Jupyter for uncertainty quantification and parameter estimation of computational models

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Background

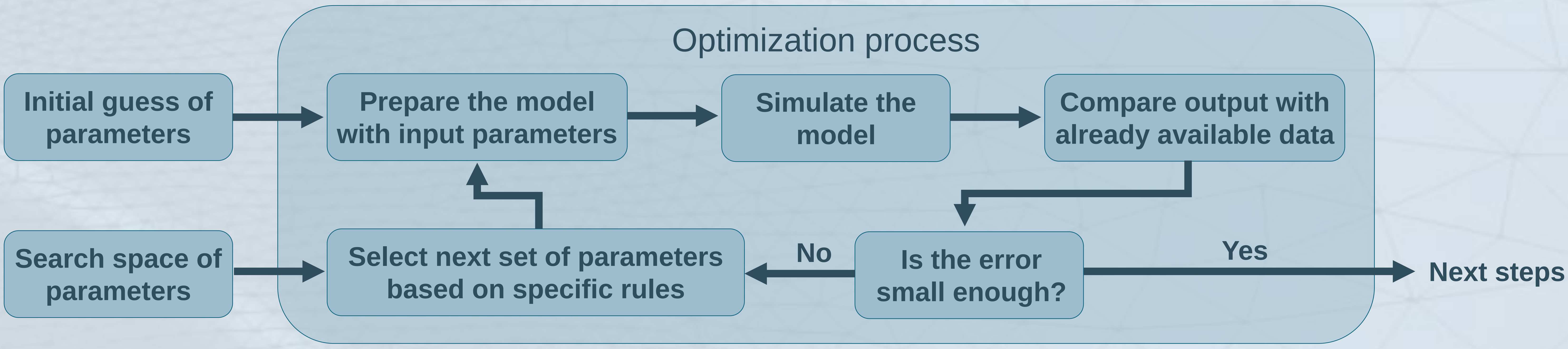
- For real-world applications, derived equations in mathematical models contain some coefficients that cannot be obtained directly from published scientific materials or experimental studies.
- One solution to obtain their values is making an inverse problem to use optimization techniques to minimize the difference of the model output and experimental data.
- Jupyter provides a unified environment for understanding, building, running, post-processing, and optimizing such a process.

$$A + 2B \rightleftharpoons C$$

$$\frac{\partial [C]}{\partial t} = \nabla . (D_C \nabla [C]) + k_1 [A][B]^2 - k_2 [C]$$

A chemical reaction and its corresponding kinetic mathematical model with unknown coefficients

