# Physics-Informed Operator Learning for Design-of-Experiments Applied to Lithium-Ion-Batteries

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## I. Introduction

**Motivation:**

- Difficulties in parameter identifiability of Lithium-Ion-Battery (LIB) surrogate models cause high expenses in time and cost for R&D and pose a challenge for on-board estimation of State-of-Health (SOH) or specific degradation modes.
- Design-of-Experiment (DoE) methodologies can improve parameter identifiability by maximizing the information provided by measurements, which can, e.g., be quantified via Fisher-Information-Matrices (FIMs).

**Goals:**

- Evaluate Physics-Informed Deep Operator Networks as parametrized surrogate models for varying current profiles and diffusivity parameters.
- Demonstrate their accuracy and inference speed in approximating FIMs.

## II. Methodology

**Single-Particle-Model (SPM):**

- Partial Differential Equation (PDE) to describe Li-concentration $c_j(r,t)$ in two spherically symmetric particles for anode (j=n) and cathode (j=p):

$$\frac{\partial c_j(r,t)}{\partial t} = \frac{D_j}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial c_j(r,t)}{\partial r}\right).$$

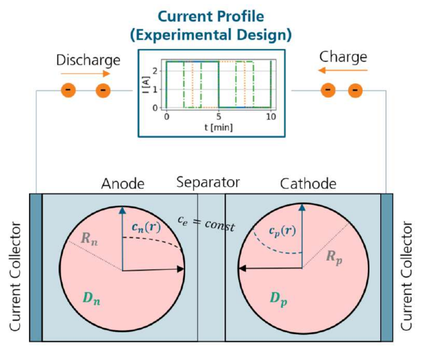


**Figure 1:** Single-Particle-Model.

- Initial (IC) and Boundary Conditions (BCs):

$$c_j(r,0) = c_j^0,\ \frac{\partial c_j(0,t)}{\partial r} = 0, \qquad \frac{\partial c_j(R_j,t)}{\partial r} = \pm\frac{I(t)}{AL_jFD_ja_j}.$$

- Voltage response via

$$V(t) = U_p^{\mathrm{OCP}}\left(c_p(R_p,t)\right) - U_n^{\mathrm{OCP}}(c_n(R_n,t)) + \eta_r(t).$$

- Open-circuit-potentials $U_j^{\mathrm{OCP}}$, overpotential $\eta_r$ and further parameters are assumed from a cylindrical 21700 cell (LGM50) characterized by Chen et al. [1].

**Physics-Informed Deep Operator Network (PI-DeepONet):**

- Data-free training via minimization of PDE, IC and BC residuals.
- Branch: Encoding discretized current profiles $I(t)$ describing three use cases: Constant current (CC), Gaussian Random Fields (GRF) and pulse profiles.
- Trunk: Encoding spatio-temporal domain $(r,t)$ and diffusivity domain $(D_n, D_p) \in \left[10^{-15}, 10^{-13}\right]^2$.

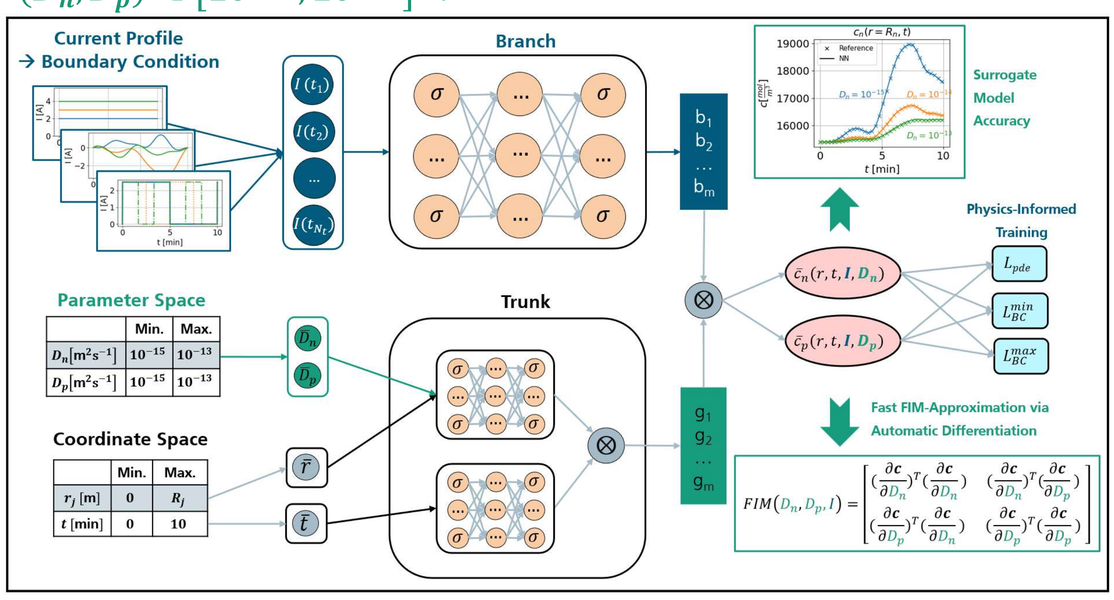


**Figure 2:** Parametrized PI-DeepONet for prediction of SPM solutions for varying current profiles (branch) and diffusivities (trunk).

