Sustainable scientific software: experiences of the PCRaster research and development team

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The open-source PCRaster environmental modelling platform (http://www.pcraster.eu) is a long-time developed toolbox for the construction of earth science simulation models, providing tailored model building blocks with main application focus in hydrology, ecology or environmental health. With a development team consisting of software engineers and environmental scientists, we cover the full spectrum from developing multi-paradigm spatio-temporal modelling concepts, their design and implementation into research software, up to the application of PCRaster in scientific studies.

The broad range of topics combined with a small team, however, faces a series of challenges. Amongst others, we have the increasing scientific demand for developing and analysing multi-disciplinary models, e.g. calculating personal human exposures to environmental variables by modelling human activity patterns and environmental variables. Consequently, a traditional raster-based toolbox as PCRaster needs to be enriched with support for agent-based modelling. From the technical perspective, we have to manage, for instance, the conflict of integrating these new features while providing continuous maintenance of our legacy software, or the need to reimplement our algorithms to take full advantage of multicore or distributed computing resources. From the user perspective, examples of challenges include the need to consider avoiding too disruptive changes for our user base and hence the models they build, and the requirement to involve the international modelling community in the PCRaster development. Our team resides in an academic environment where additionally traditional tasks such as writing scientific publications and research proposals, and teaching need to be performed. For project management this implies that all issues must be arranged with simultaneous consideration of available staff, knowledge, time planning, available hardware resources, and the scarcity in funding of software engineering projects.

In our presentation we give an overview of the 30 year development history of PCRaster, the major challenges in synchronising scientific and technical progress, and our approaches thereto. We also briefly touch upon our latest developments and prototypes concerning the integration of agent-based and field-based modelling and our new underlying data model, which are gradually integrated into our modelling platform.