Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew
Gatlinburg, Tennessee, April 6-11, 2003, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2003)

MIX AND MATCH WITH MCNPX

John S. Hendricks and Gregg W. McKinney
D-10, Nuclear Systems Design, MS K575
Los Alamos National Laboratory
Los Alamos, NM 87545
jxh@lanl.gov ; gwm@lanl.gov

Franz X. Gallmeier
Oak Ridge National Laboratory MS 6474
Oak Ridge, TN 37831
GallmeierFZ@ornl.gov

ABSTRACT

The mix and match problem has been solved in the MCNPX Monte Carlo radiation transport code. Such codes typically use tabular data for low-energy (20 MeV–150 MeV) neutrons, protons, and other particles and physics models at high energy. MCNPX can now mix physics models and tabular data. Consequently, transport can be performed in nuclides where no tabular data are available, such as germanium in bismuth-germanium-oxygen (BGO) detectors. Further, MCNPX can now match the upper end of tabular data to the corresponding physics model, making the transition more accurate between the upper tabular data bound and the physics model.

We describe MCNPX, the Monte Carlo N-Particle eXtended version of MCNP4C3, and the mix and match problem. We then provide an example of how solving the mix and match problem significantly enhances radiation transport calculations for a wide variety of problems.

Key Words: Monte Carlo, radiation transport, computer models

1. INTRODUCTION

The Los Alamos National Laboratory Monte Carlo N-Particle eXtended (MCNPX)[1] radiation transport code now solves the "mix and match" problem. The mix and match problem arises when computer modeling codes simulate physical interactions with both physics models and tabulated data. Until now, MCNPX* has required users to specify a "table cutoff energy" below which data tables are used and above which physics models are used. Now, when tabulated data are missing, physics models may be mixed with the tabulated data. When tabulated data are available in a variety of energy ranges, the physics models can now pick up where the data tables leave off.

[1]MCNPX and MCNP are trademarks of the Regents of the University of California, Los Alamos National Laboratory.

MCNPX is a computer code that models all kinds of interactions between radiation and matter. It is a time-dependent, continuous-energy radiation transport code for nearly all particles up to the terravolt energy range. The energy ranges for various particle types are illustrated in Figure 1. MCNPX is a complete superset of MCNP4C3[2] and MCNPX2.3.0,[3] both available at the Radiation Safety Information Computational Center (RSICC[4]) in Oak Ridge, Tennessee. The new mix and match capability is a modification to MCNPX2.4.0,[5] which was released to RSICC August 1, 2002, and which has many additional significant capabilities beyond those of its constituent codes.[6,7]

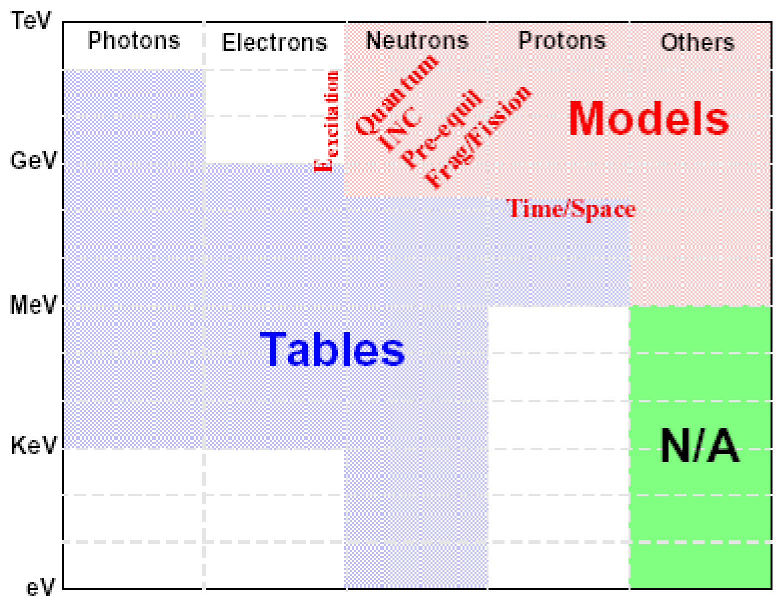

Figure 1. MCNPX PARTICLE ENERGY RANGES

2. THE MIX AND MATCH PROBLEM

There are two components to the MCNPX mix and match problem:

