KU Leuven Open Science Day

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

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Abstract

Reproducible research is gaining attention as a crucial aspect of open science in recent years, emphasizing the core idea that the results of research should be reproducible and replicable by everyone given the original dataset, code, and software. This becomes even more important in computational sciences, where researchers can claim a wide range of different output without providing enough details for reproducibility. In this field, the need for reproducible research comes from a common belief that *“never believe anything unless you can run it”*.

Making computational research partially or fully transparent will increase its outreach. One way to achieve this is by making the developed tools and models available as open source codes, but meanwhile, an even better approach is to publish the building blocks of the research in a reproducible manner. Doing this helps other researchers to understand the techniques used internally in research projects. One of the best approaches in this regard for scientific computing and data science research projects is taking advantage of Jupyter environments, in which researchers can provide a full representation of their work and enrich it with extra descriptions. Additionally, the interactive nature of Jupyter Notebooks makes it easy to convert the reproducible research into valuable educational materials.

In this presentation, an example use case shows how Jupyter Notebooks facilitate the process of uncertainty quantification and parameter estimation, an inevitable aspect of computational modeling projects, especially the ones dealing with ordinary or partial differential equations (like the models we develop in our research lab, focusing on tissue engineering processes, such as neotissue growth, engineered organs, and biodegradable implants). Jupyter increases the transparency of the entire process, especially for the people who are not deeply familiar with the field, and, at the same time, makes it easier to fine-tune the output to obtain more accurate results. The example use case is a practical implementation of a parameter estimation process using a Bayesian optimization approach, which we frequently use in our research. We will have a look at how Jupyter provides a unified environment for understanding, building, running, post-processing, and optimizing such a process.

Slides

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Author biographies

[Mojtaba Barzegari](#) (KU Leuven) is a PhD researcher in the field of computational biomedical engineering. His research is mainly focused on developing mathematical models and high-performance numerical simulations of tissue engineering systems. He uses solely open source packages and frameworks in his research. Besides from technical advantages, this enables him to contribute more efficiently to open science communities. He also [shares his work](#) via reproducible science disciplines, one important part of which is a collection of Jupyter Notebooks with Python and C++ kernels.

[Liesbet Geris](#) (KU Leuven) is Collen-Francqui research professor in Biomechanics and Computational Tissue Engineering at the university of Liège and KU Leuven. Her research focusses on the multi-scale and multi-physics modeling of biological processes. Together with her team and their clinical and industrial collaborators, she uses these models to investigate the etiology of non-healing fractures, to design in silico potential cell-based treatment strategies, and to optimize manufacturing processes of these tissue engineering constructs. Liesbet is scientific coordinator of the Prometheus platform for Skeletal Tissue Engineering (50+ researchers). She has edited several books on computational modeling and tissue engineering. She is the current executive director of the Virtual Physiological Human Institute and in that capacity she advocates the use of in silico modeling in healthcare through liaising with the clinical community, the European Commission and Parliament, regulatory agencies (EMA, FDA), and various other stakeholders.