Computational Methods Working Group

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During the Cold Moderator Workshop several working groups were established including one to discuss calculational methods. The charge for this working group was to identify problems in theory, data, program execution, etc., and to suggest solutions considering both deterministic and stochastic methods including acceleration procedures.

Over the past years, geometry setup and checkout, especially in Monte Carlo codes, has been a very time consuming operation. This problem only becomes worse as more and more details are added to the geometry. Design errors can creep in which can lead to catastrophic differences between the engineering and the neutronic models. A solution to this is to interface the CAD system to the MC program. However, this is not an easy problem since it has been worked on in the past, and at present no suitable solution has been found. In addition, the information needed/received from a "CAD/Geometry" system is not necessarily the proper information needed for the transport of the particles through the system. Additional work in this area is greatly needed.

Code systems like CALOR (HETC, EGS, and MORSE or MICAP or MCNP) and LAHET/MCNP, developed at the Oak Ridge National Laboratory (ORNL) and the Los Alamos National Laboratory (LANL), all have different media defining inputs between the various components. This diversity can have dire consequences since it leaves open so many avenues by which errors can be introduced. Efforts are currently underway to redefine these systems into coherent modular codes which will make the programs much more user friendly. The CALOR00 code will be JAVA/FORTRAN based, modular, and will cover the entire energy range ($0<E<20$ TeV). Furthermore, the new code will take maximum advantages of user/computer interfaces, i.e., debugging, inquiries during execution, graphic output during execution to check status, etc. CALOR00 has 3 specific applications--target, detector, and shielding design and analysis. The developers of the MCNPX code will initially strive to incorporate into the package the best available data/models for the energy range 0 to a few GeV. This package, like CALOR, has a specific purpose—to design the best targets/shielding for the APT project. The principal investigators on these code development projects have agreed to share information.

Regardless of how well a high-energy ($\gtrsim$20 MeV) radiation transport code package (or any detailed design program) is designed and built, approximations in terms of models, etc., must be included. Therefore, a detailed knowledge of the codes' weaknesses are needed. For example, it is general knowledge that the particle energy spectra calculated in the backward direction when using the "classical" intranuclear cascade model is too soft when compared to experimental data. This deficiency can lead to an underestimation of the backward shielding requirements. It is recommended to novice users that they remain in close contact with the developers and experienced users of the codes until a sufficient learning curve has been established.

Deterministic codes like DORT/TORT and TWODANT/THREEDANT are also valuable assets for solving radiation transport problems. These codes are able to give "exact" solutions $\phi(\boldsymbol{r}, \Omega, E)$ for the Boltzmann Transport equation. However, like the MC method, these multidimensional codes are very CPU time consuming, require large amounts of input and cross section data, have no fast way to determine the time dependence, and cannot at present handle charged particles "accurately." To use these codes at high energies ($\gtrsim$ 400 MeV) coupling between charged and neutral states must be included.

In the development of codes, test and benchmark problems and specifications are invaluable. In the interests of cold moderator development, a set of simple benchmark problems should include coupled and decoupled 2-D and 3-D moderator assemblies. An example of a "simple" problem would be the determination of time eigenvalues (α-calculation) for a decoupled moderator, and also for a coupled (target, reflector, and moderator [TRAM] assembly). Such calculations yield the asymptotic time decay and the corresponding space, angle, and energy dependent flux distributions. For the coupled calculation, including the entire TRAM assembly, a nodal code option (DORT/TORT) should be used. In addition, a simple source calculation can also be included in this series. This would yield a direct comparison between deterministic (DORT/TORT) and Monte Carlo methods.

For a complex benchmark problem, the system to be characterized should be tied to an experimentally measured quantity or distribution. The experimental data should include the following:

A. Moderator leakage spectrum [ϕ(E, t)] measurements. The experiment should be described in great detail (input file preferably created by the institute at which the measurement was made) and be a test of all the code modules. The full code sets LAHET/MCNP or CALOR95 can be tested in this way. Measurements carried out on (γ, n) sources can be as valuable as those based on spallation or other charged particle sources except for the possible difficulty of providing relevant normalization. This is true, as long as the spectral region is well below the primary source energy. Accurate measurements made at KENS, ISIS, IPNS, and/or LANSCE would be the most desirable.

B. N/P measurements of the source zone. Recent measurements at SATURNE on both lead and tungsten could be used as benchmarks for this case. These measurements predominately test the high-energy transport codes.

C. Energy deposition: Measurements of energy deposition suitable for benchmarking the code system should be found.

D. In general, descriptions of benchmark problems should include the following information:

1. For the inter-comparison of deterministic calculations and their comparison to experiments:
   - Description of the geometry, boundary conditions, and desired outputs.
   - A suggested energy group structure and order of anisotropy in the scattering matrix. In the ideal case a proposed cross section library (exercising NJOY) should be included.
   - In the case of DSN codes (DORT and TORT) the angular quadrature should be defined (order and weighting scheme). This would reduce the sources of "error" or differences between the various participants.

2. For the complex benchmarks an input description (input file) created by the measuring institute would be the ideal solution. Failing this, a description yet to be agreed upon will be required.

3. A standard set of scattering kernels should be used by all analysts. LANL has agreed to furnish this data.

The participants who have agreed to coordinate this work in the future include Hans Ludewig, Phil Ferguson, and Lowell Charlton.