Reduced Order Modelling for Lithium Sulfur Batteries

Modelling Optimization Using Numerical Techniques

Dharshannan Sugunan, Michael Cornish, Monica Marinescu

Abstract

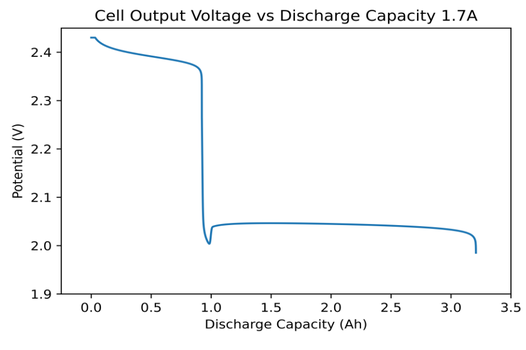
Lithium-sulfur (Li-S) batteries offer promise for advanced energy storage due to their high theoretical energy density and cost-effectiveness. Yet, practical implementation faces challenges like polysulfide shuttle effects, capacity fade, and low Coulombic efficiency. Numerical modeling is essential to understand and tackle these challenges to maximize the potential of Li-S batteries.

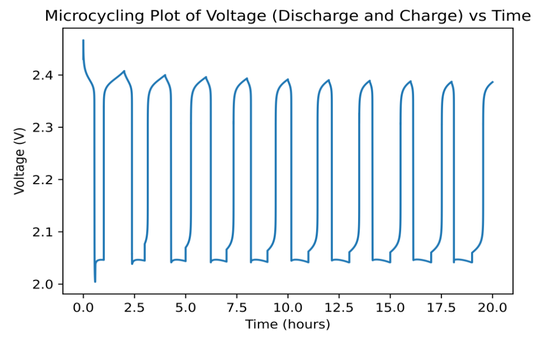
Many researchers in the battery and energy storage field use PyBaMM, an open-source Python library employing the Casadi solver for DAE simulations. However, this DAE solver exhibits limited stability, particularly with the most recent Li-S models. This may lead some researchers to favor data-driven models trained with machine learning due to their numerical robustness, even though they lack the valuable insights provided by physics-based models.

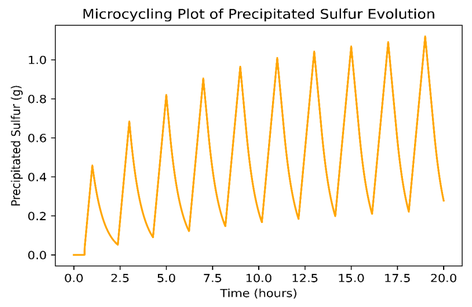
In this research endeavor, we introduce an alternative model solver optimized through numerical techniques including Parameter Backtracking, Adaptive Step Sizes, and Line Search (for Step-Size Optimization). The outcomes of this novel solver offer significant insights into both model stability and the solver's performance.

Simulation Testing 1

- The solver is initially tested using an older formulation of a 0 dimensional model (derived using the Nernst and Butler Volmer electro-chemical equations) as proposed in [1].



