Building Bespoke Physical Models from Scarce Observations

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Motivation

- The evolution of physical phenomena in nature is often modeled through partial differential equations.
- While differential equations are often known, its parameters are typically unknown or evolve with wear and tear.
- Real-life problems exhibit **Multiphysics** interactions, **nonlinear** dynamics, and **limited observations**.
- Conventional inverse-modeling via sparse identification or physics-informed machine learning struggles to train/learn.

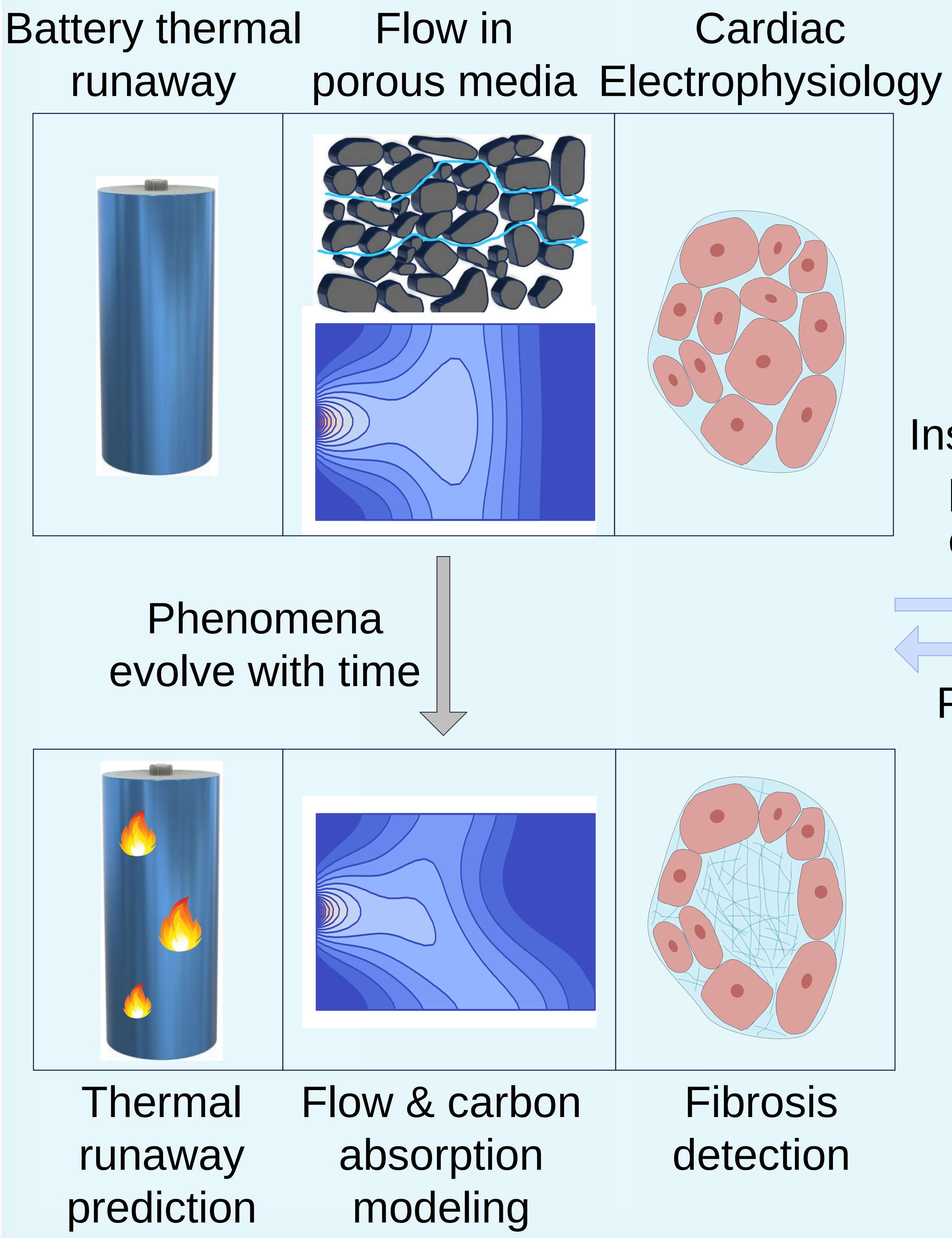
Highlights

- Proposed NeurO-Pest, a neural operator to estimate field parameters & build bespoke physical models.
- Scarce observations as low as 40 measurements.
- **100**× more accurate **dynamic response** predictions and **extrapolation** compared to PINN baselines.

