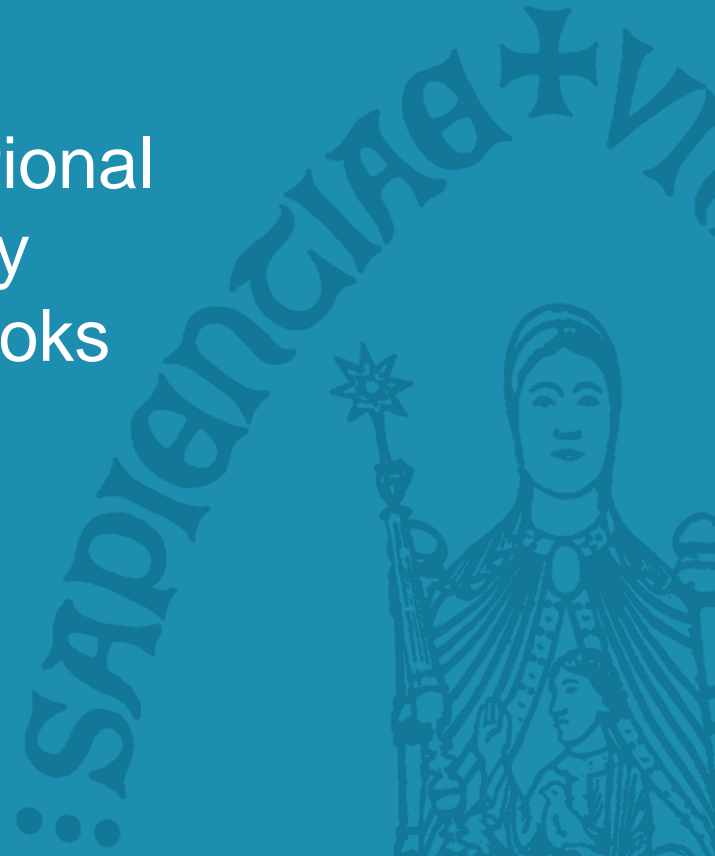


# Reproducible research in computational sciences: A use case for uncertainty quantification using Jupyter notebooks

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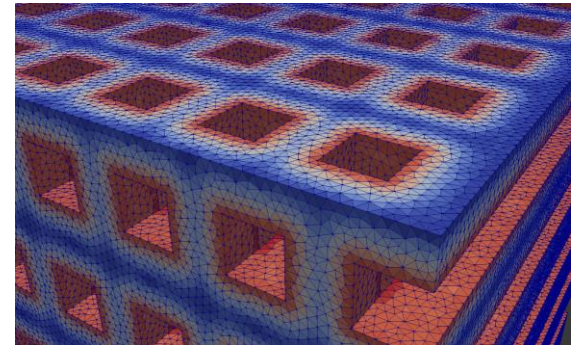
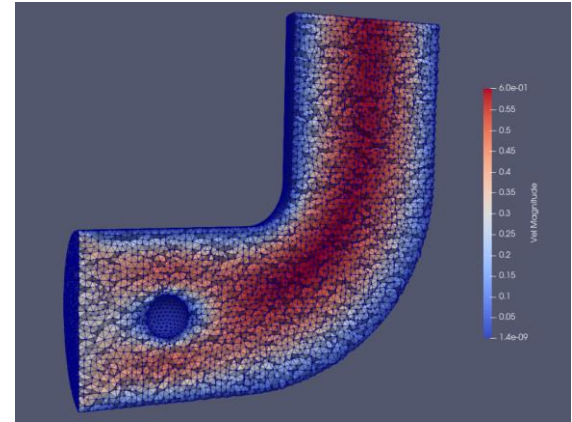


# Reproducible Research

- A crucial aspect of open science in recent years
- Core idea: the results of research should be reproducible given the original dataset, code, and software
- In computational sciences: “never believe anything unless you can run it”

# Reproducibility in Computational Sciences

- Transparency increases the outreach
- Traditional way: making the developed models available as open-source codes
- Better approach: publishing the building blocks in a reproducible manner



