

# PRACTICAL ADVICE ON MODELING COMPLEX SYSTEMS IN MCNP

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## ABSTRACT

This paper is based on practical experience of neutron and gamma calculations supporting design work on ITER, the International Thermonuclear Experimental Reactor. This is a very large and very complicated system with a geometry that can be modeled adequately only in a Monte Carlo calculation. MCNP4B<sup>1</sup> is currently used. Due to the complexity of the geometry, the amount of calculations required and the limited time available, it is necessary to have several people working on the model. Experience has shown that this requires explicit agreement on certain guidelines. Since this may also be relevant to other cases where large and complex systems have to be modeled using MCNP, some such guidelines are described here and illustrated with examples.

The system should be broken down into zones, each with its own range of cell, surface, universe, transformation and material numbers. Basically, each zone should be the responsibility of one modeler. However, it will still be necessary for each modeler to be able to understand the other parts of the model, so certain guidelines for modeling within each zone are also needed. The cells should be kept simple and small enough to provide sufficient resolution for importances or weight windows. The model should be well commented, using a hierarchical system of comments. As far as possible, the surfaces bounding cells should be ordered in a consistent fashion.

## 1. BACKGROUND

The subject of this paper is how to cope with the problems arising when many people have to work on the same MCNP model. Such a situation arose in connection with the nuclear analysis of the International Thermonuclear Experimental Reactor, ITER. This is a very large and very complicated system. Some locations of interest are more than ten meters from the plasma, where the source is

located, and more than a thousand cells are necessary to model even a minimum sector (9 degrees for the original design with 20 toroidal field coils).

There are several reasons why many people have to be involved in this work, notably:

- There are many different quantities that need to be calculated at many different locations. All this work would be beyond the capacity of any one person.
- Since mistakes are easy to make, especially in modeling such a large and complicated system, it is desirable to make at least two calculations of each quantity of major interest to provide crosschecks.
- When calendar time is critical, it is necessary to involve many people in the construction of the basic model, describing the reactor as a whole, since it would take too long for one person.

However, having more than one person working on the same model also leads to problems. Each one will have his/her own style of modeling, and it's difficult for one of them to understand the parts modeled by another. Also, it becomes both more difficult and more important to maintain a consistent numbering scheme, so that the same number doesn't get assigned to two cells or two surfaces. There is, of course, in addition the possibility that the model may be inefficient, especially if one or more of the people involved doesn't have a good grasp of how to construct an efficient MCNP model.

In addition, one must take into account that, in the design stage, the system to be modeled will be changing all the time. In the words of one frustrated modeler, "Modeling ITER is like trying to paint a portrait of a puppy. It won't stay still long enough." This accentuates the need for a model that is easy to understand and modify.

Thus it is necessary to agree on some guidelines before starting construction of an MCNP model of a complex system. This will be illustrated with reference to the provisional recommendations drawn up concerning how to model the reduced cost version of ITER in MCNP. The recommendations may seem obvious, but experience has shown that they are necessary.

## 2. OBJECTIVES

The model should fulfill the following requirements:

- (1) It must be easy to:
  - (1a) construct as a cooperative project, involving several modelers;
  - (1b) understand;
  - (1c) modify;

(1d) debug.

(2) It must be fast, which requires:

(2a) simple cells, with few surfaces (for fast tracking);

(2b) sufficient spatial resolution for weight windows.

The codes identifying these requirements are used below at the ends of some paragraphs as a shorthand way of justifying the decrees therein.

### 3. HOW TO ACHIEVE THE OBJECTIVES

- Make the basic model for one sector stretching in the toroidal direction from the midplane of an equatorial port to the midplane of an adjacent toroidal field coil ( $360 \text{ degrees} / 2n$ , where  $n$  is the number of field coils. This is the basic symmetry sector of the machine.) However, keep in mind that strict  $2n$ -fold symmetry does not always pertain, so be prepared to cope with larger sectors. (1c)
- Divide the geometry into several zones, each of which is the responsibility of one modeler. These zones must be bounded by surfaces agreed on by everyone. Within each zone, use 4-digit surface and cell numbers within a given range, reserved for that zone. (Typically 1000 numbers, all with the same first digit, would be available for each zone, but other methods may be used. However, it is desirable that the surface numbers and the cell numbers for each zone should form a contiguous range and that the range should be the same for both surface and cell numbers. The range(s) for each zone should be specified in the top-level comments identifying the zones.) Zone boundary surfaces will have numbers of less than 4 digits, as may some special cells. (1a,b,c)