Method

- The neural network predicts important field parameters controlling the dynamic response.
- PDEs are discretized into systems of ODEs, utilizing finite difference method (FDM).
- The resultant errors (loss) between observations and spatial-temporal predictions are minimized.

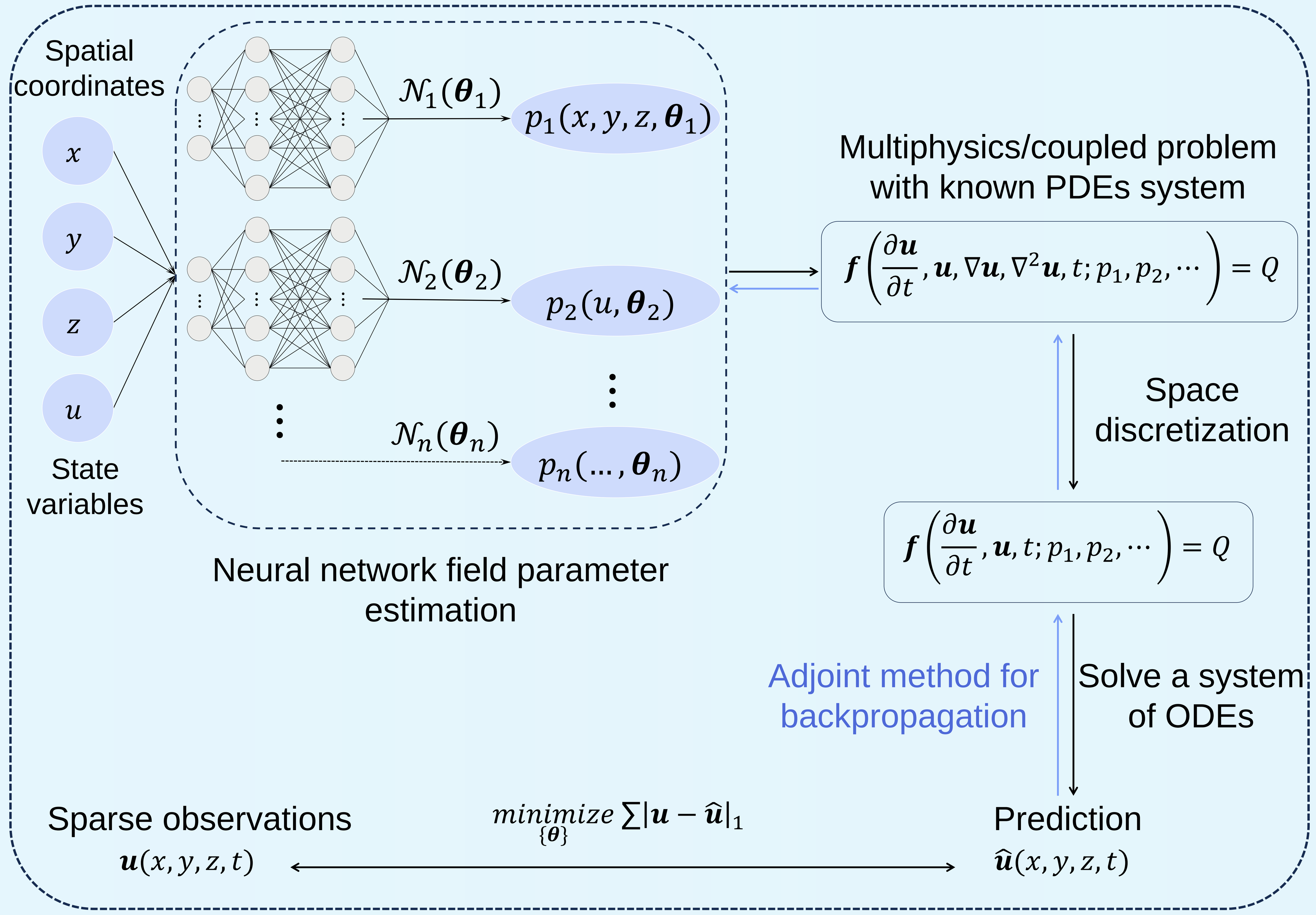
Physical Phenomena



Instantaneous parameter estimation

Predictions

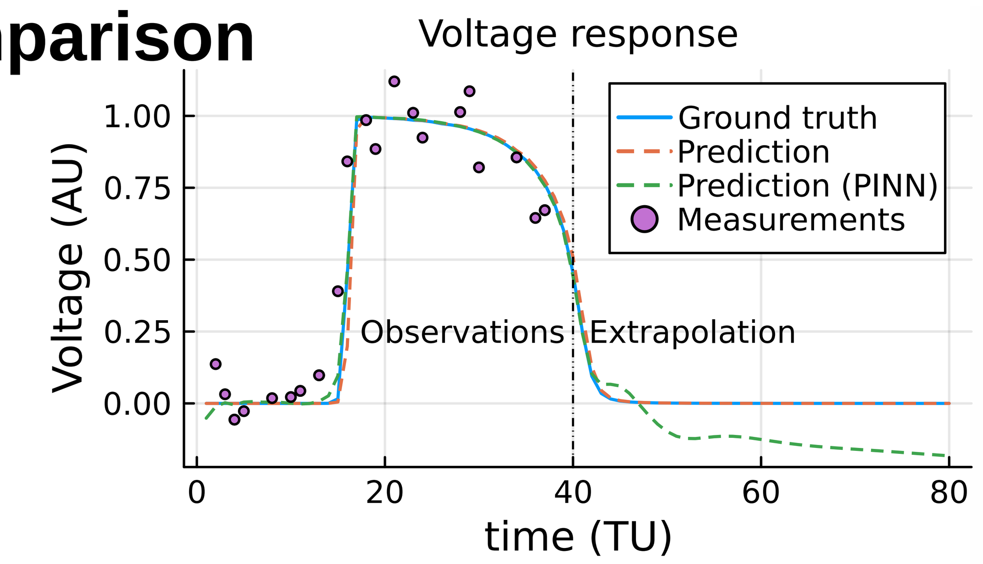
Bespoke Physics Model

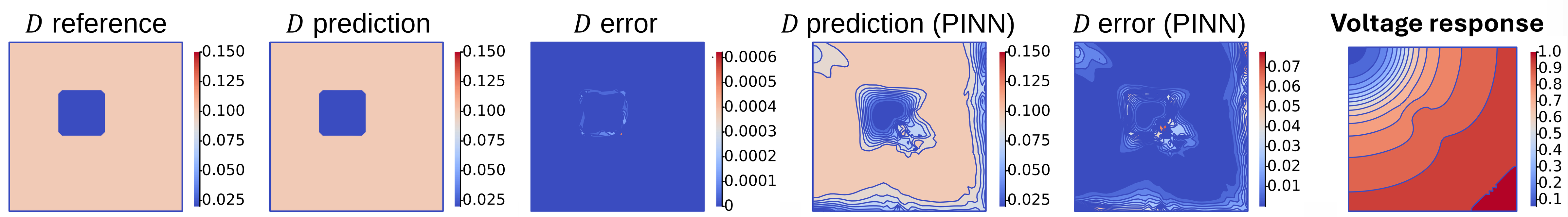


#1. Cardiac Electrophysiology & PINN Comparison

- **Fibrosis**, arrhythmias, and atrial fibrillation often present as variances in cardiac tissue properties.
- Electrical conductivity heterogeneity & electrical signal propagation are coupled in the **canine ventricular Aliev-Panfilov model**,

$$\frac{\partial V}{\partial t} = \nabla(D\nabla V) - k_0 V(V-a)(V-1) - VW$$
$$\frac{\partial W}{\partial t} = \varepsilon + \frac{\mu_1 W}{V + \mu_2}(-W - k_0 V(V-b-1))$$