Mix nuclides:

The mix problem is that only one set of neutron and proton nuclides can be specified for a given calculation. In MCNPX, nuclides are specified by a "ZAID" number of the form ZZZAAA.nnT, where ZZZ is the atomic number, AAA is the atomic mass, nn is the evaluation descriptor, and T is the cross-section table type (n for neutrons, h for protons, p for photons, u for photonuclear, and e for electrons.) Without mix and match, if natural carbon 6000.24c is used for neutrons, then isotopic carbon 6012.24h cannot be used for protons; if tritium 1003.24c is requested for neutrons, there is no nuclear data table for 1003.xxh, and a model cannot be used unless all proton physics is done with models. Our solution to the mix problem enables the substitution of nuclides and models for any material.

Consider, for example, a material composed of carbon and tritium. We could specify the material with neutron nuclides 6000.24c and 1003.24c and then override it with 6012.24h for protons and use a physics model instead of a data table for the proton tritium interactions.

Match energies:

The match problem is the requirement of a single table energy bound below which all physics is done with nuclear data tables and above which all physics is done with models. Historically, this table cutoff has been 20 MeV for neutrons and 0 MeV for protons. For photonuclear events, only tables were used; above the table limits, the values at the highest table energy were extended. With these defaults, all proton data table information was ignored and only models were used; and all neutron data table information above 20 MeV was ignored.

If users set the table energy cutoffs to some other values, there were still problems. For example, suppose the neutron table energy bound is set to 120 MeV in a problem where ^{1}H, ^{9}F, and ^{12}C are specified. The maximum energies for these data tables are 100, 20, and 150 MeV, respectively. Then model physics will always be used above 120 MeV, even though there is a nuclear data table for ^{12}C up to 150 MeV. Also, the nuclear data table information for 100 MeV for ^{1}H will be used between 100 MeV and 120 MeV, and the data table information for 20 MeV for ^{9}F will be used in between 20 MeV and 120 MeV. Extending data from the highest table energy to the specified cutoff is inaccurate. Using models where tabular data exist may be a poor approximation. For protons the presently available data libraries all go up to 150 MeV, but once the table cutoff energy is specified at 150 MeV, all protons below 150 MeV must be transported with data tables. Because there are presently only 41 proton and 12 photonuclear data table nuclides distributed with MCNPX, problems were limited to these nuclides.

3. MIXING NUCLIDES

The "mix" part of the mix and match problem has been solved by (1) allowing a nuclide substitution capability and (2) allowing tables and models to be used in the same energy range.

Perhaps the best way to describe the new nuclide substitution capability is by example, and so we describe the exact MCNPX input used. Note that nuclide substitution has been available for several years for photonuclear problems.[6] The nuclide substitution capability introduces a new user input card, MX, that is an extension of, and replacement for, the MPN card for photonuclear data:

MXn:p zaid1 zaid2 ...

where n = material number of an Mn card, which *must* precede the MXn card;
p = particle type (n, p, h for neutron, photonuclear, and proton); and
zaidn = replacement nuclide for the nth nuclide on the Mn card.

Only particle types n (neutron), p (photonuclear), and h (proton) are allowed. No substitutions are allowed for photoatomic (p) and electron (e) data because those data sets are complete. The MXn:p card is an exact replacement of the MPNn card, and specified photonuclear nuclide substitutions (library type u.) zaidn = 0 is allowed on MXn:P (photonuclear substitution) to specify no photonuclear data for a specific photoatomic reaction. zaidn = model is allowed on the MX card to allow models to be mixed with tabular data.

