

Toward Virtual Modelling Environments using Notebooks for Phenotyping and Simulation of Plant Development.

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Introduction - Functional-Structural Plant Models give new opportunities to understand plant growth and interaction with their environment. In the last decade, dedicated modelling platforms allowed the creation of a multitude of models, built upon series of dedicated tools for the representation, acquisition, analysis and simulation of plant growth and functioning. Such integrative platforms usually relied on software modules built using multiple computer languages or formalisms. While some efforts have been made for the distribution of these tools over multiple operating systems, the resulting models were usually poorly documented and organized. Models were either created as scripts or scientific workflows. The visual representation of workflows gives an overview of the modelled processes. However, their reuse by non-experts was usually limited to the modification of parameters. Reproducibility was also limited due to deployment and installation complexity on new computers with different configurations. Until recently, no cross-platform packaging suite was robust enough to manage modules built with multiple languages. In a new initiative to alleviate these problems, we explored, in the context of the OpenAlea platform (Pradal et al., 2008), the use of the Jupyter framework (Kluyver et al., 2016) to create virtual research environments for plant modelling.

Material and Methods – Our approach is based on Jupyter Notebooks, an increasingly popular web-based interactive computational application. Notebooks allow to formalize modelling scenarios as “computational narrative” (Perkel, 2018) by combining code with clear documentation based on the markdown language that includes illustration and mathematical formula rendering capability. Users can customize the narratives by editing cells of code and execute these cells in any order to refine operations. Notebooks can combine different modelling languages such as Python, R or Julia. Jupyter, combined with web deployment services such as Binder or Google Colaboratory, allow users to manipulate modelling narratives within web browsers while executing them on the cloud. To ease cloud deployment, OpenAlea packages are built and distributed from the Conda management system over multiple platforms. This allows building deployable virtual environments from docker images. Continuous integration services, based on Travis-CI and AppVeyor, deliver new releases on code update after automatic compilation and tests. Jupyter Notebooks have been extended to allow interaction with FSPMs. Using this approach, computational narratives for plant modelling can be formalized as notebooks and can be re-executed with an up-to-date virtual research environment by the community.

Results - Illustration of this approach will be presented on two modelling pipelines. First, we developed a software pipeline to characterize apple tree architecture from point clouds

acquired using terrestrial laser scanner. For this, architectural traits of each tree were extracted from their scan and their heritability was then assessed. This example illustrates standard pipelines where analyses are combined and applied on a large dataset. Scalability can be achieved using distributed computation on the cloud (Heidsieck et al., 2019).

For the second illustration, we integrate L-Py, a L-systems simulation package, into Jupyter Notebooks. By providing specific widgets, different steps of the simulation can be computed and the resulting 3D structures and associated properties can be iteratively visualized and analysed. 3D visualization of complex vegetal structures through client-server protocol was an important challenge. We developed optimized methods that minimize the size of data to exchange and allow interactive visualization of complex scenes. During the design stage, interaction and responsiveness are of main importance when exploring model parameters space. For this, graphical controls are generated within notebooks to allow tuning of parameters. A use case will be presented on the simulation of a mango tree over several growing cycles.

Discussion and Conclusion - Our aim was to provide tools to deliver models as notebooks to improve reproducibility and dissemination of FSPM. Documented and interactive notebooks provide interesting didactic tools to teach or test different types of FSPMs. Good code practices are however necessary to generate appropriate notebooks (Rule et al., 2019). Database of models start being constituted (<https://openalea.rtd.io/en/latest/tutorials>). Such an approach can provide a standard for model documentation published with scientific papers to enhance scientific reproducibility.

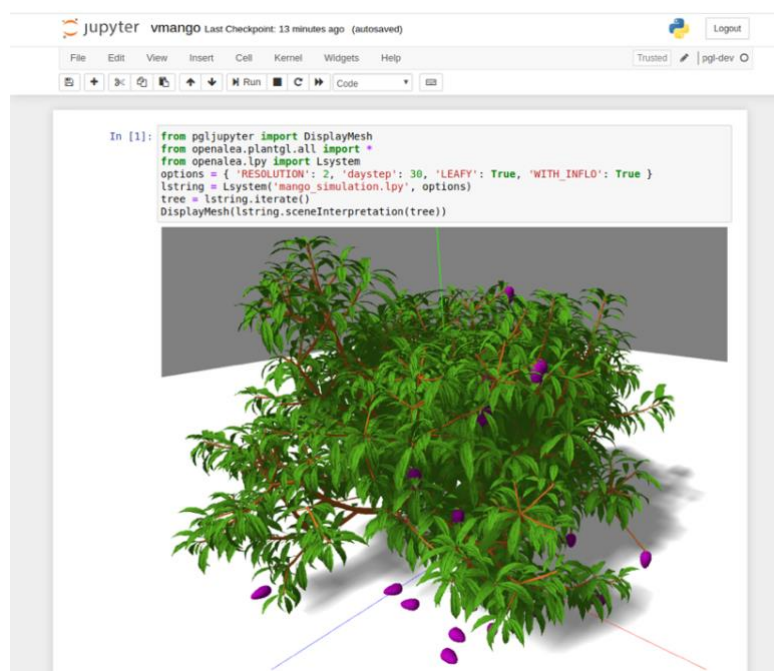


Figure: A notebook presenting a 3D view of a simulation of a mango tree after two growing cycles.

References

- Heidsieck et al. 2019. *Dexa*. doi: 10.1007/978-3-030-27618-8_33
 Kluiver et al., 2016, *Positioning and Power in Academic Publishing: Players, Agents and Agendas* 87-90, doi: 10.3233/978-1-61499-649-1-87
 Perkel, 2018, *Nature* 563, 145-146 doi: 10.1038/d41586-018-07196-1
 Pradal et al., 2008, *Functional Plant Biology* 35(10), 751-760, doi: 10.1071/FP08084
 Rule et al., 2019, *PLoS Computational Biology* 15(7). doi: 10.1371/journal.pcbi.1007007

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