What do I know about MCNPX?

Overview

MCNPX is an extremely useful tool for shielding or energy deposition calculations. It is relatively easy to "learn," is continually being 'upgraded,' and has a large world wide user community. It has satisfactory de-bugging facilities and error detection. The combination of a *small* MCNPX 'Manual,' any of the *large* MCNP manuals (I currently use MCNPB), and the constant flow of e-mail messages between members of the 'users forum' provide good documentation.

At BNL, the 'gatekeeper' of MCNPX is Mike Todosow and members of his group. I have dealt mostly with Arnie Aronson. When any validated 'beta tester' at BNL needs code or cross-sections associated with MCNPX, it is supposed to come through this group, and requests should be made to this group. One may not become a beta tester without approval of someone at LANL. Laurie Waters is usually the person who grants permission.

Physics

The physics options associated with hadron interactions are described in the MCNPX manual; the physics for photons and electrons in one of the MCNP manuals. In the version I have used (MCNPX 2.1.5) I have used only the default physics. (Earlier attempts to explore other hadron options above about 5 GeV using 2.1.4 were very unsuccessful – the code would crash!)

I am also using neutron cross-sections which go from thermal to 20 MeV. Thus, what neutrons below 20 MeV do is governed by these cross sections files, and above this energy, some model is used. The default physics model at very high energy (> 5 GeV) is an old version of FLUKA. Unfortunately, political considerations have inhibited upgrades to newer versions.

I have had some discussions regarding the quality of physics models with a very sophisticated MCNPX user (an alpha user!) named Paul Goldhagen. (Both Don Lazarus and Henry Kahnhauser know Paul). In his opinion, if one is mostly interested in neutrons, the 'best physics' would be to use Bertini together with the 150 MeV cross sections. (I think what I am doing is better *given* that I do not have the 150 MeV cross sections.) This should be possible 'any day' if Steve Kahn gets new code and the cross sections from Arnie. To choose this option (if one had the 150 MeV cross sections), the input data described in the MCNPX manual should have ipreq set to 1 on the 'lca card' and the first 4 entries on the 'lcb card' set very high.

Geometry & Tallies

Chapter 3 of the MCNP manual describes what must be in an input file. This includes a description of the geometry of the problem. The beginning for a new user is to learn how to describe the geometry. This is easily learned from reading chapter 1 of an MCNP manual (especially the introduction) and the beginning of Chapter 3. The idea is simply that one chooses *surfaces* from the list in chapter 3 to enclose regions of space called *cells*. Each cell has an importance for each particle type being transported. An importance of 0 means the cell is a sink for any particle entering the cell. Every geometry must be completely surrounded by 0 importance space (for all particle types) to avoid going 'forever.'

Another part of the input file is simply a description of what output is wanted. Output is called *tallies* by MCNP(X). There are various types of tallies. Mostly I have used tally types 2 (flux on a surface) and 6 (energy deposition in cells). One slightly tricky point is that, in order to get a valid surface tally, the surface must be used in the definition of a cell. Surfaces can be (and are for good reasons) defined without regard to cells, but if you try to get a tally on a surface not part of cell definition, the result is always 0 and nothing like an error message appears!

Estimating Dose

A flux can be modified by what MCNP calls a 'dose function.' In fact, I have estimated dose (equivalent) by multiplying by such a function. The MCNP manual gives flux to dose conversion functions only for low energy neutrons and photons. I have used different flux to dose conversion functions for hadrons – those given by Stevenson – simply because they are the only such functions I am aware of that include protons and pions, and go to very high energy.

Similarly for photons, an appendix of the MCNP manual goes to 15 MeV. I have used MCNPX itself (energy deposition in tissue with QF = 1) to generate flux to dose numbers, but I have never had a need to go higher than 100 MeV.

The input file records ('cards' – MCNP goes back a long ways) for hadrons I have used are:

```
c Flux to dose conversion for neutrons (in 10-10 )
c
de2 1.0e-8 3.0e-7 2.0e-6 7.0e-4 2.1e-3 1.1e-2 .112 1.122 7.079 &
22.39 35.48 70.79 281.8 891.2 1778. 8912. 28180. 112200.
df2 7.7 10.4 10.3 6.2 6.3 10. 78.8 339.2 423.43 623.85 524. &
321. 344. 677. 1005. 2130. 3500. 6290.
c
c Flux to dose conversion for protons(in 10-10 )
de12 1.0 5.0 10. 35.5 70.8 141.3 447. 562. 1122. &
8912. 28180. 112200.
df12 1.0 15.0 1000. 3130. 1825. 1230. 828. 898. 1125. &
2480. 3870. 6690.
c
c Flux to dose conversion for pions(in 10-10 )
de22 1.0 5.0 10. 35.5 70.8 141.3 447. 562. 1122. &
8912. 28180. 112200.
df22 1.0 15.0 1000. 1640. 1445. 1355. 1330. 1331. 1345. &
2520. 3910. 6720.
```

And for photons are:

```
c Photon Flux to dose (Mcnpb manual - same units - crap on
c low end of the spectrum)
de0 .00001 .001 .01 .015 .02 .03 .04 .05 .06 .08 .10 .2 .3 .4  &
.5 .6 .8 1.0 2. 3. 4. 5. 6. 8. 10. 11. 13. 15. 30. 50. 100.
df0 .0001 1.0 7.72 3.08 1.63 .71 .43 .33 .31 .33 .41 .96 1.54 &
2.14 2.53 3.17 4.08 4.97 8.42 11.1 13.2 15.4 17.4 21.4 25.3 28.6 &
32.8 36.9 70. 120. 160.8
```

(Note that a c in column 1 followed by one or more blanks is a comment record, and that an ampersand indicates continuation onto the next 'card')

These records define simple functions. The first record for the neutrons says that, applied to tally number 2, a fluence of 1 n/cm^2 with energy 10^{-8} MeV corresponds to 7.7×10^{-10} rem (note the units of 10^{-10} in all cases). For the photons, the '0' in de0 and df0 means that the dose function applies to all tallies.