The restriction to 4 rather than 5 digits is a provision for possible requirements to cope with larger sectors. Each 9-degree part of such a larger sector can then be identified by the first digit of a 5-digit number. (1c)

Each zone should also have its own range of material numbers, universe numbers and transformation numbers. However, since the same material may occur in several zones, using the same material number in different zones rather than defining the same material several times is allowable, provided the modelers responsible agree explicitly on this. For each such common material, one modeler responsible for keeping it up to date should be designated. Changes amounting to making it a different material rather than updating it are permitted only if all modelers agree. Use of the same universe or the same transformation in different zones is best avoided, unless the same modeler is responsible for all zones in question. (1a,b,c)

It is possible that the above procedure may lead to the same surface being defined several times, with different numbers, in different zones. This is no problem.

- For speed of tracking, cells should be simple, with few boundary surfaces. If any cell has more than 8 surfaces, consider simplifying it. In particular, the union operator (:) should generally be avoided. Break up composite cells into several simpler ones. (1b,c,2a)

One case where the union operator is acceptable is where the radius of curvature of a surface changes. In such cases, a composite surface (rather than a composite cell) will often make modeling easier than if the cell is split in two. The ambiguity surface delimiting the parts of the composite surface should be given just before and just after the union operator for clarity. An example is given in Section 5.

It should also be noted that a complex description of the outside world makes less difference to the tracking time than a complex description of a cell in which particles actually have to be followed.

- To provide sufficient resolution for importances or weight windows, cells should not be too thick in the direction in which importances/weights vary, usually the direction of the neutron current. (Note that this no longer applies when superimposed importances are used, as in A3MCNP.) For ITER the recommended maximum thicknesses are 4.5 cm in materials without penetrations through which neutrons can stream and 7.5 cm when small penetrations are present, based on the observation that these are typical values for the shielding thicknesses needed to halve the fast flux, thus appropriate spacings for a doubling of the importance. Note that in some cases it will be necessary to apply this restriction in two dimensions, when there is a need for the importances to vary in both. An example is the walls of the equatorial port, where the importance may have to vary both lengthwise along the port (in those places where shielding is present inside the port) and through the wall. (2b)

To make the cell descriptions easier to understand, the surfaces should be given in a consistent order and, as far as possible, arranged in columns so that equivalent surfaces of different cells are below each other. For instance, for hexahedral (box-like) cells the surfaces might be ordered as: y+ y- z+ z- x+ x-, where y+ denotes the upper limit for y etc. (1b,c,d)

## 4. OTHER RECOMMENDATIONS

Never give densities with more than 4 significant digits. It's a pointless waste of space, the densities are never that accurate anyway.

Whether one uses atomic or mass densities is pretty much a matter of taste. However, for water mass densities are preferable. That way it's easier to see if the effect of temperature and pressure on density has been taken into account. (1d)

One of the more troublesome causes of input error is accidental blank lines. To make these easier to spot, one should designate some column that will never be empty except on blank lines, so that all a user needs to do is to scan the input along this column to find blank lines. (Finding blank lines may sound easy, but it is not if you are dealing with thousands of lines and have to look at each one individually.) Column 6 may be a suitable candidate, at least when importances are not used. Alternatively, column 54 may be suitable in the cell block when importances are included on the cell cards. (For the sake of

neatness and convenience in changing importances, it's a good idea to let all importances begin in the same place. Somewhere around column 54 is suitable if both neutron and gamma importances are used.) (1c,d)

Generous use of comments is recommended. A hierarchical comment system should be used to make the structure clearer, for instance:

```
C
C      -----
C      | CELL BLOCK |
C      -----
C
```

(similarly for the surface and data block)

```
C
C      ===== FIRST LEVEL COMMENT =====
C
```

```
C
C      SECOND LEVEL COMMENT
C
```

```
c
c      ----- third level comment -----
c
```

```
c      fourth level comment
```

First level comments should be used to identify the zones mentioned above and lower levels within the zones. This comment system should be used at least in the cell and surface blocks and, as applicable, in the data block as well. (1b)

In this paper we have often referred to importances rather than weight windows. Actually, weight windows are usually preferable, but, unless energy-dependent weight windows are required, letting the program calculate the weight windows from given importances, using the SWITCHN parameter on the WWP card, is often the most convenient method of specifying the weight windows.

