Physics-Informed Learning: Accelerating Scientific Modelling and Discovery

From Data-Driven AI to Physics-Constrained Intelligence

Remus Teodorescu

Professor, Department of Energy | Aalborg University, Denmark

The AI Revolution in Science: from data to physics!

2016
AlphaGo

Defeats world champion Lee Sedol — AI masters strategic reasoning

2021
AlphaFold 2

Solved 50-year protein folding problem — 200M+ structures predicted (acceleration)

2022–
Reasoning LLMs

GPT Claude, GROK, Gemini reads, writes, and reasons science at PhD level! (topic- and language-agnostic!)

2026–
Scientific LLMs

ROSALIND

- the life sciences counterpart to OpenAI's general-purpose frontier models — bringing deep reasoning to drug discovery, genomics, and translational medicine

SciSpace

- Combining the reasoning slills of ChatGPT/Claude is the most comprehensive AI-powered research platforms for accelerating scientific research (literauture discovery, hypothesis generation and research planning)

Physics-Informed Neural Networks (PINN) – 2019 (Raissi et al.)

- Combines the representational power of neural networks with the constraints and structure of physical laws — delivering models that generalise from sparse data while respecting conservation laws, PDEs, and boundary conditions.
- AKA learning to play piano from both hearing (data) and teacher/method (physics)
- Relevant for engineering as most of the governing physics laws are already ..discovered!

Two Paradigms — One Synthesis

Pure Data-Driven ML

✗ Learns purely from data — no physics knowledge

✗ Requires massive datasets (millions of samples)

✗ Black-box: no interpretability or guarantees

✗ Fails to extrapolate beyond training distribution

✗ Violates physical constraints (energy, mass, momentum)

Classical Physics Modelling

✓ First-principles PDEs — interpretable and trustworthy

✓ Works with zero data — pure physics

✓ Computationally expensive: hours to days per simulation

✓ Cannot incorporate noisy real-world sensor data

✓ Requires perfect knowledge of all parameters

PIML Synthesis:

Data efficiency of ML + Physical fidelity of PDE solvers = Real-time, trustworthy surrogates

Karniadakis et al., 2021 | Raissi et al., 2019

What is Physics-Informed Learning? — The Core Idea

Composite Loss Function

L_total = L_data + λ · L_physics

1. **L_data — Fit the observations**

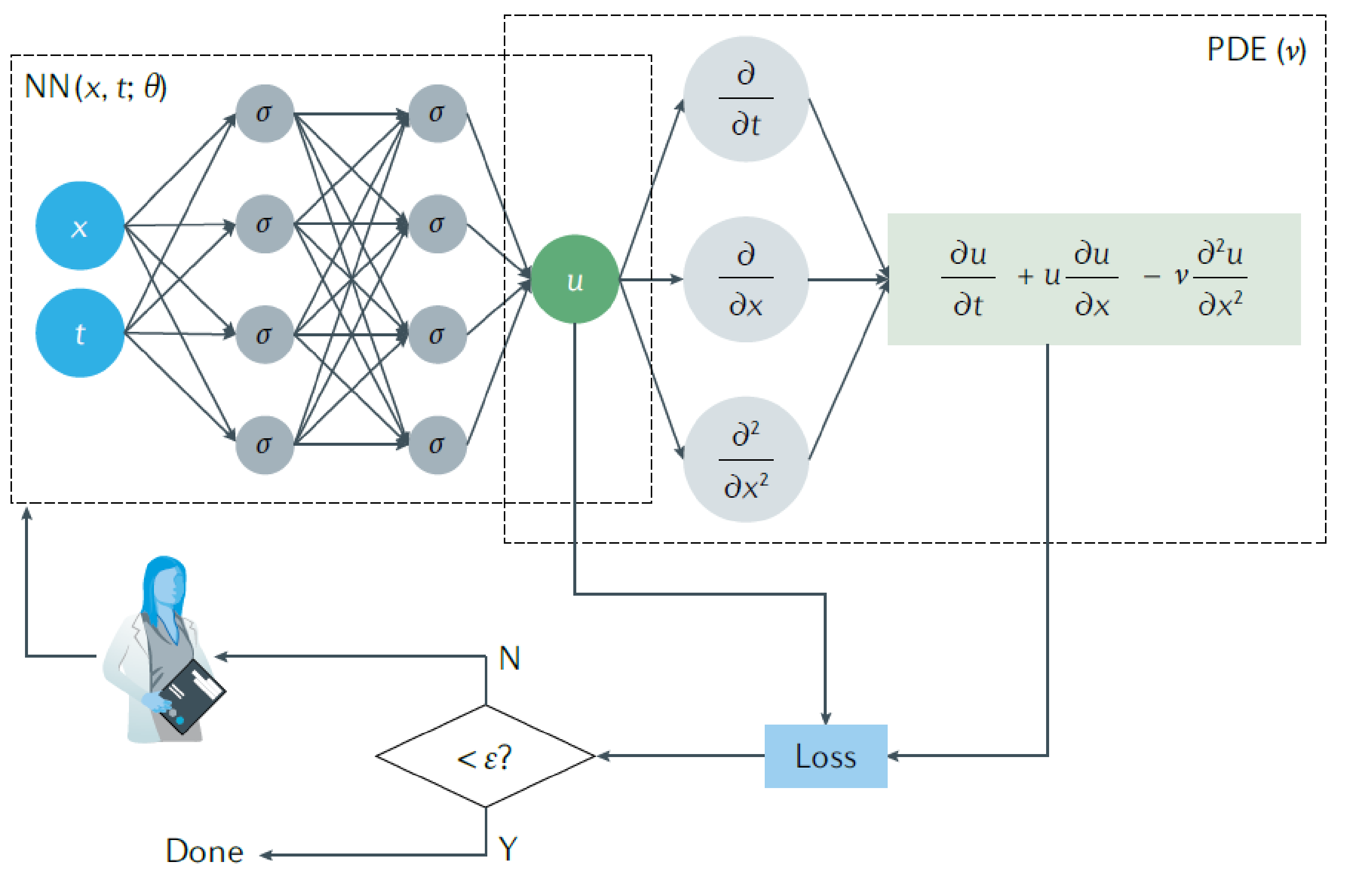
   Mismatch between network predictions and measured data (V, I, T)