The following example illustrates the use of the new MX card to mix models and data tables and to substitute nuclides. The "j" entry is a jump indicating to use the value from the m1 card.

```
m1      1002 1   1003.6 1 6000 1   20000 1  nlib .24c
mx1:n   1002     1003     j       j
mx1:h   model    model    6012     20040
mx1:p   6012     0        6012     20040
```

Results are summarized by a new print table in the problem output:

Particles and energy limits Print Table 101

Particle type			Particle cutoff energy	Maximum particle energy	Smallest table maximum	Largest table maximum	Always use table below	Always use model above
1	N	Neutron	0.000E+00	1.000E+37	2.000E+01	1.000E+05	2.000E+01	1.500E+02
2	P	Photon	1.000E-03	1.000E+03	1.000E+05	1.000E+05	1.000E+37	1.000E+37
		Photonuclear	1.000E-03	1.000E+03	1.500E+02	1.500E+02	1.500E+02	1.500E+02
3	E	Electron	1.000E-03	1.000E+03	1.000E+03	1.000E+03	1.000E+37	1.000E+37
9	H	proton	1.000E-00	1.000E+03	1.500E+02	1.500E+02	0.000E+00	1.500E+02

The above problem is for neutrons, photons, electrons and protons from 0 MeV to 1000 MeV with photonuclear physics turned on. Print Table 101 shows the range of upper data table limits and the range of energies where data tables and models will be used.

In this example, both data tables and physics models are used for protons. That is, both data tables and physics models are mixed in the same energy range. This mixing is done by the "match" solution described in the next section.

4. MATCHING ENERGIES

MCNPX now allows for the matching of energies so that physics models are used seamlessly above the energy range of data tables. When the various nuclides in the same material have different upper table energies, then the data tables are used for the nuclides where data are available and the physics models are used for those above the tabular data range. The new capability applies to neutrons, protons, and photonuclear events. Data libraries are available for the entire range of photons, and currently, MCNPX merely extends the 1-GeV electron data to higher energies rather than using models. The other particles transported by MCNPX, such as pions, muons, kons, neutrinos, deuterons, tritons, and alphas, have no data tables and always use physics models.

The simplest case is for the matching of photonuclear events. Photonuclear events are not particle transport: they generate other particles for transport. Thus, mix and match for photonuclear events entail determining the photonuclear interaction cross-section and particle production.

Consider a material composed of M nuclides. Let T_m be the maximum energy of the data table for the *mth* nuclide. Then for a photonuclear event at energy E, set the table cross section to zero if $E > T_m$ and set the physics model cross section to zero if $E < T_m$. Note that the photonuclear physics models exist at this time only for the new CEM2K[7,8] (Cascade-Exciton Model) MCNPX physics model and not for the older MCNPX FLUKA, BERTINI or ISABEL models. Then the probability of a data table collision is proportional to the nonzero data table cross sections, and the probability of a physics model collision is proportional to the nonzero physics model cross sections. If a data table collision is selected, then the nuclides are sampled from the nonzero data table nuclides. If a physics model collision is selected, then the nuclides are sampled from the nonzero physics model nuclides. The rest of the photonuclear reaction is then performed in the usual way for tables or models. A complication is that the nuclides for the physics models are different than the nuclides for the data tables because all elemental data are converted to isotopic data according to natural abundances.

