

Managing reproducibility in computational experiments

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It is often difficult to reproduce computational experiments from papers due to a lack of detailed in how such experiments are documented. Even when researchers publish their code along side a paper, key information is often not well documented: *What version of an external software library was used? What value should be given to an undocumented model parameter? Which specific version of the code produced the results?*

In the NUMA research group at KU Leuven, we are developing a set of workflows for software development and computational experiments which attach this key information to our computational results as metadata. On a technical front, we have integrated Git with the iRODS data management software. We will reproduce our experimental results by reconstructing the exact computational environment that we used to produce our results. We will employ a Docker based reproducibility package for this purpose. In this presentation we will present our technical solutions, as well as our experiences in integrating these technical approaches with researchers' workflows.

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