

Computational Research

This area spans theoretical and applied sciences, where researchers perform computer simulations and develop models and software. Algorithms and code are often regarded as the main types of data. In principal, reproducibility is given by the scripts and there is not always the need to store and preserve input data and results. However, simulations can be very expensive, meaning that they are running for a long time or require large computational resources. This is especially the case for High Performance Computing (HPC). Since there are substantial costs associated with HPC, there is usually the need for at least a minimal amount of data management planning to estimate the required computing time, hardware and storage space for a given project.



Simulation software commonly provides some automatic metadata through log files containing version number and input parameters, for example.

Code and software are being developed for both internal use and for a broader community. The degree of documentation varies and is mostly up to the individual developer. Since most of the programs serve very special purposes, they are mainly targeted for experts in the respective field, who would understand how to use them by reading the source code. Bigger pieces of software are presented in specialized journals, which are frequently being cited. Smaller parts can be published as algorithms. Most software is managed by version control through software repositories like SVN, GitLab, GitHub or BitBucket.

There is a strong tradition for open science in computational research. Software and tools are often made publicly available with open licenses on the group's website or in community-specific repositories. However, software can also have a commercial value and should therefore not be made openly available. Deciding whether software has potential for commercialization is often very difficult and needs to be done case by case with help from innovation advisors. Some software is also directly being developed for commercial partners as part of innovation and consultancy.