2. **L_physics — Enforce the laws**

   Residuals of governing PDEs/ODEs computed via automatic differentiation

3. **Result: Physics-consistent predictions**

   Generalises with limited data — no physics violation, better extrapolation



PINN architecture: neural network + PDE residual loss

Raissi et al., 2019 | Karniadakis et al., 2021

The PIML Revolution

1: Accelerating Complex Modelling

PIML surrogates replace expensive PDE solvers — delivering real-time inference at a fraction of the cost.

2: Acceleraating Scientific Discovery

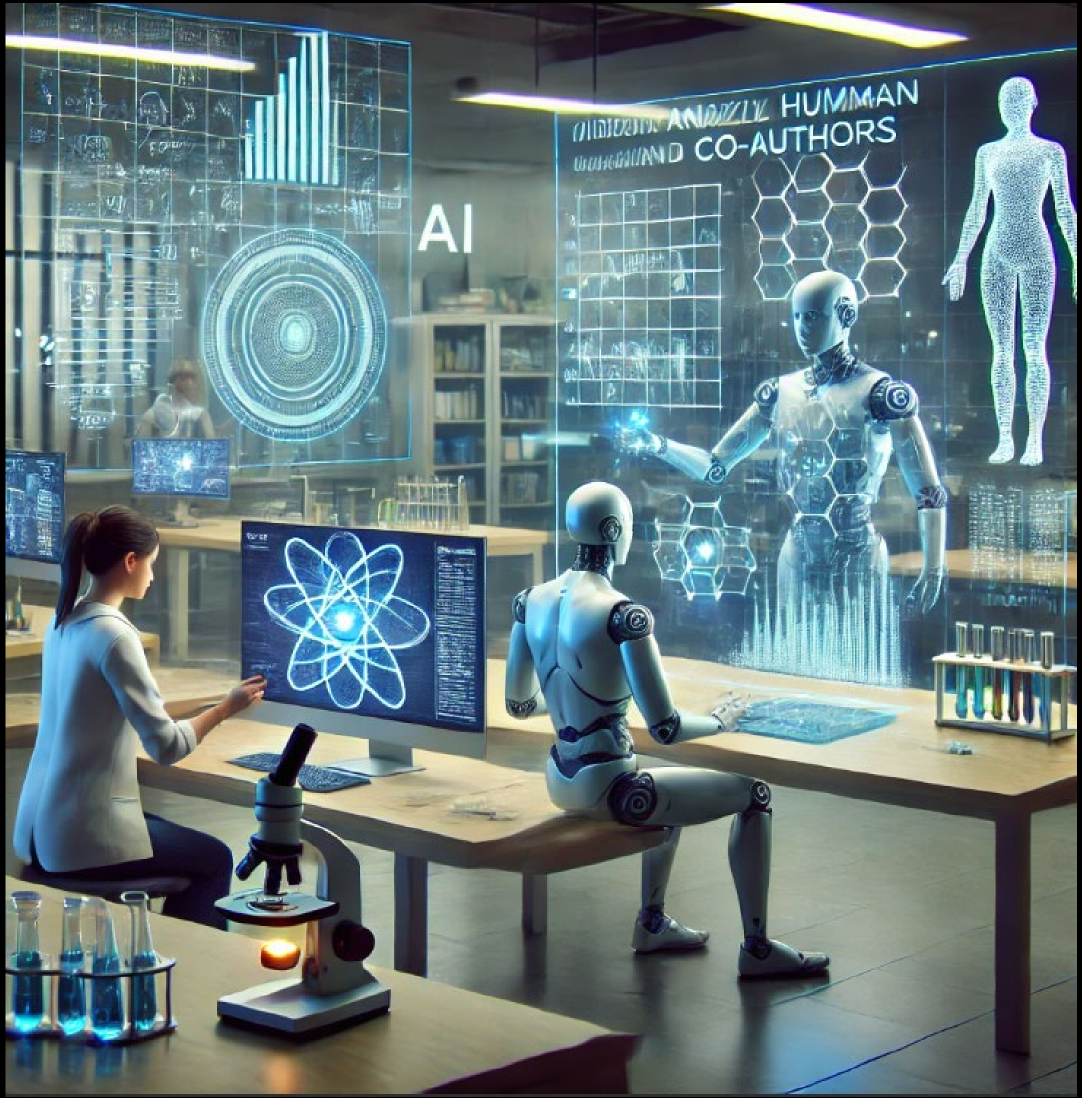
Inverse problems: infer new physics equations from sparse observations, new materials