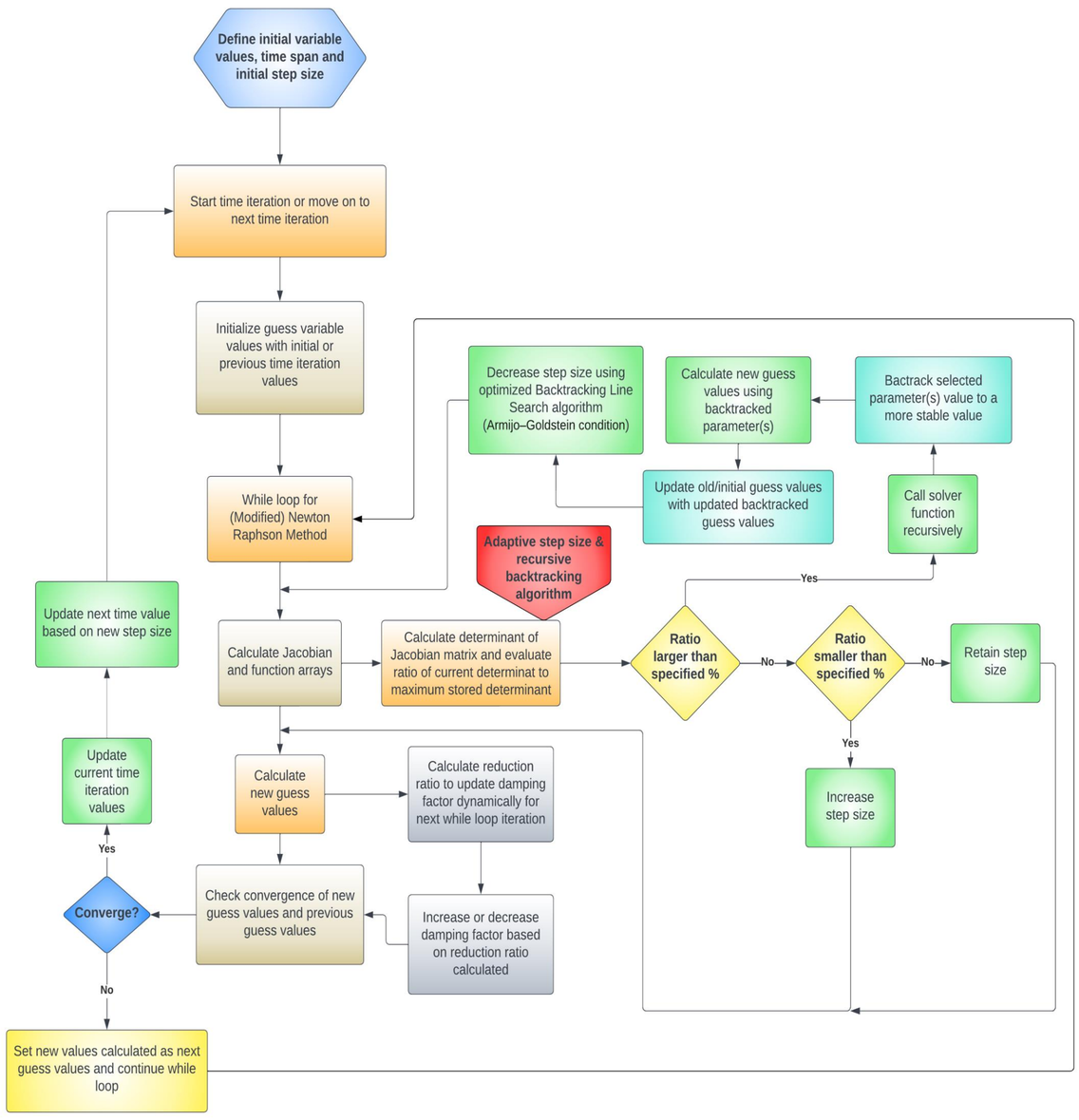




- The solver is tested for single discharge and charge cycles to verify its stability.
- It is then used to simulate a micro-cycling procedure of alternating discharge and charges over a span of 20 hours (on a laptop simulation only takes approximately 10mins).

