ICANS XIV
June 14-19, 1998
Starved Rock Lodge
Utica, IL, USA

Working Group on Monte Carlo Simulation of Neutron Scattering Instruments

R. K. Crawford

This working group session can be regarded as the second in a series of meetings aimed at establishing an international collaboration to develop improved Monte Carlo neutron tracking software for neutron scattering instrument simulation. The first meeting in this series was a workshop held at Argonne National Laboratory November 13-14, 1997.[1]

Many of us have developed Monte Carlo software to solve specific problems in the past. However, now we are beginning to need much more sophisticated software, capable of realistically tracking neutrons through an instrument from moderator to detector while including the possibilities that a variety of low- to high-probability events will occur along the way. Uses envisioned for such software include instrument design and optimization, experiment design, data analysis, diagnosis of problems in experimental data or instrument performance, and training of users. A very large amount of effort is required to develop such broad software capabilities, and it no longer makes sense for any one laboratory to try to do it all by themselves. This realization is driving the current effort to establish a collaborative mode for the development of such software.

Issues addressed at this ICANS working group meeting included the setting of standards for such software, providing centralized support for software maintenance and for communications among the collaborators, validation of the software, and funding for this process. A particularly useful feature was the participation at this session of people involved in source calculations. This enabled exchange of information to help define the source calculations needed and the nature of the interface between the source calculations and the instrument simulations.

Standards

The first major set of issues that need to be addressed is the development of standards. Of highest priority is to define the architecture for this software, and to identify at what levels within this architecture collaboration is to occur. We can envision four different layers to this software:

- The physics modules that describe the neutron source or the interaction of the neutron with a given component on the instrument
- The geometry of the instrument including the position and orientation of the different components, surfaces, and regions, and the materials involved in each
- The actual Monte Carlo calculation engine that moves the neutron between components, handles statistics, enables the saving of histories to identify the sources for problems, etc.
- The user interface that allows definition of the instrument, control of the simulation, and visualization of the output.

Standards for each of these layers and for the interfaces between them will define the architecture. At the moment there is some disagreement concerning the architecture that is appropriate. Resolution of this disagreement and definition of the architecture standards is required before most other collaboration activities can proceed, and is of the highest priority. The goal is to define a preliminary set of standards, at least for the architecture, by September 30, 1998. This is addressed in the action items below.

It is envisioned that a primary role of this collaboration will be to develop the physics modules for the components. This lends itself well to a division of labor according to the components of greatest interest at each of the different laboratories. Development of these modules at several different laboratories requires the establishment of standards and standard templates for such modules and for how the geometry and coordinate systems will be handled. Such modules should include documentation, and should be self-describing so they can be properly

integrated with the other layers of the software. Standards for the calculational and visualization layers will enable different versions of these to be developed at different laboratories as the need arises. These standards should make it possible for any new visualization or calculational software to work with previously created physics modules.

Maintenance

An immediate need is for an improved means of sharing information among the persons interested in collaborating on this project. ANL agreed to set up a web page for this purpose, and the meeting also generated a mailing list of additional persons interested in being kept informed. The complete mailing list will be posted on the web page. A centralized repository for validated code and for the currently approved standards will need to be established. Centralized tracking of the status of development and validation will be important. Management of the process for code and standards approval requires some central authority. In some of the proposed architectures, one or more layers of the software will be maintained and run on a central web server rather than on the users' client systems. All of these activities require the definition of a process and the identification of some group to assume the responsibility.

A model that was suggested for this centralized operation was that of a "journal", with an individual code module corresponding to an article being submitted by a particular author. The central organization would serve as "editorial board" to send each submitted module to "reviewers" for testing. When the module was accepted, it would then be added to the centralized repository. This model seemed to the group to make sense, but it needs wider circulation and discussion before being adopted. Groups to assume each of these activities for the collaborative project have not yet been identified. LANL is currently providing some of these services for the Monte Carlo software they have been developing.

Validation

Most of the existing Monte Carlo codes have not been benchmarked against existing data. There is a need to perform and document such validation both for existing codes and for newly developed modules. Both the individual modules and the integrated software packages need to be validated. To assist in this process measured data needs to be assembled for several "standard" instruments. This information should include a complete description of the geometry and materials comprising an existing instrument, similar information for one or more samples measured on this instrument, and files of data resulting from these measurements for each sample.

Resources and Funding

In the U.S. there are at present three groups funded for development of Monte Carlo instrumentation simulation software. These are groups at LANL, ORNL, and ORNL scientists working at ANL on the SNS project. Other U.S. laboratories also work on Monte Carlo codes, mostly on an ad hoc basis, and any such development in the future could probably be designed to conform to the collaborative standards with little difficulty. In Europe, the ESS project will provide some activity in this area, and other laboratories continue to develop their own codes as the need arises. In Japan both KEK and JAERI are interested in the development of such codes, but have not yet started any serious activity on this. The potential exists to funnel significant resources into this collaboration if the necessary standards and procedures can be put in place. In particular, the SNS project has expressed the intent to devote a significant amount of effort over the next six years to develop Monte Carlo software and the ESS project also expects increased levels of effort in this area.

A means must still be found to fund the central maintenance activities discussed above. Charging a subscription fee to the collaborating laboratories was discussed as one possible mechanism. The submission of a proposal to external funding agencies was also suggested. When the level of centralized activity that must be supported becomes better defined, it may also be possible that this activity could be sustained by funds available within one or more of the collaborating laboratories and projects. All of these routes should be explored.

Status

At the Monte Carlo workshop last Fall an international advisory committee was established to set up the framework for the collaboration and to guide collaboration activities. Members of this committee were Kent

Crawford (ANL, chair), Ulrich Wildgruber (BNL), Luke Daemen (LANL), Lee Robertson (ORNL), Ian Anderson (ILL), and Mark Hagen (ISIS). At that time the absence of a committee member from Japan was noted, and it was agreed to add a representative from Japan as soon as practical. One concrete accomplishment of this working group session was to add Masatoshi Arai (KEK) to this advisory committee.

A second concrete accomplishment of this meeting was the agreement of ANL to set up a web page for the continued dissemination of information about this Monte Carlo collaboration. Participants in this working group session who wanted to be kept informed about the Monte Carlo project added their names to the Monte Carlo e-mail list, which also currently includes names of the attendees at last Fall's workshop. This mailing list will be used to notify people when the web page is operational.

A third concrete accomplishment was to agree to the set of action items outlined below.

Action Items

1. A meeting of representatives from ANL, ORNL, and LANL will be set up as soon as possible, preferably in July 1998, to resolve the philosophical differences concerning the architecture to be adopted for this collaboration and to define a preliminary standard for this architecture. Luke Daemen will take the lead in organizing this meeting.
2. A Monte Carlo web page will be set up at ANL. The Monte Carlo mailing list will be posted on this web page. Ken Herwig will take the lead on this.
3. A list of proposed standards for "non-controversial" items requiring standardization, such as format to be used for documentation (the working group recommended PDF), order of parameters used in subroutines, etc., will be circulated to those on the Monte Carlo e-mail list for approval. Luke Daemen will take the lead on this.
4. Additional meetings will be scheduled as needed to continue the development of other necessary standards and of the centralized management process. This awaits the outcome of item 1.

References

[1] "Report on the Workshop on Monte Carlo Simulation of Neutron Scattering Instrumentation", Argonne National Laboratory, November 13-14, 1997. SNS Technical Report ANL/SNS/97-2.