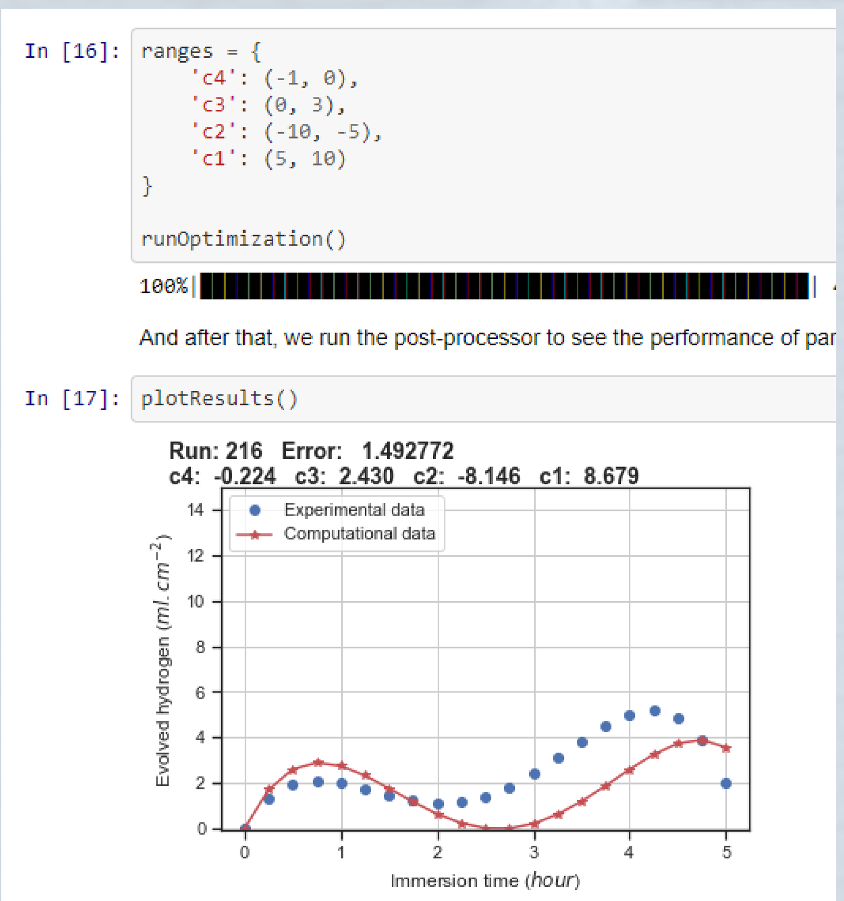
Methodology

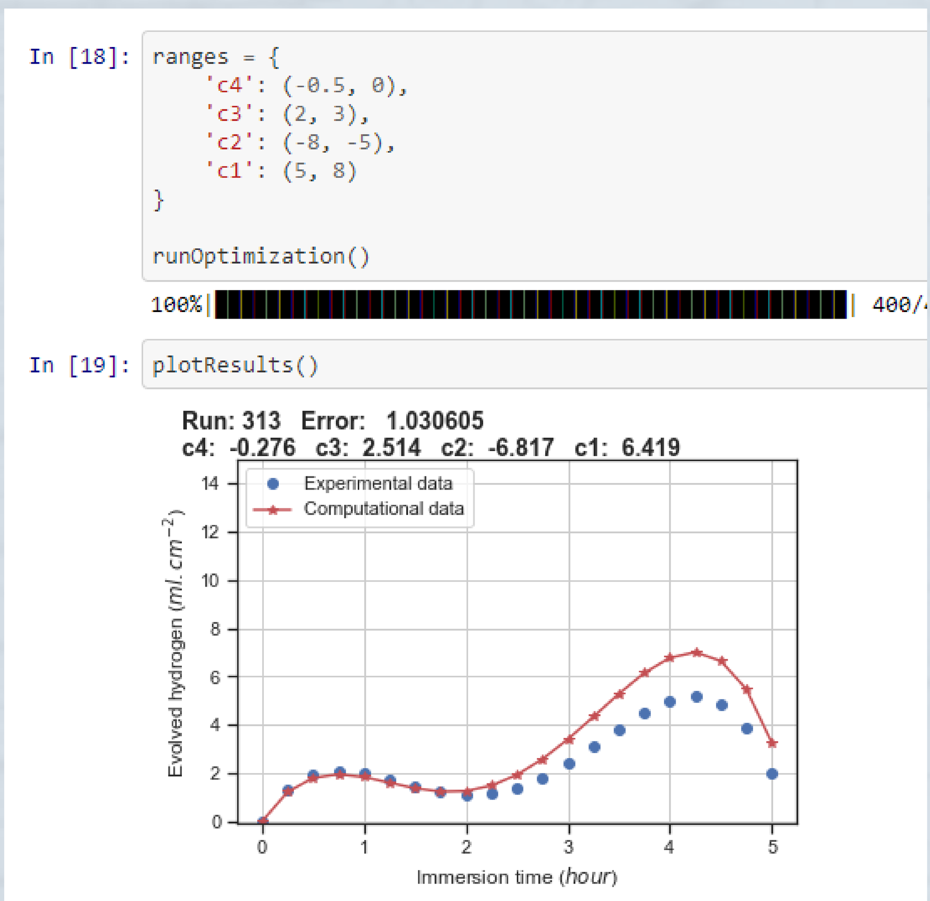


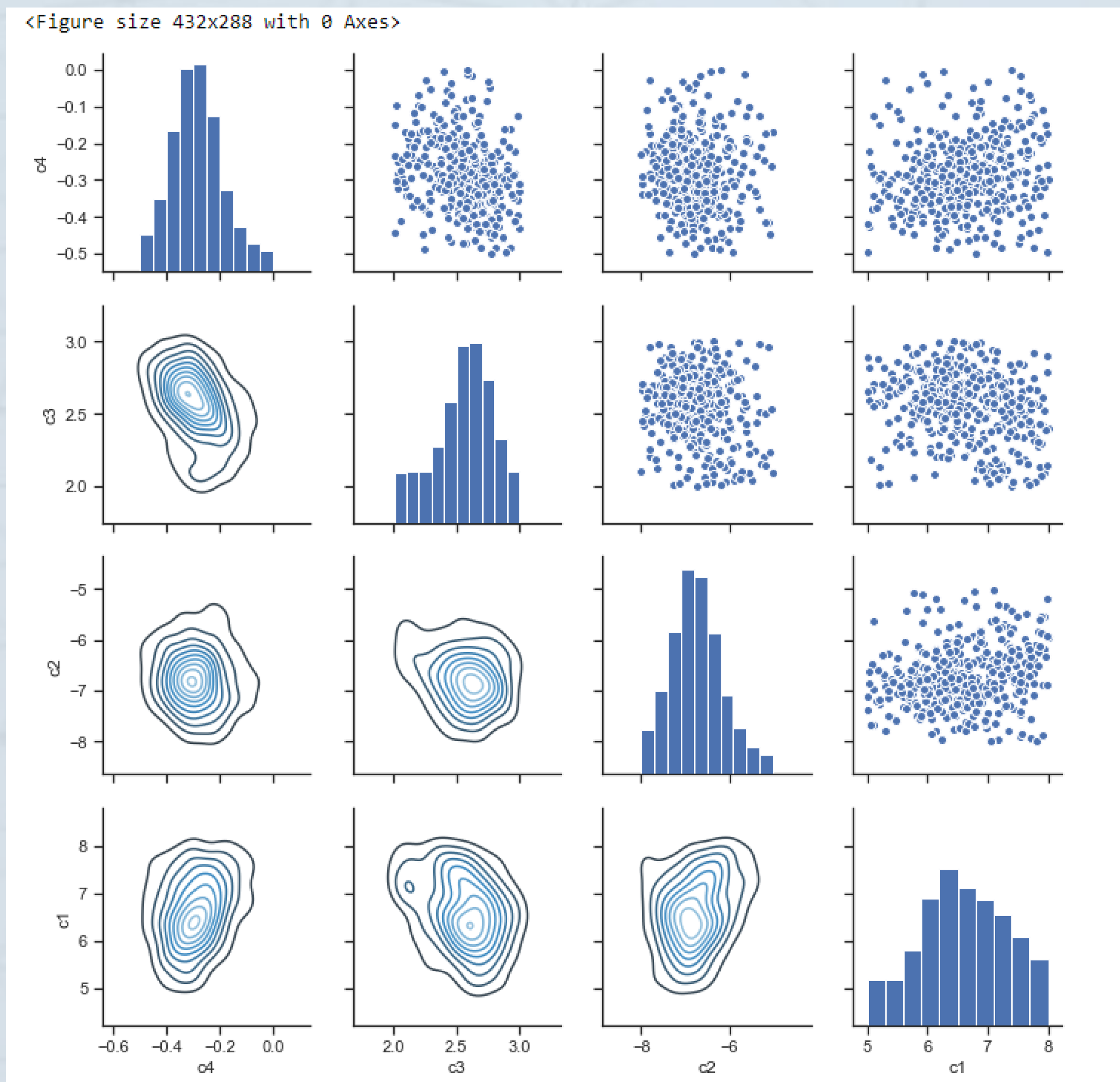
- Implementing this iterative process in Jupyter increases its transparency, especially for the people who are not deeply into the field, and at the same time, makes it easier to fine-tune the output to obtain more accurate results.

An example application

- Jupyter allows the whole process be implemented in a reproducible way.
- It also helps to keep track of the output and tune the process more efficiently.
- It's usually required to fine-tune the search space multiple times, and Jupyter provides a modern way to compare all the differences in one place.







Developed notebook at a glance

- Available at this repository: https://github.com/mbarzegary/educational-bayesian
- Implemented a full parameter estimation based on Bayesian optimization principles (using HyperOpt package) for a simple fitting problem
- In our research, the code has been extensively used for parameter estimation of finite element models

This research is financially supported by the PROSPEROS project, funded by the Interreg VA Flanders - The Netherlands program, CCI grant no. 2014TC16RFCB046.

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