For neutrons and protons, mix and match is achieved similarly to photonuclear events. The table cross section is set to zero if $E > T_m$, and the physics model cross section is set to zero if $E < T_m$ Then the probability of a data table collision is proportional to the nonzero data table cross sections, and the probability of a physics model collision is proportional to the nonzero physics model cross sections. If a data table collision is selected, then the nuclides are sampled from the nonzero data table nuclides. If a physics model collision is selected, then the nuclides are sampled from the nonzero physics model nuclides. The collision physics is then done by data tables for data table nuclides and by physics models for physics model nuclides. The previous subroutine for physics model treatment of neutrons is gone: all neutrons are transported in the data table history tracking subroutine with appropriate calls to the physics models from the collision subroutine when a physics model nuclide is chosen. The previous subroutine for data table treatment of protons is gone: all protons are transported in the physics model charged particle subroutine with appropriate calls to the data table collision routines as required. Care has been taken to ensure exact tracking—identical computational results—when all collisions are in either the data table energy range or the physics model energy range. Results differ from previous MCNPX versions only when collisions occur in the energy range that is above some data tables and below others. Users can still set a table cutoff energy above which only physics models are used and below which only data tables are used, even when the data table values must be extended above their range up to the cutoff energy. This option makes it possible to track exactly earlier MCNPX versions over the entire energy range.

Mixing of nuclides with physics models and nuclides with data tables is enabled by treating the physics model nuclides with an upper table energy of zero.

5. RESULTS

A bismuth-germanium-oxygen (BGO) detector problem is a good example of the new MCNPX mix and match capability. There is presently no germanium, Ge, cross section available to MCNPX. The best available oxygen, O, cross-section table goes up to 150 MeV, but the best available bismuth, Bi, cross-section tables goes up to only 20 MeV. The example problem consists of a cylindrical can of height 8.433 cm and radius 3.932 cm. The 100-MeV neutrons are a monodirectional point source on the bottom center of the can, and we tally the neutron and photon currents out of the top of the can and the photon heating in the can. Previously users had three unpleasant alternatives:

1. Substitute some other nuclide for germanium, such as arsenic, As, and use data tables. Above 20 MeV, the cross section values at 20 MeV would be used for Bi and As. Above 150 MeV, the highest energy of the O data table would be used. Results above 20 MeV are incorrect. This solution is the only available MCNP4C alternative.
2. Use physics models for all energies. Below 150 MeV, the physics models are inferior to the O data tables. Below 20 MeV, the physics models are inferior to the Bi data tables. Below around 10 MeV, the models become poor, and they are unreliable below 1 MeV.
3. Substitute some other nuclide for Ge, such as As, and use physics models for everything above some table cutoff energy, say 20 MeV. The physics model for As rather than Ge will be used.

The new mix and match capability makes it possible to use a physics model for Ge for the entire energy range, a data table for Bi up to 20 MeV and a physics model above, and a data table for oxygen up to 150 MeV and a physics model above.

Figure 2 is an MCNPX tally coplot of the neutron current escaping out of the top of the BGO can from the 100-MeV monodirectional neutron source impinging upon the bottom of the can. The solid black line is the MCNPX result with the new mix and match capability just described. The dashed blue line uses option 3 above: Arsenic is substituted for Ge, and physics models are used above 20 MeV. The dotted red line uses option 3 above with As substituted for Ge and physics models used above 150 MeV, which is above the problem range.

