Computational battery modelling with differentiable quantum circuits

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Abstract

In this work we demonstrate the use of a **hybrid quantum-classical algorithm** for solving **systems of Partial Differential Equations** relevant to the **battery simulation** problem. We show that the algorithm is able to achieve **accurate solutions** and we study the **curvature** of the loss landscape of the problem via the **Hessian eigenspectrum**, also performing a comparison of different **optimizers**.

Introduction

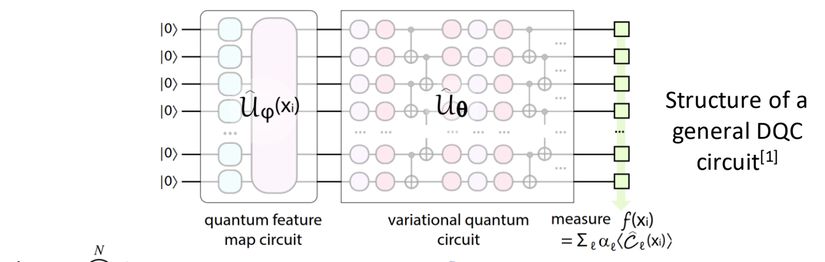
- Many scientific problems can be formulated as systems of **Partial Differential Equations** (PDEs). **Quantum Scientific Machine Learning** (QSciML) is an emerging field offering an alternative approach to conventional mesh-based PDE solvers. **Differentiable Quantum Circuits**[1] (DQCs) is a QSciML algorithm which draws inspiration from **Physics-Informed Neural Networks** (PINNs), encoding the solution to the PDE system in a Quantum Neural Network (QNN) instead of a classical NN. DQC offers the potential for a **spectral basis-set size** that can **scale exponentially** with the number of qubits, enabling accurate fitting of solutions even in higher-dimensional problems, while remaining NISQ-compatible.
- We benchmark the DQC algorithm with a **relevant industrial use case**, namely solving a standard computational battery model known as the **Single Particle Model**[2]. We show that DQC is able to obtain **accurate solutions** with a relatively small QNN, and we compare it with a classical NN and the Finite Volume Method. The **local curvature** of the loss landscape around the minima is studied via the lens of the **Hessian eigenspectrum** and the performance of different optimizers is compared, showing that **Quantum Natural Gradient**-based optimizers[3] that take in account the geometry of the parameter space perform very well compared to conventional optimizers.

Differentiable Quantum Circuits

DQC is a **hybrid quantum-classical algorithm** that can be used to **solve differential equations**. It prepares trial solutions encoded in the **expectation value** of an observable in the QNN, which is trained to minimize a loss function with a classical optimizer. Its main components are:

- **The feature map (FM) encoding.** Input data is encoded in the quantum circuit via a **non-linear quantum feature map,** avoiding amplitude encoding. The FM derivatives can be exactly calculated through **automatic differentiation**, circumventing approximation errors of numerical differentiation.
- **The Quantum Neural Network (QNN)** containing the trainable parameters. The solution is encoded as the **expectation value of an observable.**
- **The loss function** that measures the quality of the solution generated by the quantum circuit. When solving PDE systems, the loss function measures how well the PDE, and boundary conditions terms are satisfied.

In this work we employ a **4-qubit** quantum circuit w. Data is encoded with a **Chebyshev** feature map and the variational circuit consists of 4 layers of a **Hardware-Efficient Ansatz** (HEA) which is trained with the **ADAM** optimizer. We use the **average Z-magnetization** of the qubits as the cost operator.



Structure of a general DQC circuit[1]

Our specific choices for the feature map and the QNN architecture in this work

Computational battery modelling

- We solve the **Single Particle Model**[2] (SPM) for a **Lithium-ion** (Li-ion) battery. The SPM is a simple full-battery model that captures the basic physics of the battery.
- DQC achieves slightly better performance than the classical PINN with approximately 1/3 of the trainable parameters (48 in DQC vs 141 in classical PINN).

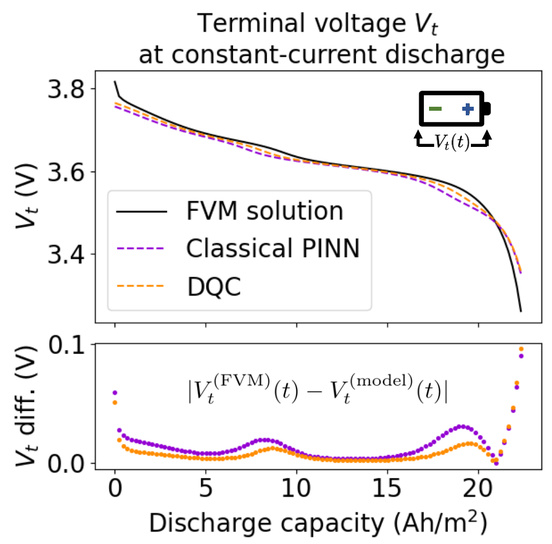
Single Particle Model PDE system

$$\mathcal{C}_{\mathrm{k}} \frac{\partial c_{\mathrm{s,k}}}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial c_{\mathrm{s,k}}}{\partial r} \right)$$