## 5. EXAMPLES

Figure 1 shows an example of how a zone structure could be implemented. This figure is a vastly simplified image of ITER. Non-void regions are hatched. The details of the geometry and the actual cell structure are not shown; each of the zones shown could include several hundred cells, though not all of them would be visible in a single cut through the system. Many major features of ITER are entirely missing from this figure, which is merely intended to serve as a rough illustration of the principle of

zoning. The zone boundaries are shown as thick red lines, and the non-void parts of different zones are shown in different colors.

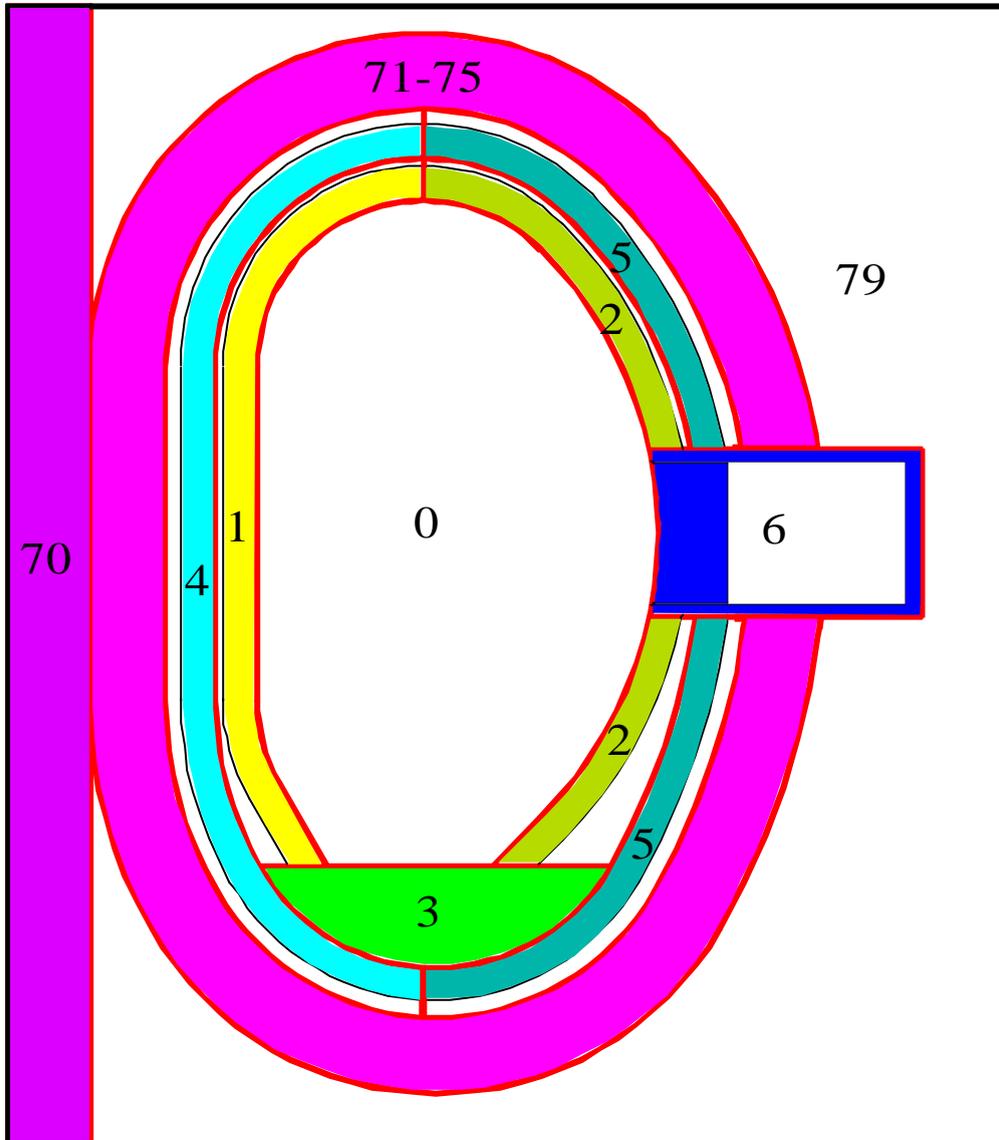


Fig. 1. A Simplified Example of a Zone Structure

Specifically, the zone structure would in this case be as follows:

Cell numbers	Zone
0xxx	Plasma
1xxx	Inboard shield/blanket
2xxx	Outboard shield/blanket
3xxx	Divertor
4xxx	Inboard vacuum vessel
5xxx	Outboard vacuum vessel
6xxx	Equatorial port with contents
70xx	Bucking cylinder, central solenoid
71xx to 75xx	Toroidal field coils, inter-coil structure
79xx	Surrounding voids

Each modeler could then concentrate on one or more zones without having to worry about the details of how the other zones were modeled.