**DoE Framework:**

- The FIM quantifies the information provided by a given experimental design $I(t)$, e.g., for identifying parameters $(D_n, D_p)$ from the model response

$$\boldsymbol{c} = \left(c_n\left(R_n, t^k, D_n, I\right), c_p\left(R_p, t^k, D_p, I\right)\right), \qquad k = 0, \dots, 600,$$

$$\mathbf{FIM}\left(D_n, D_p, I\right) = \begin{bmatrix} \left(\frac{\partial \boldsymbol{c}}{\partial D_n}\right)^T\left(\frac{\partial \boldsymbol{c}}{\partial D_n}\right) & \left(\frac{\partial \boldsymbol{c}}{\partial D_n}\right)^T\left(\frac{\partial \boldsymbol{c}}{\partial D_p}\right) \\ \left(\frac{\partial \boldsymbol{c}}{\partial D_p}\right)^T\left(\frac{\partial \boldsymbol{c}}{\partial D_n}\right) & \left(\frac{\partial \boldsymbol{c}}{\partial D_p}\right)^T\left(\frac{\partial \boldsymbol{c}}{\partial D_p}\right) \end{bmatrix}.$$

- The scalar "D-optimality" can be maximized for optimal experimental design:

$$\mathcal{D}^{\mathrm{opt}}\left(D_n, D_p, I\right) = \log\left(\det\left(\mathbf{FIM}\left(D_n, D_p, I\right)\right)\right).$$

## III. Results

**Surrogate model accuracy:**

- Comparison with reference solution from *PyBaMM* [2] via Normalized-Mean-Absolute-Percentage-Error at particle surfaces and Root-Mean-Squared-Error on the resulting voltage response ($N_t = 101$):

$$\mathrm{NMAPE}^{\mathrm{surf}} = \frac{1}{2}\sum_{j\in\{n,p\}}\frac{1}{N_t}\sum_{i=0}^{N_t}\frac{\left|c_j^{\mathrm{NN}}(R_j,t_i) - c_j^{\mathrm{ref}}(R_j,t_i)\right|}{\max\left(c_j^{\mathrm{ref}}(R_j,t)\right) - \min\left(c_j^{\mathrm{ref}}(R_j,t)\right)} \cdot 100\%,$$

$$\mathrm{RMSE} = \sqrt{\frac{1}{N_t}\sum_{i=0}^{N_t}\left|V(c^{\mathrm{NN}},t_i) - V(c^{\mathrm{ref}},t_i)\right|^2}.$$

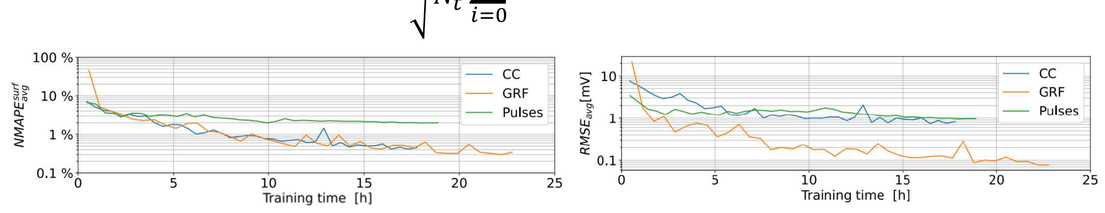


**Figure 3.** Accuracy evolution during training of PI-DeepONets for different use cases averaged over multiple current profiles I(t) in each use case, cf. Fig. 2 – top left. Training times are measured on a NVIDIA A100 GPU.