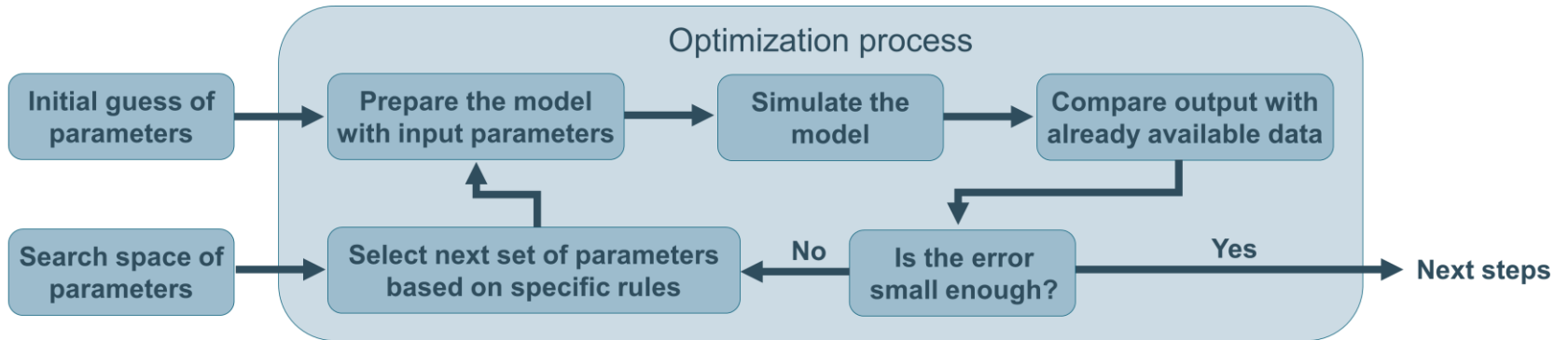
# Jupyter Comes Into Play

- Providing a full representation of the work (building blocks) being enriched by extra descriptions
- Jupyter facilitates reproducibility by increasing transparency, especially for the people who are not deeply into the field
- Bonus: its interactive nature helps converting the reproducible research works into valuable educational materials



# Use Case: Model Parameters Calibration

- A practical implementation of a parameter estimation process



# Use Case: Implementation




<https://github.com/mbarzegary/educational-bayesian>

- Showing reproducibility in a unified environment for understanding, building, running, post-processing, and optimizing processes

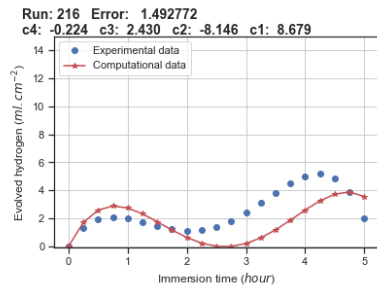
```
In [16]: ranges = {
'c4': (-1, 0),
'c3': (0, 3),
'c2': (-10, -5),
'c1': (5, 10)
}

runOptimization()
```




And after that, we run the post-processor to see the performance of par

```
In [17]: plotResults()
```

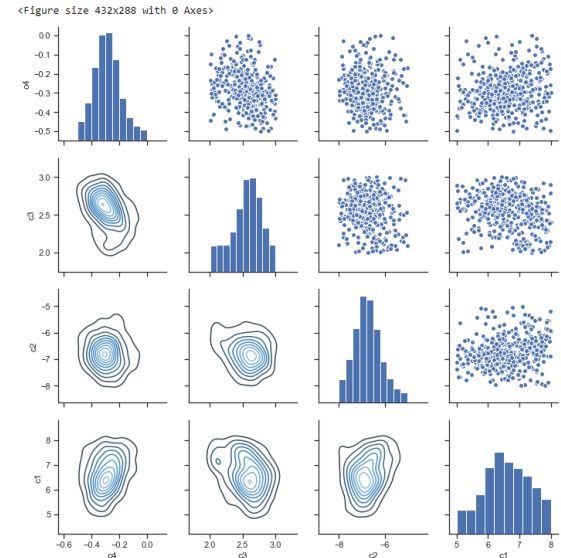
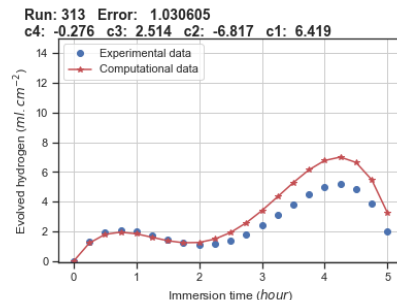


```
In [18]: ranges = {
'c4': (-0.5, 0),
'c3': (2, 3),
'c2': (-8, -5),
'c1': (5, 8)
}

runOptimization()
```



```
In [19]: plotResults()
```



# Conclusion

- Importance of reproducibility in computational research works
- The role that Jupyter plays in increasing transparency
- A use case for showing the proof-of-concept

# Thank you for your attention!



<http://mbarzegary.github.io>



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