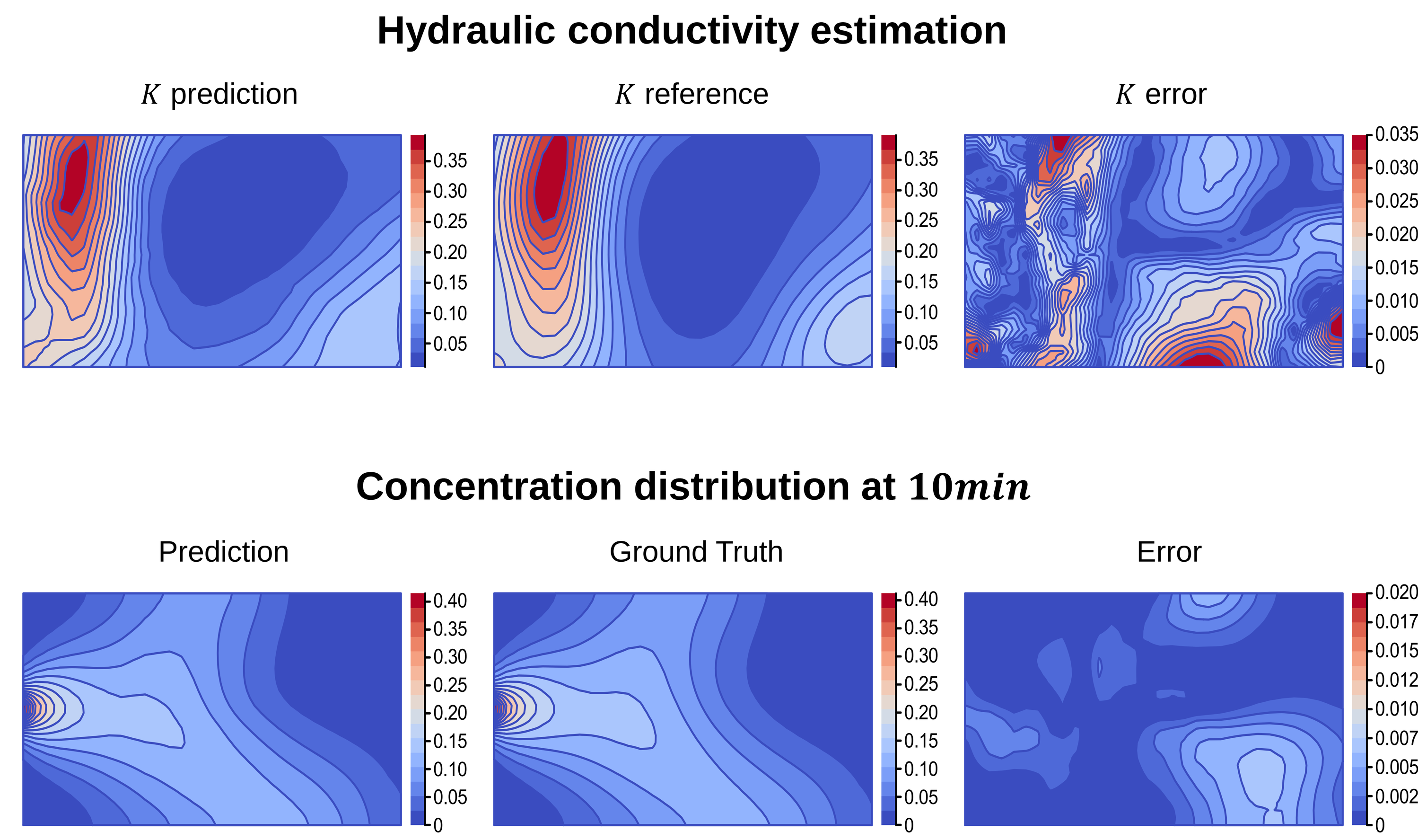


#3. Flow in Porous Media

- The particle transport is described by **advection-dispersion equation (ADE) & Darcy's law**.

$$\frac{\partial u}{\partial t} + \nabla \cdot [\boldsymbol{v}u] = \nabla \cdot [\boldsymbol{D}\nabla u]$$
$$\nabla \cdot [K\nabla h] = 0$$
$$\boldsymbol{v} = -K\nabla h/\phi$$

- Darcy's law characterizes fluid movement through porous media with hydraulic conductivity K and hydraulic head h.
- The ADE describes the concentration of particles based on the flow velocity v.