The Source Specification

Another part of the input file is the source specification 'SDEF card.' This can be tricky, and the new user is urged to read the manual carefully here. There is a great deal of flexibility in using functions defined solely by the input file in MCNPX. Especially useful are the SI, SP, and SB 'cards' which can be used to define tabular functions and sampling probabilities (SB) which differ from the actual probabilities (SP) so that 'tails' of distributions can be examined. Note also that correlations are possible – see example 6 on the bottom page 3-54 in the MCNPB manual. I have used as many as 27 distributions in one source that correlated the energy with the polar angle.

Energy Deposition

Energy deposition is not the strong point of (the current) MCNPX code, but a recent calculation I did of the MECO coil agreed very well with a modern GEANT. (CASIM did very poorly.) MCNPX does not track knock-on electrons, so that it will overestimate energy deposited in a thin window. Another characteristic that the user should be aware of is that the energy of created particles that are not transported are deposited at the spot of creation. Suppose, for example, that you are transporting only protons, neutrons, pions, pi-0's, and photons. This is done via the MODE 'card' (and photons include electrons in some approximation). When a lamdba is created, its energy will be deposited at that point. This is no big deal and usually does not motivate one to transport lambdas, but the user should be aware that this is what happens.

Weaknesses of the Code.

Besides not having the best physics models available for terrible reasons, the only weaknesses of MCNPX that I am aware of is the lack of an external magnetic field, and some difficulty doing 'deep penetration' calculations.

In fact, I have rarely found the lack of magnetic field capability to be a serious drawback. I now keep CASIM around *only* to do field-on vs. field-off to scale MCNPX results. (This is not really correct, but the best method I can think of.) Most applications have only a small correction in comparison to the usual systematic uncertainties.

Although CASIM is good at giving you an answer in deep penetration calculations, since it is wrong the benefit is of dubious value. There is actually a mechanism in MCNPX which can be very useful for doing deep penetration estimates. The user should read about the SSW (Surface Source Write) and SSR (Surface Source Read) capabilities in the MCNP manual.

Status of Code/Location of Files

As mentioned above, I have used an 'old' version (2.1.5) of MCNPX, and newer versions are available. The executable I use is just a copy of an executable I obtained from Steve Kahn.

The cross-sections I use are on the rcf computers in the directory /u0b/stevens/mcnpx/linux/Xsection. (I execute on the machine now called rplay20, but there is a continual threat to change its name.) I am not really sure whether Steve has all the data files that exist in this directory. However, it is important to note that these are old data files that only go to 20 MeV (measured neutron data), and migration to the '150 MeV' cross sections is overdue. There is no reason why Steve cannot do this; in fact, he said he was going to do this in (roughly) March of 2002, but it has not been done. Again, Arnie Aronson would provide Steve with anything he would need.

There are many example input files in the directory /u0b/stevens/mcnpx/stevensrun and the directory (on rplay20 only) /home/stevens/mcnpxrun.

Further remarks noted by Kin Yip from Alan Stevens:

(1) Flux in principle should be per cm^2 per second. And what is called "flux" in MCNP(X) should be really called "fluence", which is the time integration of flux.

(2) Alan likes to use the following densities:

   a. Soil : 1.9 g/cc
   b. Light concrete : 2.35 g/cc
   c. Steel (Fe actually) : 7.7 g/cc

   And -7.7 (-ve 7.7) means that it is in g/cm^3 instead of how many particles per volume.

(3) Files
   a. .60c → 20 MeV neutron files (c = continuous)
   b. .24c → 150 MeV neutron files (c = continuous)

New additions by Kin Yip:

1. **F5 (detector tally) is only applicable for energies below or equal to the maximum energy that the data files offer such as 20 MeV or 150 MeV, depending on what data files that one is using.**
    a. **Alan thought that this is OK in most cases because one typically uses F5 when the neutron/photon flux/dose etc. is very small and in those cases, most neutrons/photons are of low energy.**
    b. **But Laurie Waters (one of the authors) told me (~June 2004) that as long as the energy in any part of the problem is greater than the data file energy, F5 tallies would be WRONG !!!**
    c. **Most recently, MCNPX has used "isotropic" angular distribution for energies > data file energy. So, we have an approximate treatment for F5 tallies for energies above data file energy, which may be correct.**

2. **F2 tallies would be zero if the surfaces are not used in the cell definitions. That is, even if you define certain surfaces in the surface card portion but if they are NOT used in the cell card portion (and no other identical surfaces are present in the entire geometry), the F2 tallies would be zero.**

3. **If you want to see the weight window mesh when viewing the geometry (ie., using the "ip" on the command line), you need to include the line like "wwg:p" in the input file; otherwise, you would not see the weight window mesh. Alternatively, one could add wwinp=xxxx.e (where xxxx.e is the weight window file) in the command line in order to view the weight window mesh.**

4. **To plot tally results in MCNPX after the simulation is run, use the following command:**

    mcnpx n=junkv. z r=result.r

    and then enter at the 'mcplot>' prompt :

    tally 4 label "proton" coplot tally 14 label "photon" coplot
    tally 24 label "electron"

Be aware that one can't type too long a line, probably something like the FORTRAN constraint. Instead, one may put "coplot" at the end of a line and put other tallies at the next line.

5.