An Advanced, User-Friendly MCNP-McStas Coupling Interface (Joint Research development):

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Partners: *Erik Knudsen (Danish Technical University DTU-Denmark), Kim Lefmann (University of Copenhagen - Denmark) – (partners not yet confirmed).*

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

-- 9 person months over a period of 1.5 years. 50% contribution from each of the two partners (preferred option)

Two of the most commonly used software at neutron facilities are MCNP and McStas. Although very powerful and useful on their own, they are designed and optimized to serve different purposes: MCNP is mainly used for the production and transport of neutrons from the target to (and through) the moderator and the reflector. McStas is used for simulating the transport of neutrons through (supermirror) guides and their interactions with instruments on experimental beam lines. The ability to combine the two in a direct and uncomplicated way would be an extremely useful tool, allowing for types of calculations that none of the two codes can handle on its own. The difficulty in 'merging' the two codes, lies mainly on the peculiarities of the different coordinates systems used in each of them. DTU, with help from PSI and SNS have already developed a set of MCNP and McStas subroutines, that allow the two codes to communicate with each other: each of the two codes can create an output file (i.e. a list of neutron states) that the other one can read and continue from where the simulation was left off. This back and forth between the two codes can be performed as many times as needed.

Our proposal for an advanced version of the aforementioned coupling subroutines aims at a more robust and user-friendly coupling tool: among other things we want to eliminate the need for user interaction with the codes at each file exchange event (a fact that can discourage usage among general users), facilitate parallelism for the McStas coupling subroutines (not supported at the moment but greatly needed), and finally wrap the whole package in an easy to use Graphical User Interface (GUI). As the purpose of this project is to make this software interface easily available to users of the neutron community (and not only), and expand its usage beyond the current closed and limited circle of users, it would be beneficial if the development was done on a European consortium level. It

should be stressed that as McStas's development is heavily dependent and supported by user contributions - in the form of code development, bug reports, requests and suggestions - the user community can be directly involved in our activity through beta testings and requests, as our goal is to make the end product of this project as accessible and usable by the general user as possible.

At the same time such a tool would be very useful for the X-ray community, as McStas's sibling code McXtrace (x-ray ray-trace simulation package) could similarly be coupled to MCNP (also widely used within the community), providing similar benefits to x-ray simulations. It is important to mention here that our long term vision for our project, is a tool that will allow not only the communication between MCNP and McStas, but also among a moral general ‘suite’ of existing and widely used codes within the neutron and x-ray communities (such as GEANT, PHITS, SHADOW and VITESS). Therefore, development of the initial MCNP-McStas GUI proposed here, will be done in a way that can accommodate those future developments.

On a national level, this project would find a direct and immediate application within the SINQ upgrade project at Paul Scherrer Institute, which has entered its investigation phase on January 2014.