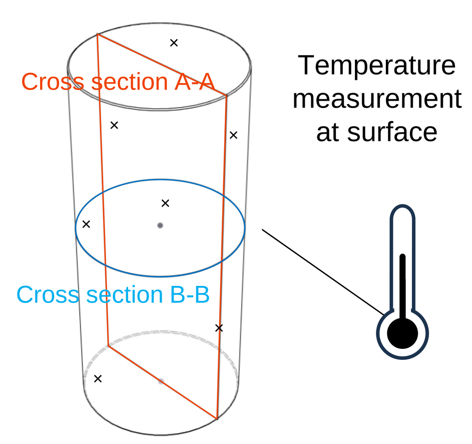


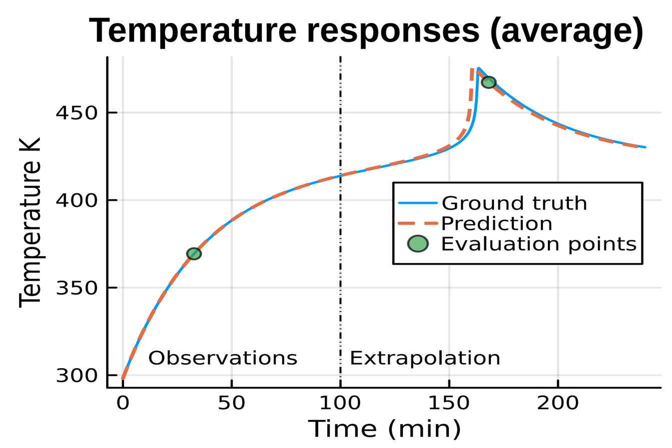
#2. Battery Thermal Runaway

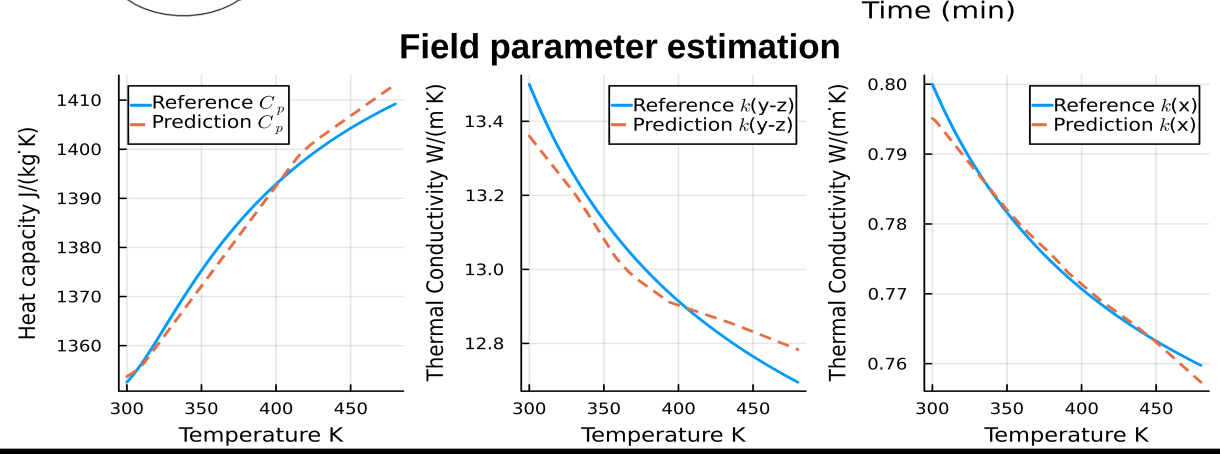
- Lithium-ion batteries in EVs possess high energy density, can easily overheat and cause fire.
- We consider two important phenomena: thermal (heat conduction) & chemical kinetics (Arrhenius law).

