Unlocking Insights in Battery Research with Digital Twin-driven Data Augmentation

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Keywords: Battery degradation, Thermo-elasticity, Inverse problem, Finite Element Method, PDE-constrained optimization, Image registration.

1 Introduction

Increasing both the amount of charge a battery can hold and the total number of times a battery can be charged are two of the key challenges that the battery sector is facing [1]. Among the many strategies to achieve this goal, dynamic experiments with X-ray tomography or Transmission Electron Microscopy (TEM) are of particular interest. Both techniques enable to non-destructively observe the ongoing processes in the interior of a battery cell while it degrades during successive charging and discharging cycles and to distil lessons to iteratively improve the design [2]. However, while they do provide morphological -and sometimes electrochemical- information, other quantities of interest, such as the internal pressure and temperature distribution, are invisible. The current study tackles this challenge by creating a digital twin of the cell to provide the missing quantities. As will be shown, the proposed methodology is generic and can be used in a wide range of applications to fill in missing data.

2 Methodology

The method was developed and tested based on a synthetic dataset mimicking the temporal evolution of a symmetric Li-Li solid-state battery cell. When such cell is charging or discharging, the chemical reactions that take place are respectively endothermic or exothermic. The local temperature variation associated with the absorption or generation of heat causes the cell to locally deform, and these geometric variations can be observed using X-ray tomography or TEM.

For testing purposes, we have generated a number of synthetic datasets that differ in the amount of heat that is locally absorbed or released, and we varied the image resolution and the image quality. In the current study we focus on a two-dimensional cross section through the cell and its evolution over time, yet the method can also be used to investigate the full cell in three-dimensions. The entire workflow is developed in Python.

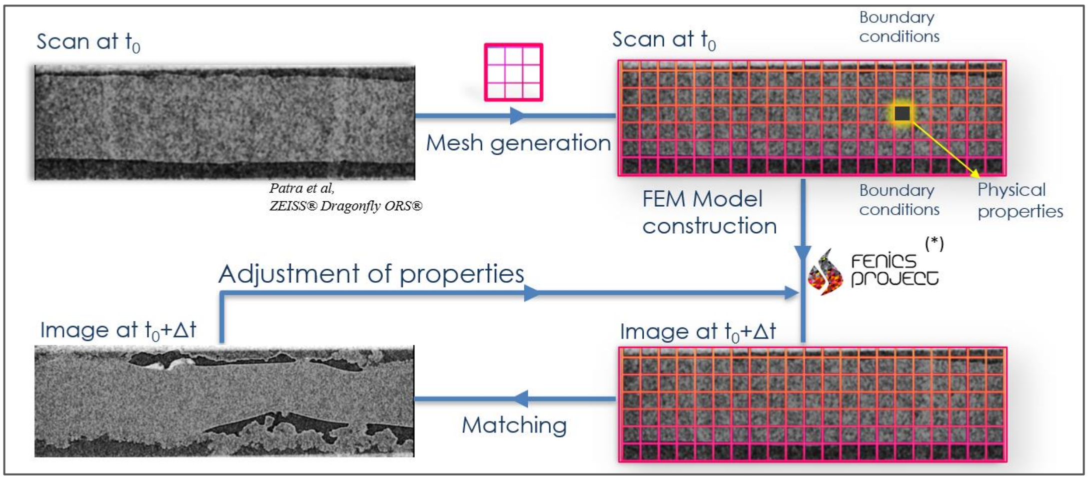

Figure 1: Schematic of the developed workflow

The first image of the sequence is automatically segmented by means of grey-tone thresholding into three phases, i.e., the electrode, the electrolyte and the surrounding air. Next, a finite element grid is constructed on top of it and physical properties are assigned to each element, corresponding to the underlying material phases. At the macroscale, the thermal deformation of the cell can be regarded as a thermo-elasticity problem, whereby an unknown heat source or sink mimics the energy exchange by the electrochemical processes during battery cycling. Complemented with initial and boundary conditions, the governing equations are solved using *FEniCS* [3], a software package that enables scientific models to be efficiently translated into a finite element code, and yield the displacement and temperature fields inside the battery cell, as well as their corresponding evolution over time. The resulting displacement field is used to warp the initial image. The latter is then compared to the next image in the sequence and the difference is iteratively minimised by adjusting the unknown heat source. The iterative optimisation procedure relies on the COBYLA-algorithm[4][5], which was found to offer consistent performance in a wide range of test cases. Once the differences between the warped and the real image are smaller than a user-defined tolerance, the algorithm moves to the next time point. The final result consists of a series of displacement fields consistent with the input image sequence, as well as temperature and heat source fields that are compatible with both the displacement field and the test conditions (i.e. initial and boundary conditions).

3 Results

The model was thoroughly tested to evaluate its robustness in the case of low-quality images i.e. exhibiting a low signal-to-noise ratio. Furthermore, we studied the impact of scale and resolution changes in the image. This evaluation allowed us to have a better insight into the robustness of the model as well as its limitations. In the case of low-resolution images, results revealed that the model showed accurate predictions (<10% error) over a range of heat source intensities between 500 and 20 000 W/kg. At higher image resolution, this reliable range extends towards smaller heat source intensities. The performance was found to degrade with increasing noise level, yet even under high noise levels (4x higher than typical tomography datasets) the predicted values do not deviate more than 20% from reality. Overall, these results demonstrate the robustness of the model and highlight the importance of both image resolution and image quality in its implementation.

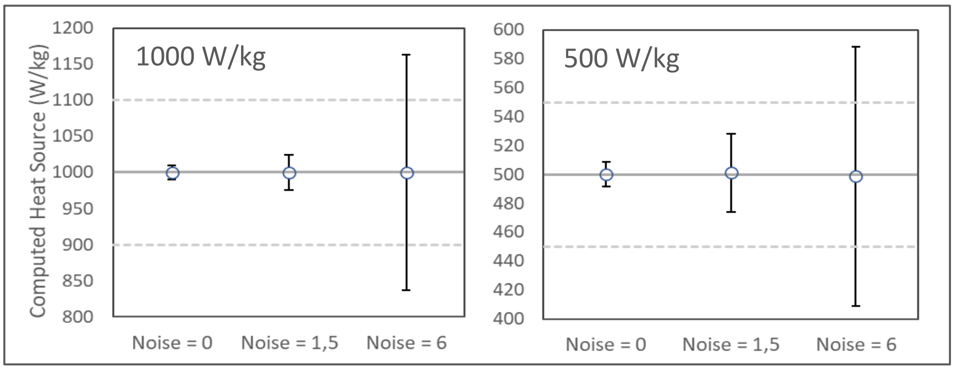

Figure 2: Sensitivity to image noise for two different heat sources.
The error bars span the range of predictions over time.

4 Conclusions and perspectives

The results show that the proposed methodology enables augmenting experimental datasets with numerical data. The proposed approach implicitly ensures that the obtained quantities respect the governing equations as well as the initial and boundary conditions. The method was tested for a wide range of heat sources, both constant and variable over time, for different image resolutions and for various image noise levels. As long as the deformations were sufficiently large to be detected at the image resolution, and sufficiently small to remain contained within the borders of the image, accurate results were obtained. Current work focuses on the application of the method on real datasets.

Acknowledgements: This research was financially supported by the European Doctoral program on ENergy and Environment (EDENE) under the European Union's Horizon 2020 research and innovation program (grant agreement No 945416). The authors also thank TotalEnergies for financial support.

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