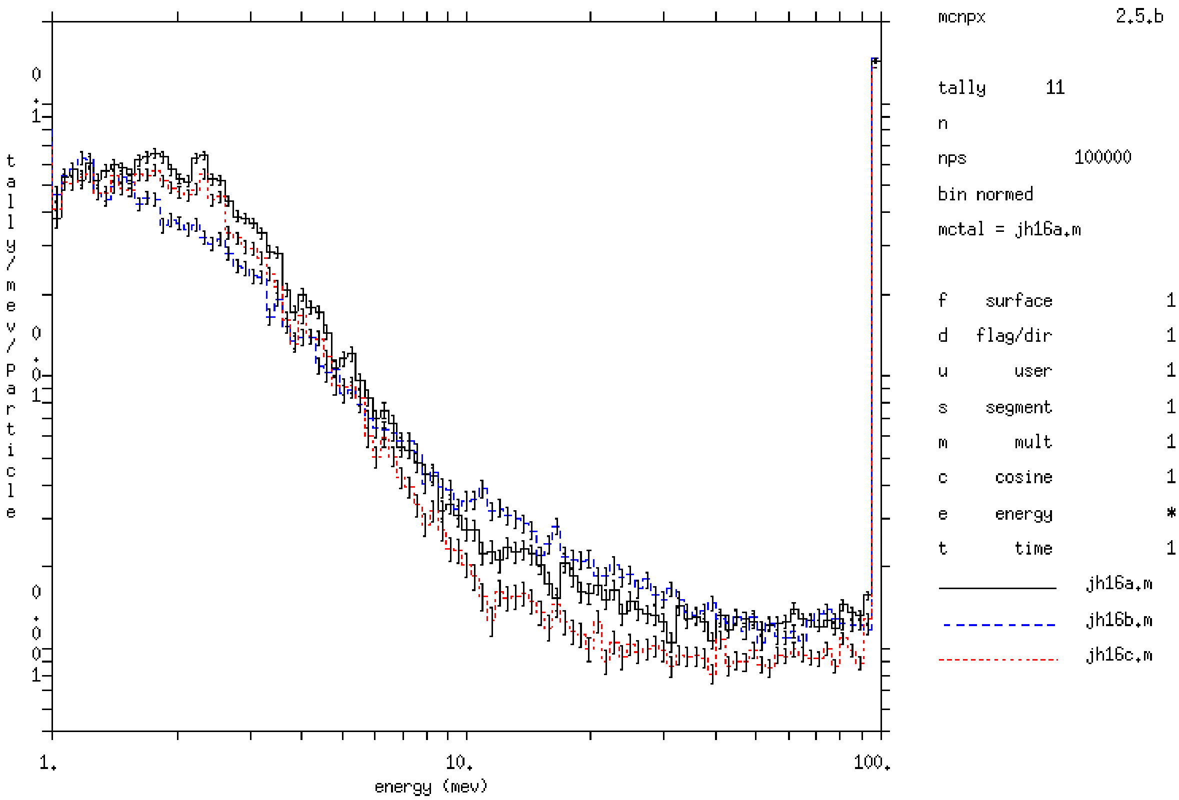

Figure 2. Neutron Current Escaping Top of BGO Can

Figure 3 shows the photon current leaking out of the top of the BGO can.

