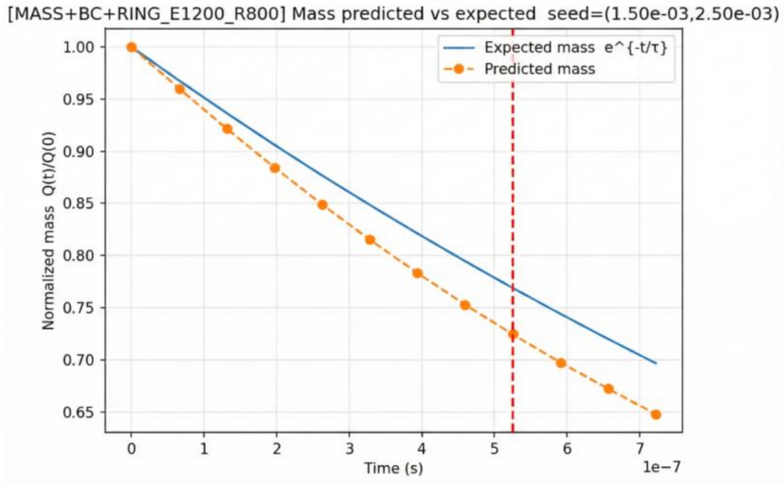
Animation: Drift, Diffusion and Absorption at the Anode

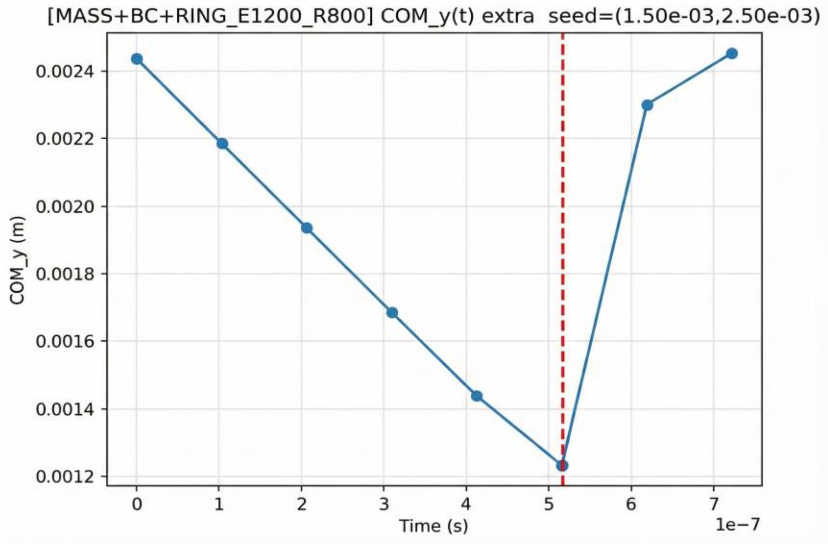


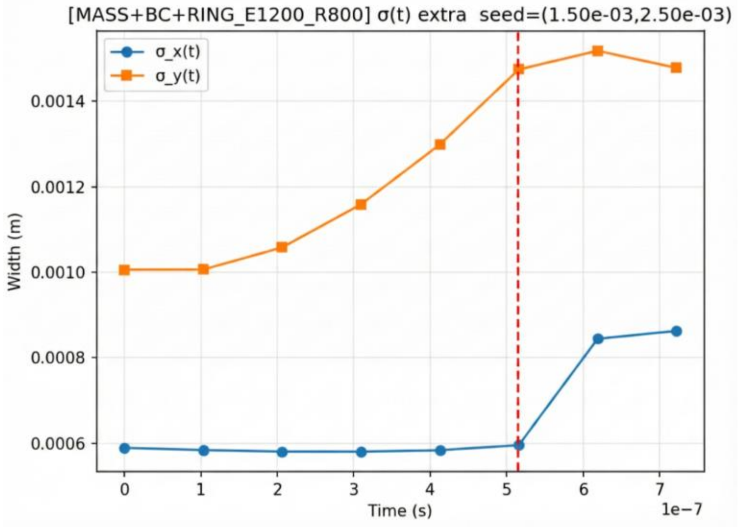


Global Physical Diagnostics: Mass, COM and Widths

- Total mass Q(t)/Q(0: monotonic decay close to exponential, slight over-absorption
- yCOM(t): almost linear drift, then apparent rebound (COM artefact after absorption)
- Widths σx(t), σy(t): diffusion broadening, stronger along y







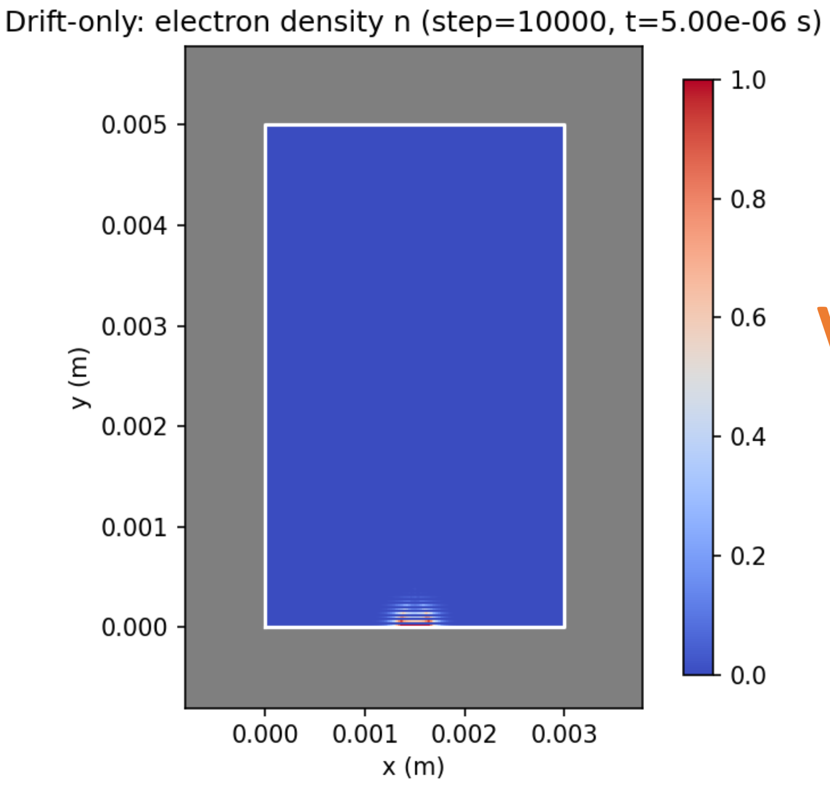
Baseline Simulator vs PINN near the Anode