$$\left. \frac{\partial c_{\mathrm{s,k}}}{\partial r_{\mathrm{k}}} \right|_{r_{\mathrm{k}}=0} = 0,$$

$$- \left. \frac{a_{\mathrm{k}} \gamma_{\mathrm{k}}}{\mathcal{C}_{\mathrm{k}}} \frac{\partial c_{\mathrm{s,k}}}{\partial r_{\mathrm{k}}} \right|_{r_{\mathrm{k}}=1} = \begin{cases} \frac{I}{L_{\mathrm{n}}}, & \mathrm{k} = \mathrm{n}, \\ -\frac{I}{L_{\mathrm{p}}}, & \mathrm{k} = \mathrm{p}, \end{cases}$$

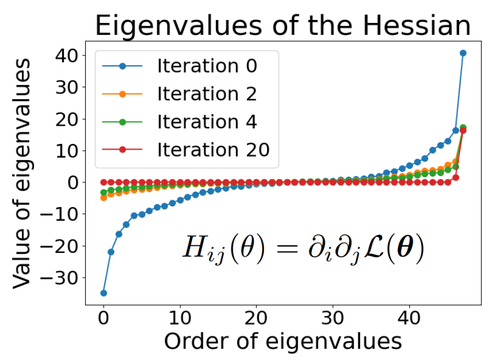
$$c_{\mathrm{s,k}}(r_{\mathrm{k}}, 0) = c_{\mathrm{s,k},0}$$



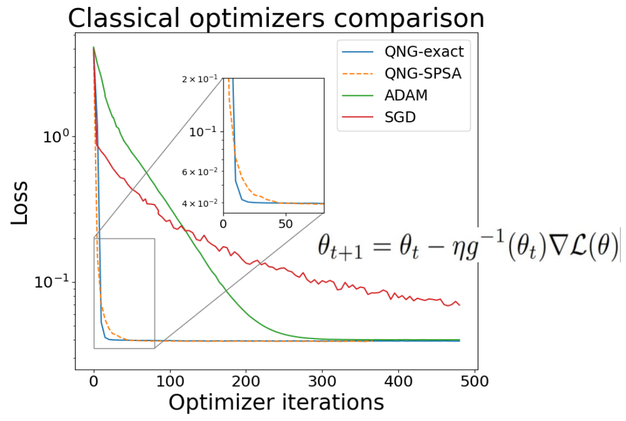
Discharge-curve at constant-current with a C-rate of 1.5C. Voltage difference is calculated with respect to the FVM solution.

Loss landscape and trainability

- The **loss landscape** of Quantum Neural Networks has been shown to be **highly non-convex**[4] in supervised learning tasks, but little is known for the Physics-Informed QML paradigm.
- We use the **Hessian eigenspectrum** to learn about the local curvature of the loss landscape. We observe that close to the minimum, most of the eigenvalues are zero with a few positive outliers, indicating that the minimum is a flat pool with a **few steep directions**.
- We find that for DQC, standard gradient-descent (GD) methods converge very slowly compared to the **Quantum Natural Gradient** (QNG), which takes into account the geometry of the parameter space. We also test a **SPSA approximation**[3] to the QNG only requiring a ***O*(1) overhead in circuit evaluations** compared to GD.



Eigenvalues of the Hessian $H_{ij}(\theta)$ during training with the QNG optimizer, calculated as the second derivative of the loss $\mathcal{L}(\theta)$. Convergence is achieved after ~20 iterations.



Convergence comparison among different optimizers. QNG updates the parameters through the inverse of the Quantum Fisher Information g^{-1}.

Outlook

- Move towards **more complex battery models** such as the Doyler-Fuller-Newmann[1] (DFN) model, including physical phenomena such as the electrolyte dynamics or thermal and ageing processes.
- More detailed study of the **algorithmic components** of DQC and their relation to the trainability of the DQC algorithm, such as different feature map encodings or alternative quantum models (e.g. quantum kernel methods).
- Adaptation of the quantum circuits to a digital-analog approach.

References

[1] *Phys. Rev. A* ***103****, 052416*
[2] *J. Electrochem. Soc.* ***166*** *A3693*
[3] *Quantum 5, 567 (2021)*
[4] *Quantum Sci. Technol. 6 025011*

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