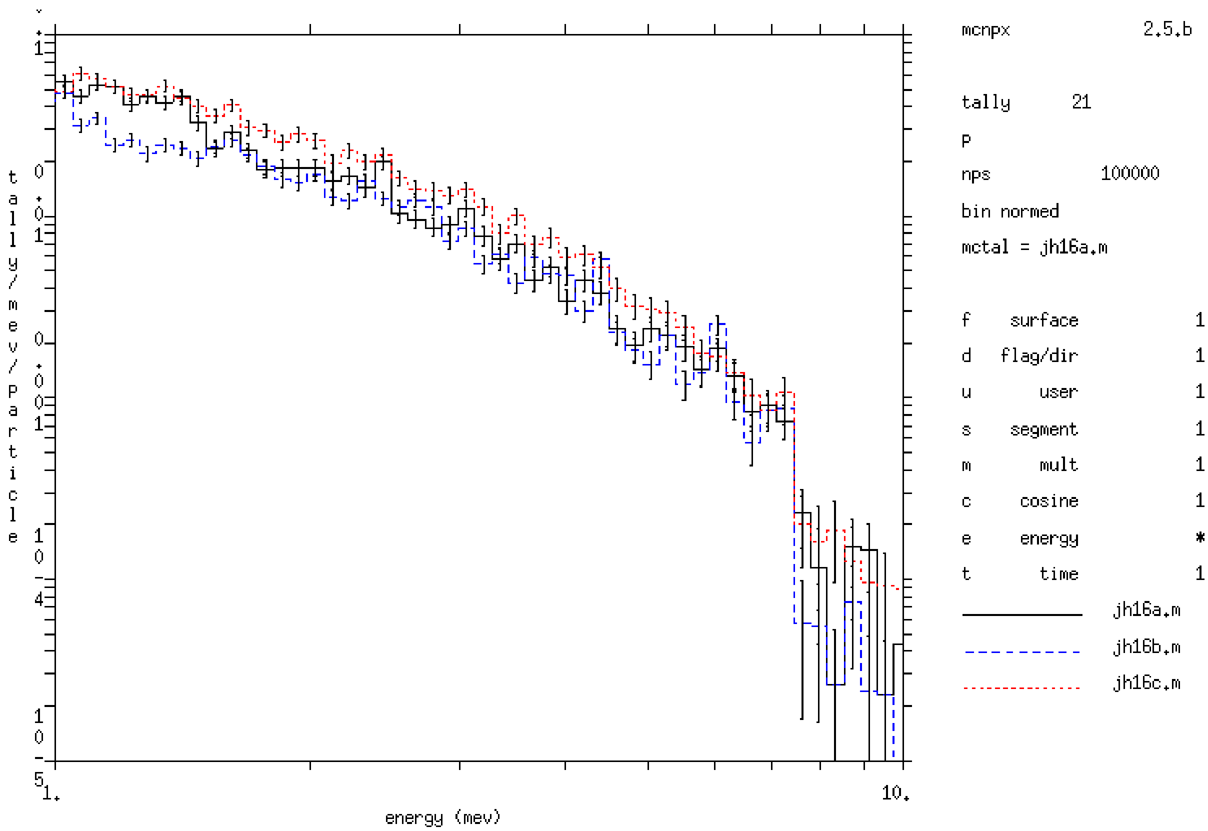

Figure 3. Photon Current Escaping Top of BGO Can

Finally, Figure 4 shows the photon heating in the BGO can. Again, results are significantly different when one substitutes As for Ge and cannot use physics models above the exact energy where the data tables run out.