3: Human-AI collaboration

PhD level AI agents can accelerate scientific discovery by humans (statistics!)

4: Accelerating Art creation

”AI Art” can co-exist with ”Human Art” not compete!



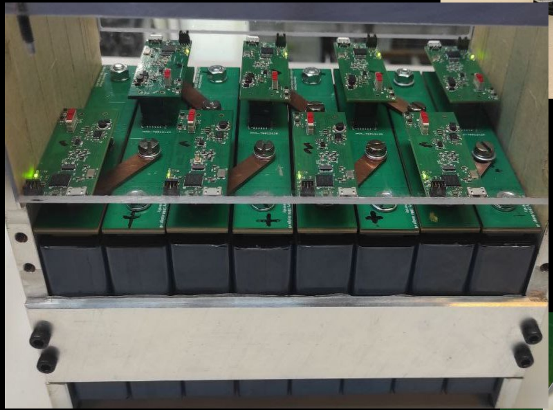
Misyris et al., 2020 | Nellikkath et al., 2023 | Li et al., 2024 | Karniadakis et al., 2021

CROSBAT AIX Resarch Group and Laboratory

Smart Battery Project (2021–2027)

- ► Funded by Villum Fonden, Denmark — 4 million EUR
- ► Team of ~10: Assistant Professors, Postdocs, PhD students
- ► Goal: Improve baterry perfomance with Power Electronics and AI
- ► Partnerships: MIT, Stanford, Imperial College London, Oxford Univ.


Main idea: independent control of cells!



Lab Infrastructure

- ► NVIDIA RTX 4050 Workstations (4 units)
- ► COMEMSO battery simulator (96 channels)
- ► Smart Battery Modules — own design |
- ► Blackwell B300 GPU cluster 1000x acceleration)

CROSBAT AIX – Scientific Impact – Top Publications

Improved diagnostic by active distrurbances:

Zheng,Y., Che,Y., Tao, S., Hu, X., **Teodorescu,R**,.- Unlocking rapid and scalable battery diagnostics through active perturbations, ***Nature Reviews Electrical Engineering*** *3, 203-204 (2026). (Impact: prove that active perturbations could elicit informative responses that improve diagnostic performance and provide mechanistic insights, unlocking rapid and interpretable diagnostics)*

Novel learning framework for deep-learning

Che,Y., Zheng,Y., Rhyu,J., Guo,J., Wang,S., **Teodorescu,R**, Braatz , R.D.- Mechanistically guided residual learning for battery state monitoring throughout life, ***Nature Communications*** *17, 855 (2026). (Impact: introduces mechanistic leading residual learners a hybrid framework combining: Real-time filtering (prior knowledge) as primary guidance, Mechanistic + statistical features as complementary inputs and Two novel pipelines: the correction model and compensation model)*

Advanced Energy Storage Management for Electric Vehicles:

Zhang, J., Che, Y., **Teodorescu, R.**, et al. (2025). "Energy storage management in electric vehicles." ***Nature Reviews Clean Technologies***, 1, 161–175.
(Impact: This comprehensive review in a leading Nature journal highlights Prof. Teodorescu's expertise in innovative battery management solutions, significantly influencing future EV energy storage research.)