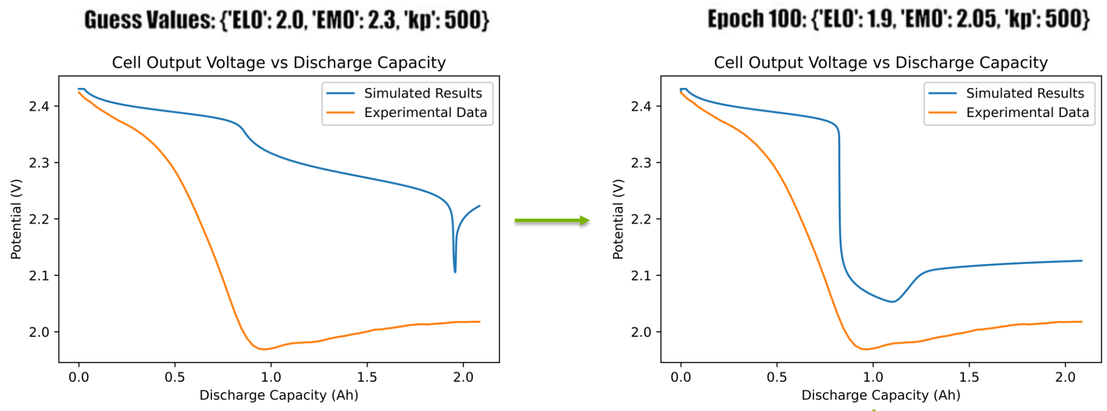
Novel Solver Logic

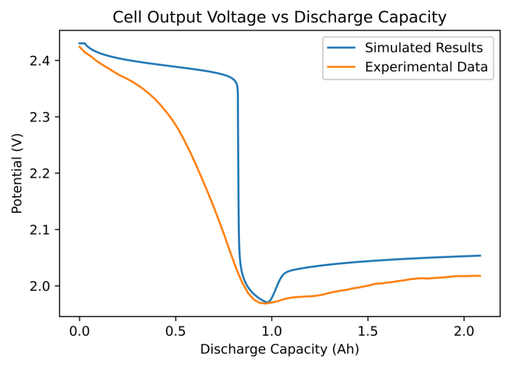
- The solver logic that were used to code the algorithms, including the optimized numerical methods are described in the flowchart below:



Simulation Testing 2

- The generalized solver is also tested via a gradient descent method to optimize parameter fitting using experimental results. The model used for this procedure is the newest 3 stage model proposed in [2].
- The gradient descent is initiated with guess values for any parameter(s) that describes the model (*in this example the Low Plateau, Middle Plateau Standard Potentials [EL0 & EM0] and the Precipitation Coefficient [kp]). The gradient descent slowly converges to the optimized parameter values to fit the experimental curve, as depicted below (simulation takes <30mins):





- NOTE: Further documentation, user manual and Python scripts for the generalized novel solver and gradient descent method can be found in the GitHub repository below:
- https://github.com/Dharshannan/FUSE_Li-S_Battery_Modelling
- The documentation and user manual documents contain information on the solver functions and how to implement them for any battery model (NOT LIMITED TO Li-S ONLY).

Conclusion and Next Steps

- The novel solver is generally stable and is capable of running simulations for parameter values that were initially problematic for the PyBaMM solver, namely when the EL0 value approaches 2.0 V and below.
- The novel solver efficiently conducts numerous simulation iterations within a short timeframe, as evidenced by the 200 iterations required for the gradient descent method to achieve optimal parameterization (solved <30mins).
- The novel solver is currently tested to simulate a newer unpublished model formulation.
- The long-term goal of this novel solver is to be released as part of or an open-source alternative to the PyBaMM solver.

References

- 1. Marinescu M, Zhang T, Offer GJ. A zero dimensional model of lithium-sulfur batteries during charge and discharge. *Physical Chemistry Chemical Physics*. 2016;18(1): 584–593. https://doi.org/10.1039/c5cp05755h.
- 2. Cornish M, Marinescu M. Toward Rigorous Validation of Li-S Battery Models. *Journal of The Electrochemical Society*. 2022;169(6): 060531. https://doi.org/10.1149/1945-7111/ac7750.

Intern bio

Dharshannan Sugunan is studying Mechanical Engineering at Imperial College London. He is currently in his final year and is expected to graduate with an MEng in summer of 2024.

Dharshannan is interested in projects involving numerical computations and simulations, optimization, machine learning and data science. He aspires to contribute to the energy industry in the future, especially in the field of computational simulations and data analysis.

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