Actual examples of comments from a model built on these principles are given below:

First level comment:

```

C
C     ===== SHIELD/BLANKET ASSEMBLY: OUTBOARD =====
C
c     numbering scheme: the first of 4 digits is 2
c     the second digit is the module number - 7
c     for the gaps separating modules toroidally, it's 0
c     for the manifold and backplate, it's 9
c     the remaining digits are, in the central modules:
c     01 for the Be
c     02 for the Cu
c     00 for the bulk shield, sometimes subdivided into 03...
c     in the external modules:
c     41 for the Be
c     42 for the Cu
c     40 for the bulk shield, sometimes subdivided into 03...
c     otherwise:
c     80... for gaps separating modules poloidally
c     90... for shielding blocks between modules

```

Second and third level comments:

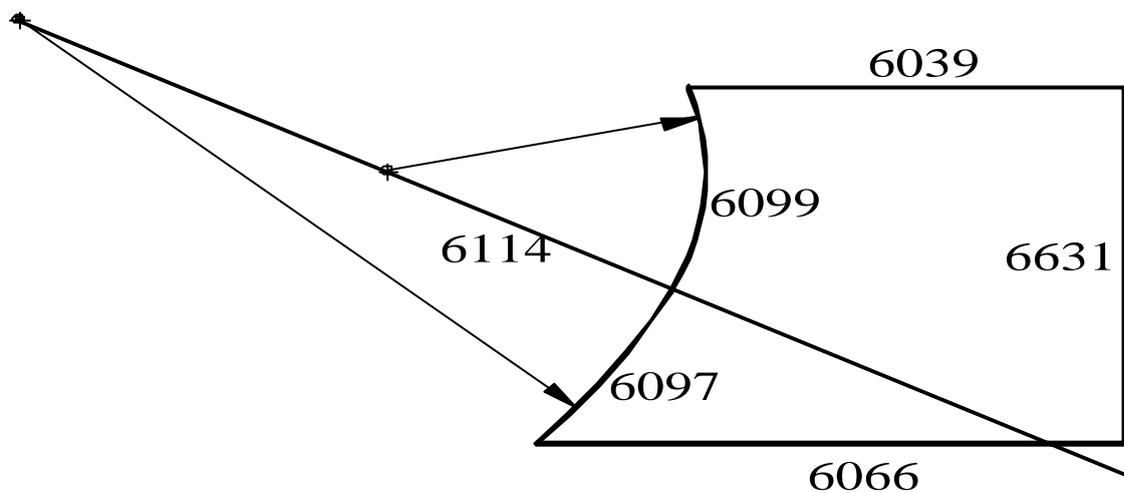
```

C
C     MODULE 8
C
c     ----- central part -----

```

Thus the first cell following these second and third level comments is cell 2101, which is the beryllium armor of the central part (01) of module 8 (8-7 = 1) of the outboard shield/blanket (zone 2).

The second example shows a cell modeled in accordance with the principles suggested here. It contains a compound surface, which requires the use of a union operator (:); otherwise it's a simple box. Other parts of the same object should be modeled as separate cells rather than making this cell more complicated. The remarks below the cell description identify the surfaces, which in this case are ordered according to the system described in Section 3.



```

cell description
6251 65 8.605e-02   -6143 6041 -6039 6066 -6631 (6097 -6114 : 6114 6099)
cell #  m#, density      y+      y-      z+      z-      x+      x-
  
```

Fig. 2. Model of a Cell With a Compound Surface

## REFERENCES

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<sup>1</sup> J.F. Briesmeister, Editor, MCNP—A General Monte Carlo N-Particle Transport Code. Version 4B. LA-12625-M, Version 4B, March 1997. Available at <http://www-xdiv.lanl.gov/XCI/PROJECTS/MCNP/manual.html>.