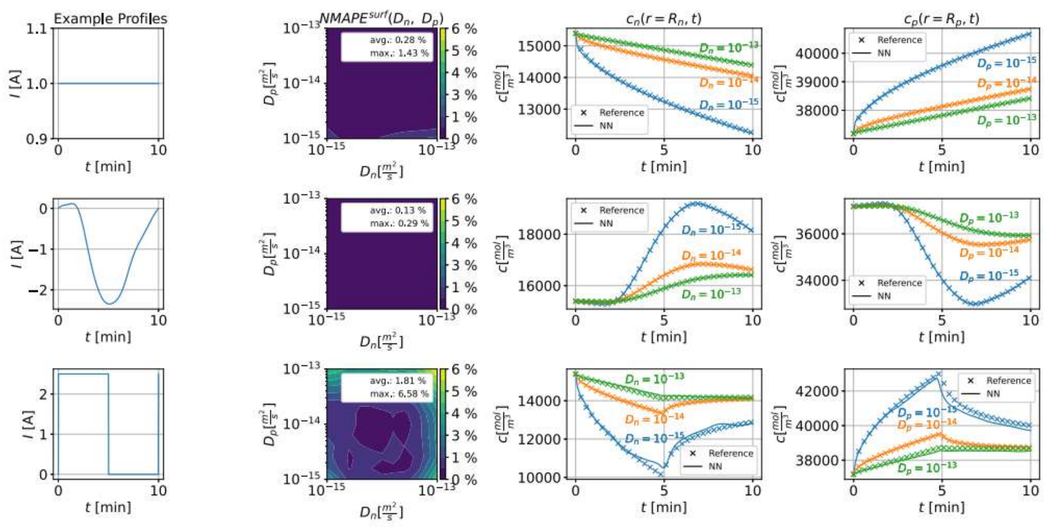


**Figure 4.** Surrogate model accuracy at particle surfaces for three exemplary profiles and varying diffusivities $(D_n, D_p) \in \{10^{-15}, 10^{-14}, 10^{-13}\}$.

**Accuracy for DoE based on FIM-Analysis:**

- D-optimalities are approximated accurately and more efficiently via AD on the trained PI-DeepONet compared to the reference based on *PyBaMM* [2]:

a) local $\mathcal{D}^{\mathrm{opt}}$: $(D_n^*, D_p^*) = \left(3.3 \cdot 10^{-14}, 4.0 \cdot 10^{-15}\right)\frac{m^2}{s}$

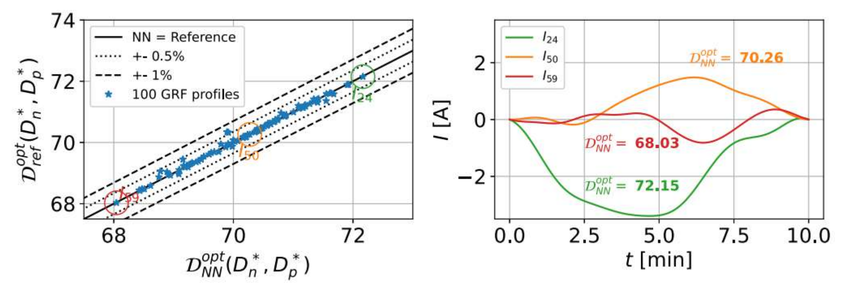


**Figure 5:** Local D-optimalities for 100 randomly generated GRF profiles (left) and three exemplary design candidates (right).

b) global $\mathcal{D}^{\mathrm{opt}}$: $(D_n, D_p) \in \left[10^{-15}, 10^{-13}\right]^2\ \frac{m^2}{s}$

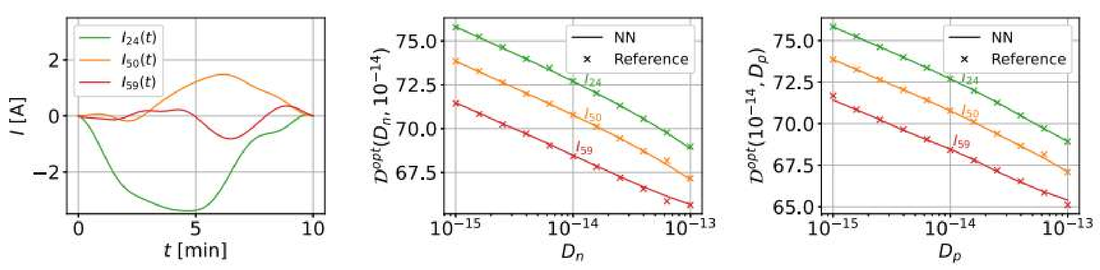


**Figure 6:** Comparison of global D-Optimalities throughout the parameter space.

**Conclusion:**

Parametrized PI-DeepONets can be accurate and fast surrogate models with inference times in the order of milliseconds and offer further potential for DoE methodologies based on Fisher-Information. See [3] for more insights and implementation details.

## IV. Outlook

- Integration of more realistic, high-frequency current profiles, variation of further (aging) parameters and a voltage-based FIM approximation.
- Demonstration of improved parameter and state estimation procedures based on PI-DeepONets and realistic application-specific voltage data.

**References:**

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[3] Brendel, P., Mele, I., Rosskopf, A., Katrašnik, T., & Lorentz, V. (2025). Parametrized physics-informed deep operator networks for Design of Experiments applied to Lithium-Ion-Battery cells. *Journal of Energy Storage*, 128, 117055, https://doi.org/10.1016/j.est.2025.117055.

**Acknowledgements:**

Co-funded by the European Union under grant agreement N° 101103755 and by UKRI under grant agreement No. 10078013, respectively. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Climate, Infrastructure and Environment Executive Agency (CINEA). Neither the European Union nor CINEA can be held responsible for them.

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Co-funded by the European Union