TITLE and type of activity (Networking, Joint Research development): Scientific Computing

Leading beneficiary: MLZ, ILL

Partners:

Please do not forget evtl University partners!

Estimated budget (in person months, other direct cost) and tentative distribution per partner

Abstract of your innovative activity: *(please make sure that you mention the following points)*

The Scientific Computing Group of Heinz Maier-Leibnitz Zentrum Garching is highly interested to deepen its cooperation with partner groups at other European neutron sources. We would like to see this cooperation based on open source, international division of tasks, code modularity and interoperability.

We suggest that tasks be divided into instrument-class specific software packages. For instance, we are right now developing software for grazing-incidence small-angle scattering. Based on this, we could take over long-term responsability to consolidate and curate data analysis software for all variants of reflectometry. We publish our software under an open-source license so that it can be freely used at other facilities. Within a funded European cooperation, we could additionally offer professional support for end users. In exchange, for other types of scattering instruments, we could then fully rely on software contributed by other partners.

We should foster the modularity and interoperability of scientific software. Currently, much software is developed time and again to fit into different frameworks; instrument users are contrieved by instrument-specific data formats to use instrument-specific tool chains. We need to facilitate code reuse. At the lowest level, our group works towards this aim by publishing solutions to specific numerical problems as separate code packages.

To enable a similarly modular packaging of more complex functions, acting on entire data sets, some standardization of data structures is necessary; this could be a rewarding task for a European cooperation. When there are different software projects with overlapping scopes, standardized interfaces will enable common tests, benchmarks and an exchange of code modules. A good example is the impressive progress in neutron guide simulation achieved by the friendly and healthy competion between the projects McStas and Vitess.