AI-based Battery Degradation Prediction:

Cai, L., Yan, J., Jin, H., Meng, J., Peng, J., Wang, B., Liang, W., & **Teodorescu, R.** (2024). "A two-stage method with twin autoencoders for degradation trajectory prediction of lithium-ion batteries." ***Journal of Energy Chemistry***. *(Impact: Introduced novel AI methods enhancing prediction accuracy and reliability for battery lifetime management.)*

Health Prognostics for Lithium-ion Batteries:

Che, Y., Hu, X., Lin, X., Guo, J., & **Teodorescu, R.** (2023). "Health prognostics for lithium-ion batteries: mechanisms, methods, and prospects." ***Energy & Environmental Science***, 16(2), 338-371. (177 citations) *(Impact: Highly cited work providing a roadmap for battery health management, significantly influencing industry practices.)*

Thermal State Monitoring of Batteries:

Zheng, Y., Che, Y., Hu, X., Sui, X., Stroe, D.I., & **Teodorescu, R.** (2023). "Thermal state monitoring of lithium-ion batteries: Progress, challenges, and opportunities." ***Progress in Energy and Combustion Science***, 100, 101120. (94 citations)
(Impact: Established fundamental insights into battery thermal management, crucial for safe and efficient battery operation.)

Physics-informed Neural Networks for Battery Modeling:

Wang, J., Peng, Q., Meng, J., Liu, T., Peng, J., & **Teodorescu, R.** (2024). "A physics-informed neural network approach to parameter estimation of lithium-ion battery electrochemical model." ***Journal of Power Sources***, 621, 23527. *(Impact: Pioneered integration of physics-based modeling and machine learning, significantly improving battery model accuracy.)*

Novel Learning framework for mechanical strain estimation in batteries:

Peng, J., , Zhao, B., Meng, J., Cai, L., Liu, H-, Lin, M., Zhang, M., **Teodorescu, R.**. Boundary evolution constrained Seq2Seq framework for lithium-ion batteries strain state estimation." ***Journal of Energy Storage,*** *146, Elsevier, 2026. (Impact: Introduced novel AI methods enhancing prediction accuracy and reliability for battery lifetime management.)*