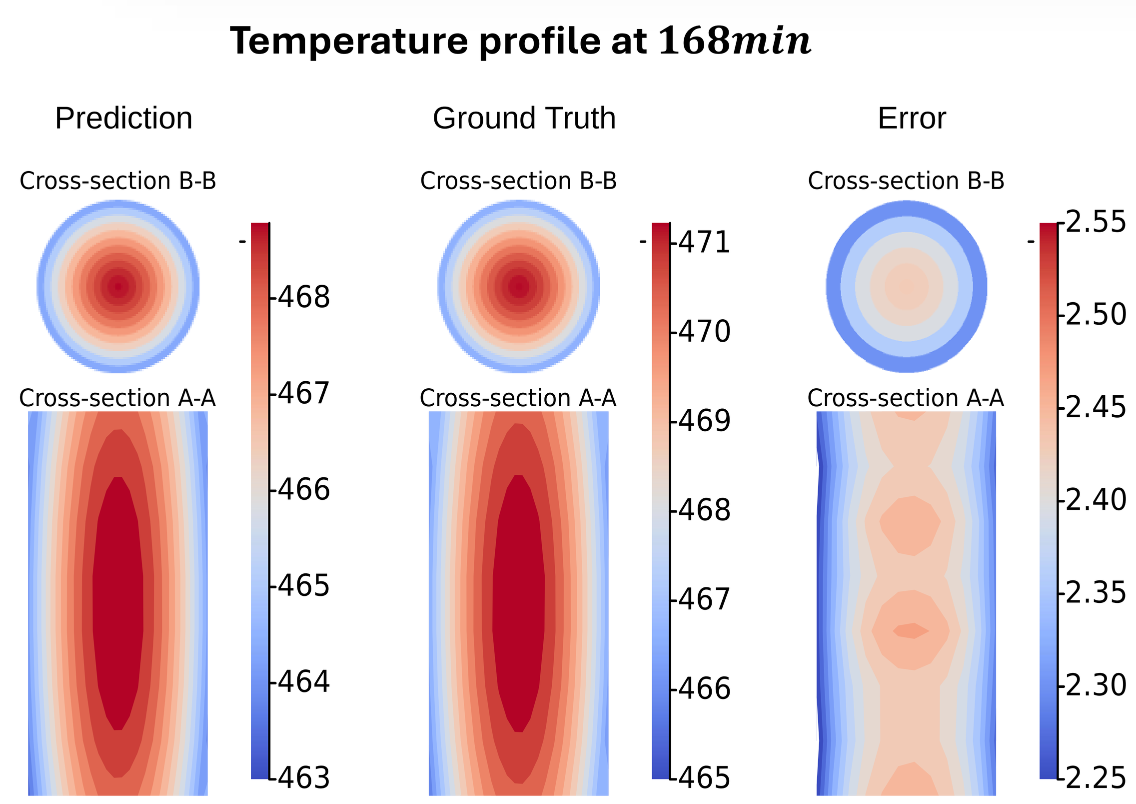
$$\rho C_p \frac{\partial T}{\partial t} = \nabla(k\nabla T) + \dot{Q}_{exo}$$
$$\dot{Q}_{exo} = HW\left(-\frac{\partial c}{\partial t}\right) = HWA\exp\left(-\frac{E}{R_c T}\right)c$$

- The **initial & boundary Conditions** are room temperature and heat flux with ambient temperature.
- **Only 32 temperature measurements** are taken.









Conclusion

- NeurO-Pest **learns unknown field parameters** via a learnable neural network & **builds bespoke physical models** within PDEs.
- **High accuracy**:
  1. Parameter estimation MAPE <1%
  2. Response prediction MAPE <1% (outperforms PINN by two orders of magnitude).
- **Superior extrapolation** performance (PINN disobey physics).
- **Less data:** <100 observations, much lower than PINN.
- The model is **versatile, flexible** and can be extended to **other PDEs**.