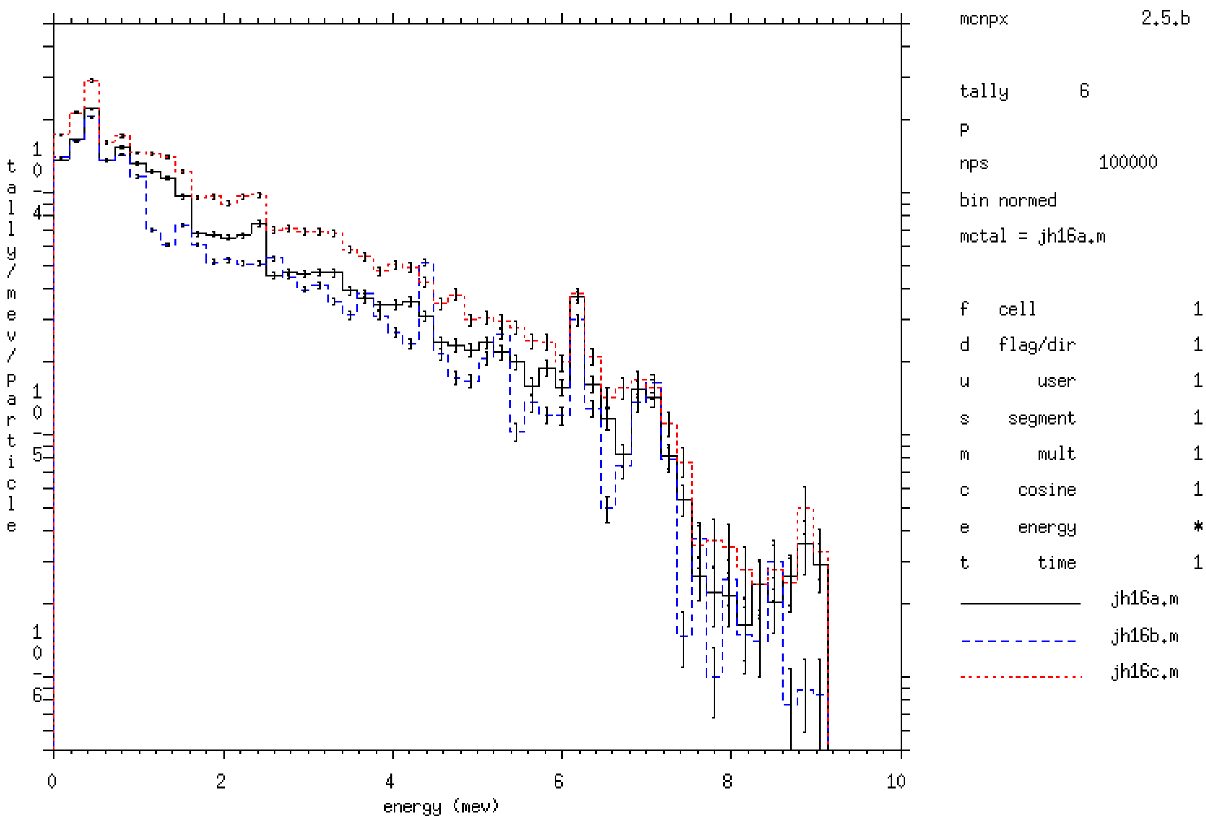

Figure 4. Photon Heating in the BGO Can

6. CONCLUSIONS

The new MCNPX mix and match capability makes it possible to use data tables when available and use physics models above the data table range or when no data tables are available. For problems such as the BGO detector, where Ge data tables are unavailable, or for nuclear waste problems where fission products are not available, we can now use physics models instead of substituting or neglecting nuclides. Proton or photonuclear problems, which were limited by having only a handful of data tables available, can now be used with physics models being utilized for the remaining problem nuclides. In particular, the Evaluated Nuclear Data File (ENDF) US standard data tables for protons and photonuclear cross sections from RSICC do not include fissionable nuclides. If the only data tables for neutrons are for elements, such as natural calcium, and the only data tables for protons are for isotopes, such as calcium-40, both data tables now can be used for the same material region. Substitution of nuclides is now possible and the mix and match problem is solved.

REFERENCES

1. MCNPX home page: http://mcnpx.lanl.gov.

2. J. F. Briesmeister, Editor, "MCNP—A General Monte Carlo N-Particle Transport Code—Version 4C," Los Alamos National Laboratory report LA-13709-M (March 2000).

3. "MCNPX 2.3.0 User's Guide," Los Alamos National Laboratory report LA-UR 02-2607 (April 2002).

4. Radiation Safety Information Computational Center, http://www-rsicc.ornl.gov/rsic.html.

5. "MCNPX 2.4.0 Manual," Los Alamos National Laboratory report LA-CP-02-408 (August 2002).

6. Morgan C. White, "Development and Implementation of Photonuclear Cross-Section Data for Mutually Coupled Neutron-Photon Transport Calculations in the Monte Carlo N-Particle (MCNP) Radiation Transport Code," Los Alamos National Laboratory report LA-13744-T (July 2000).

7. Stepan G. Mashnik and Arnold J. Sierk, "Improved Cascade Exciton Model of Nuclear Reactions," Proceedings of the Fourth Workshop on Simulating Accelerator Radiation Environments (SARE4), Knoxville, TN, September 14–16, 1998, T. A. Gabrioel, Ed., ORNL, pp. 29–51 (1999).

8. Stepan G. Mashnik and Arnold J. Sierk, "Recent Developments of the Cascade-Exciton Model of Nuclear Reactions," International Conference on Nuclear Data for Science and Technology, October 7–12, 2001, Tsukuba, Japan. Los Alamos National Laboratory report LA-UR-01-5390 (2001).