PIML for Battery Internal Temperature Estimation

Spatiotemporal distribution prediction — enabling Health Scan in AI-BMS

The Challenge

► Complex multiphysics: electrochemistry, thermal, mechanical strain

► Limited sensing: only surface temperature T_s and T_c measurable

► Core temperature T_core critical for safety — not directly accessible

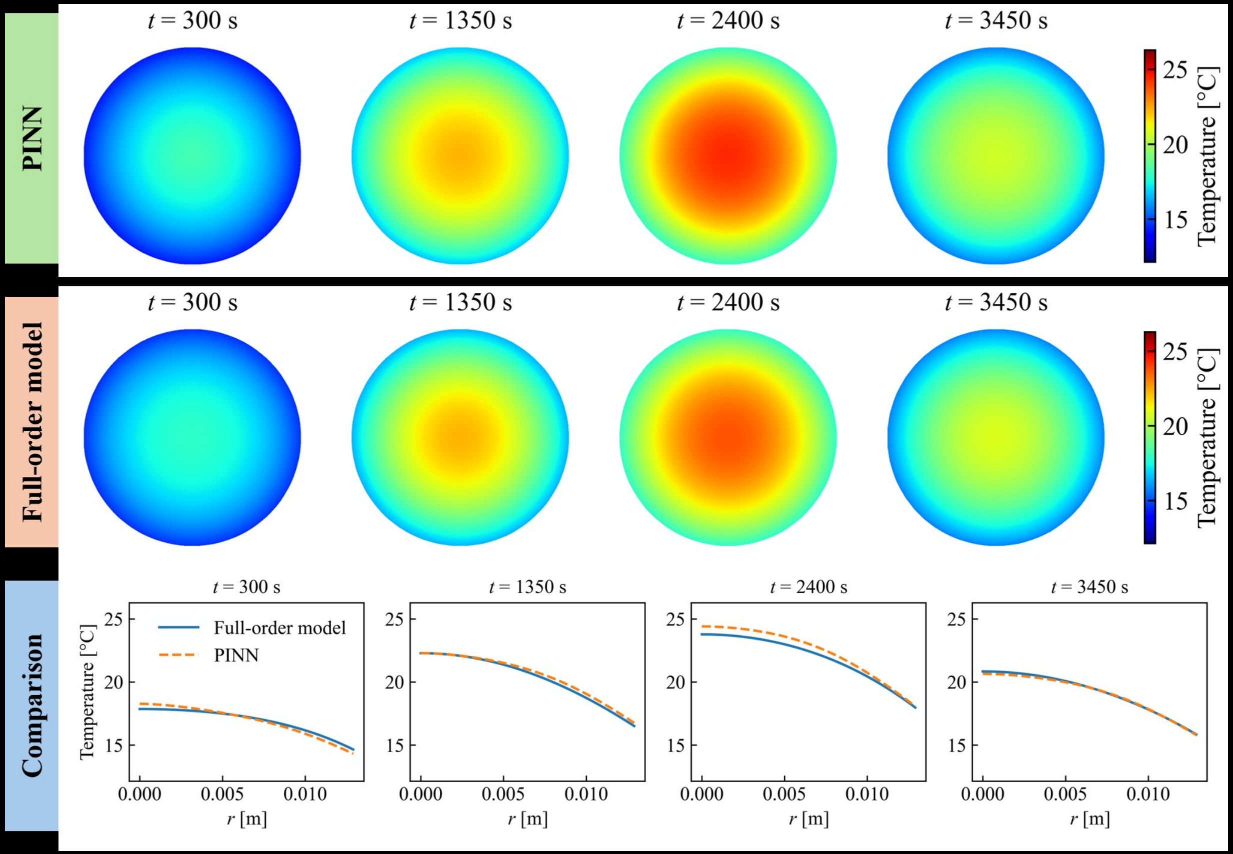
The PINN Solution

► Inputs: r, t, I^2, V, T_s, T_f — from standard BMS sensors

► Physics loss: cylindrical heat equation PDE + boundary conditions

► Output: full spatiotemporal temperature distribution T(r,t)

► Target: implementation in AI-BMS health scan module (NXP)



PINN vs Full-order model: internal temperature distribution at t = 300, 1350, 2400, 3450 s (Zheng et al., INTELEC 2025)

>15%
Accuracy gain vs. data-driven baseline

Real-time
Capable inference for BMS deployment

Zheng, Che, Hu & Teodorescu, INTELEC 2025 | Liu et al., 2024

PINN-Accelerated Single Particle Model (SPM)

Electrochemical surrogate for real-time BMS

The Method

- ▶ PINN replaces finite-difference solver for SPM PDEs
- ▶ Physics loss: solid-phase diffusion + Li-ion flux BCs
- ▶ Inputs: applied current I(t) → Output: SoC, voltage V(t), concentration c(r,t)
- ▶ Training: 500 synthetic charge/discharge cycles

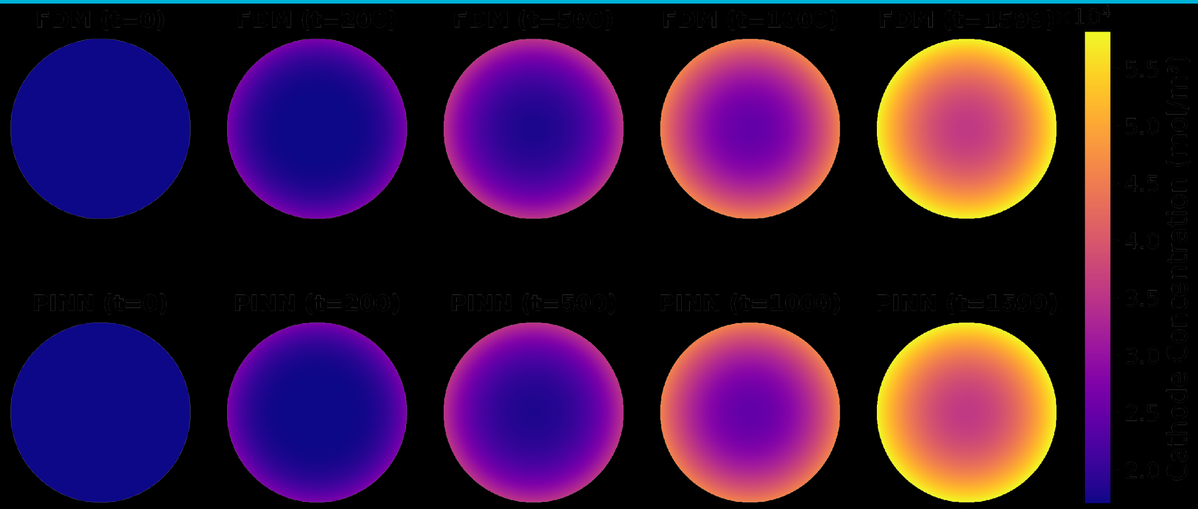
Results

- ▶ ~50× speedup vs FDM solver at equivalent accuracy
- ▶ SoC error < 1% across C-rates 0.5C to 3C
- ▶ Voltage prediction RMSE < 5 mV on unseen profiles
- ▶ Enables real-time electrochemical state estimation in BMS