Baseline drift solver

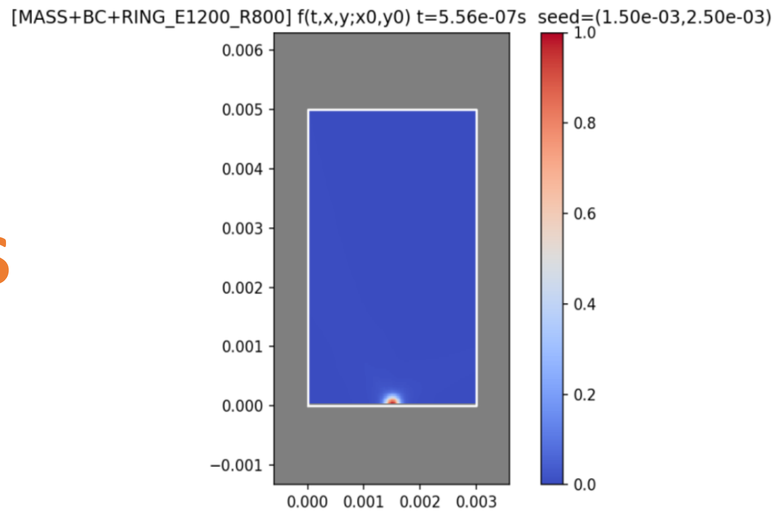
- Simple, deterministic reference on a fixed grid
- Not differentiable w.r.t. geometry/parameters
- Boundary artefacts near the anode (reflected packets)

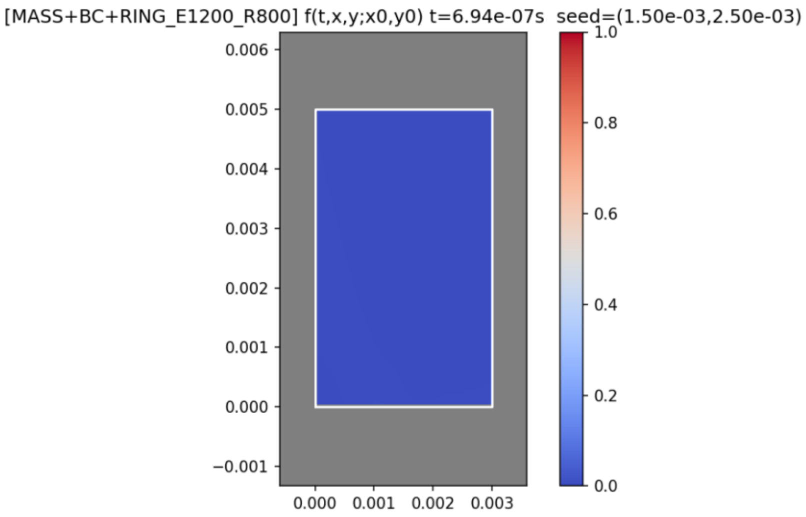
PINN surrogate

- Training is costly and solution is approximate (non-zero PDE residual)
- Mesh-free, fast to evaluate for many interaction points
- Differentiable and smoother behaviour near the anode thanks to BC + ring losses



VS





Limitations

Limitations of the Physical Model

- Simplified 2D planar slab with uniform electric field
- Only electrons modelled; holes and complex trapping ignored
- Trapping represented by single homogeneous lifetime
- Shockley–Ramo signal formation not included
- Model is a proof-of-concept, not a full TCAD replacement

Limitations of the PINN Implementation

- Composite loss mixes terms with different scales and units
- Uniform collocation sampling ignores most critical regions
- PDE residual RMS remains finite (~10^2)
- Network capacity finite; with non-uniform accuracy across de sensor
- Ablation and tuning based on limited number of runs

Future Work

Future Work: Physics Extensions

- Use realistic electric and weighting fields from Poisson / TCAD solvers
- Extend from planar 2D geometry to 3D pixel detectors
- Include Shockley–Ramo signal formation and CIE maps
- Model both electrons and holes with position-dependent trapping
- Train a PINN for transport towards a small anode

Future Work: Methods and Applications

- More exhaustive ablations and longer training runs
- Residual-based adaptive sampling of collocation points
- Explore alternative architectures (Fourier features, ResNets, operators)
- Domain decomposition (cPINNs) for larger or 3D domains
- Integrate PINN into inverse problems and design/optimisation loops

Summary and Take-Home Messages

Proof-of-concept 5-input PINN surrogate for CdZnTe charge transport – a solid starting point for more realistic detector modelling and future optimisation studies.

Thank you very much for your attention
I’ll be happy to take any questions.

Bachelor thesis presentation

- Josep Coll – Degree in data science and engineering – DTU
- Context: i-RASE project