Scientific Software – the role of best practices and recommendations

Bernadette Fritzsch (1), Erik Bernstein (4), Wolfgang zu Castell (2), Markus Diesmann (3), Holger Haas (4), Martin Hammitzsch (5), Uwe Konrad (6), David Lähnemann (7), Alice McHardy (7), Heinz Pampel (8), Kaja Scheliga (8), Andreas Schreiber (9), and Dirk Steglich (10)

(1) Alfred Wegener Institute, Helmholtz Centre for Polar and Marine Research, Bremerhaven, Germany (Bernadette.Fritzsch@awi.de), (2) Helmholtz Zentrum München, (3) Forschungszentrum Jülich, (4) Deutsches Krebsforschungszentrum Heidelberg, (5) GFZ German Research Centre for Geosciences Potsdam, (6) Helmholtz-Zentrum Dresden-Rossendorf, (7) Helmholtz Centre for Infection Research, (8) Helmholtz Association, Helmholtz Open Science Coordination Office, (9) DLR, (10) Helmholtz-Zentrum Geesthacht

In Geosciences – like in most other communities – scientific work strongly depends on software. For big data analysis, existing (closed or open source) program packages are often mixed with newly developed codes. Different versions of software components and varying configurations can influence the result of data analysis. This often makes reproducibility of results and reuse of codes very difficult. Policies for publication and documentation of used and newly developed software, along with best practices, can help tackle this problem.

Within the Helmholtz Association a Task Group “Access to and Re-use of scientific software” was implemented by the Open Science Working Group in 2016. The aim of the Task Group is to foster the discussion about scientific software in the Open Science context and to formulate recommendations for the production and publication of scientific software, ensuring open access to it. As a first step, a workshop gathered interested scientists from institutions across Germany. The workshop brought together various existing initiatives from different scientific communities to analyse current problems, share established best practices and come up with possible solutions. The subjects in the working groups covered a broad range of themes, including technical infrastructures, standards and quality assurance, citation of software and reproducibility.

Initial recommendations are presented and discussed in the talk. They are the foundation for further discussions in the Helmholtz Association and the Priority Initiative “Digital Information” of the Alliance of Science Organisations in Germany. The talk aims to inform about the activities and to link with other initiatives on the national or international level.