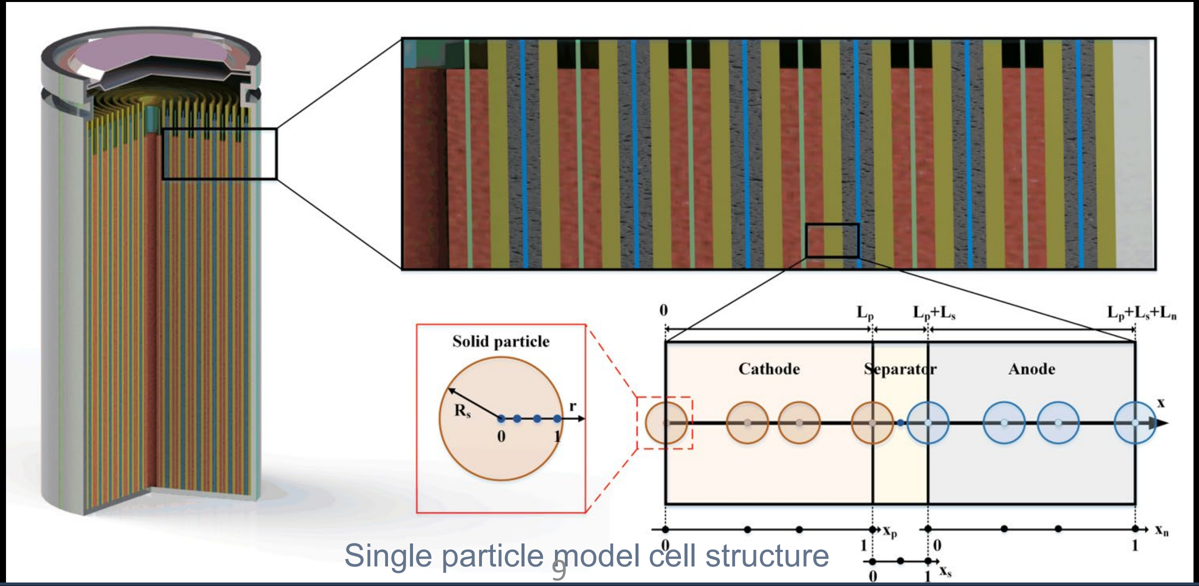
~50×
Speedup vs FDM

<1%
SoC error

<5mV
Voltage RMSE



Cathode concentration evolution: FDM vs PINN (Zheng et al., 2025)

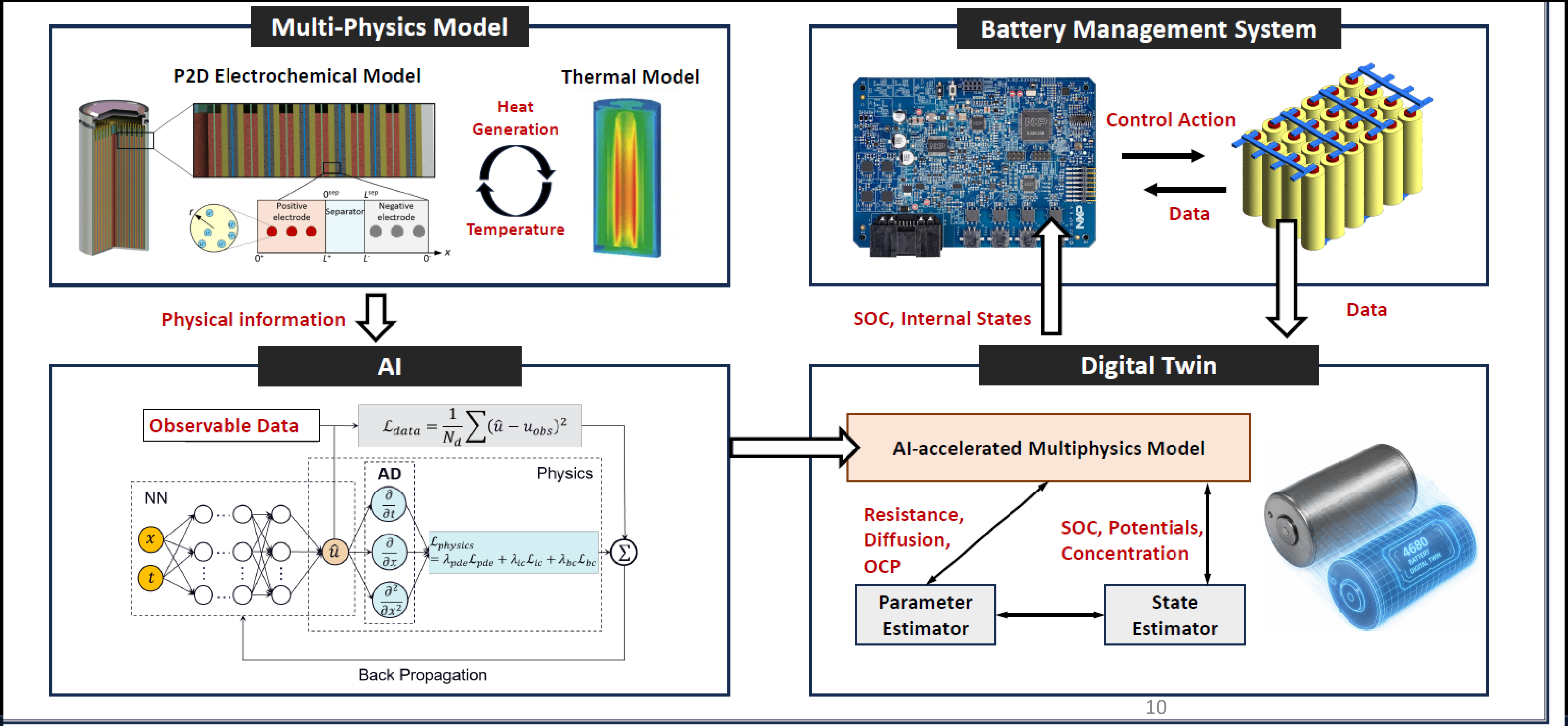


Single particle model cell structure

Zheng et al., 2025

PIML-base Digital Twin for future BMS of large packs

The complex physics models are executed online and support the optimal operation



Multi-Physics Model

P2D Electrochemical Model

Thermal Model

Heat Generation

Temperature

Physical information

AI

Observable Data

$$\mathcal{L}_{data} = \frac{1}{N_d}\sum(\hat{u} - u_{obs})^2$$

$$\mathcal{L}_{physics} = \lambda_{pde}\mathcal{L}_{pde} + \lambda_{ic}\mathcal{L}_{ic} + \lambda_{bc}\mathcal{L}_{bc}$$

Back Propagation

Battery Management System

Control Action

Data

SOC, Internal States

Data

Digital Twin

AI-accelerated Multiphysics Model

Resistance, Diffusion, OCP

SOC, Potentials, Concentration

Parameter Estimator

State Estimator

PIML Applications in Power Grid Systems

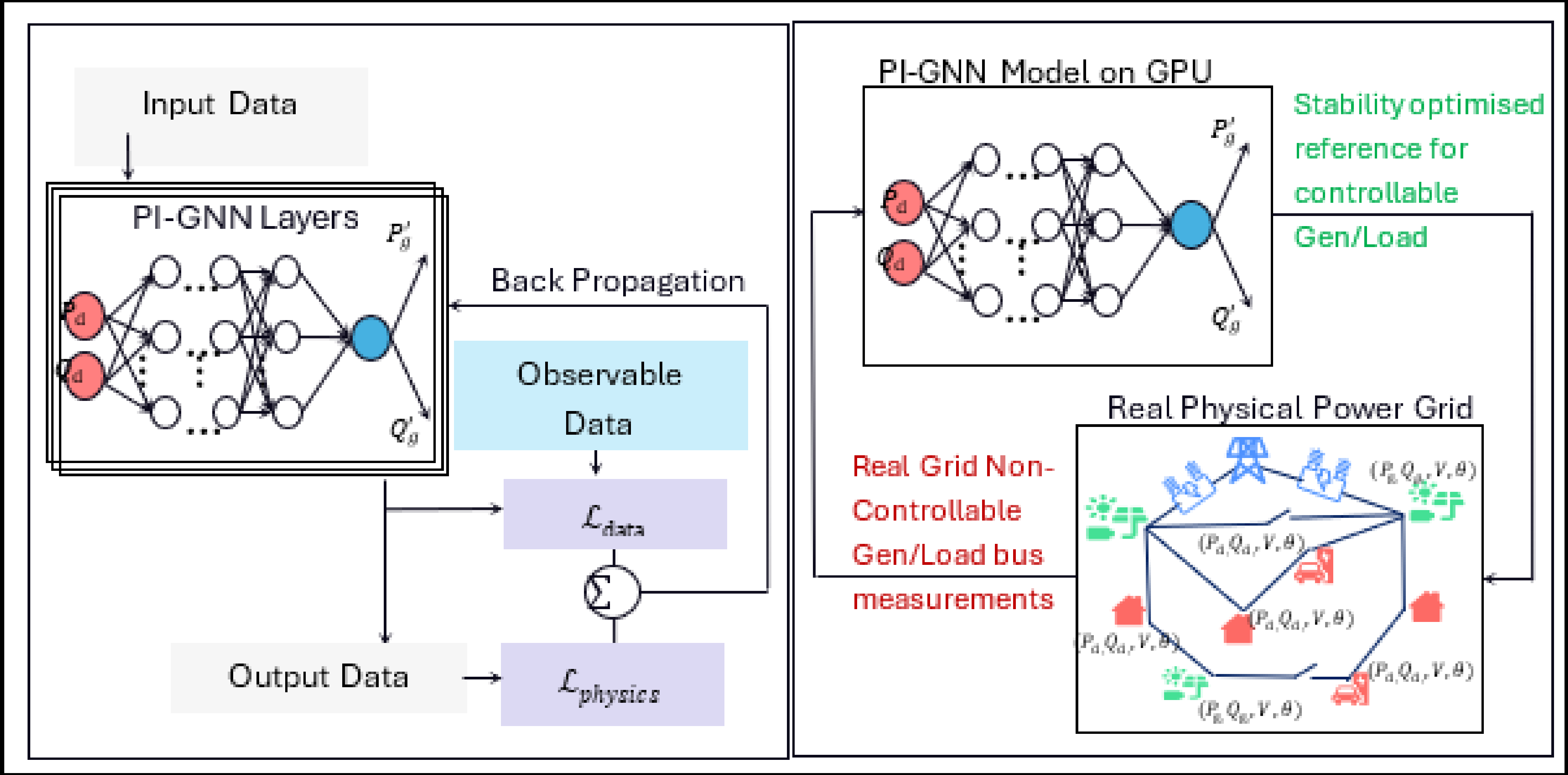
From real-time stability to optimal power flow

PINNSim — Real-Time Dynamics	87× faster rotor angle and frequency solutions vs ODE/DAE solvers. Enables real-time grid control and contingency analysis. (Misyris et al., 2020)
Transient Stability & PLL	Over 100× acceleration for PLL dynamics and region-of-attraction computation. Critical for inverter-dominated grids with high renewable penetration. (Nellikkath et al., 2023)
AC Optimal Power Flow (OPF)	PINN-based OPF with provable constraint satisfaction. Solves non-convex AC-OPF in real-time with physics guarantees. (Nellikkath & Chatzivasileiadis, 2022)
Parameter Estimation	Identify unknown grid parameters (line impedances, load models) from PMU data. Enables digital twin calibration for real power systems.
Frequency & Inertia Modelling	PINN models frequency dynamics under low-inertia conditions. Supports grid planning for high-renewable scenarios.

Misyris et al., 2020 | Nellikkath et al., 2023 | Nellikkath & Chatzivasileiadis, 2022

PIML for Power Grid Prediction and Optimization

Power Grid Is a Network. GNN can encode both topology and electrical distances (impedance)



Perspectives - PIML

1 **Dramatic Acceleration**

Order of magnitudes speedups enabling faster design and real-time control

2 **Discovery Tool**

Inverse problems: infer hidden parameters and laws from sparse observations

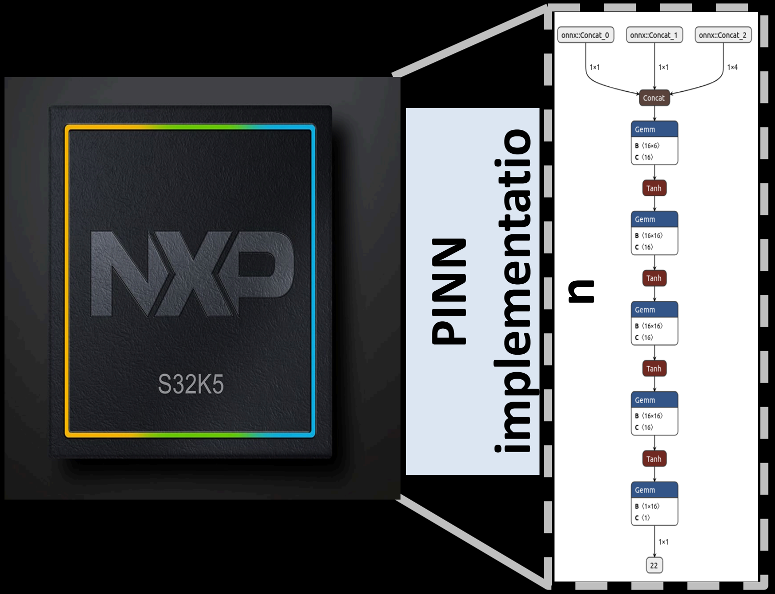
3 **Application to engineering**

Large Energy Models (SOA GPU)

RT controller (DT) of energy devices

The question is:
How will we use it?

Blackwell B300 for training/inference
Source: www.nvidia.com



AI-accelerated MCU/NPU
Source: www.nxp.com