# MONTE CARLO ADVANCES FOR THE EOLUS ASCI PROJECT

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## ABSTRACT

The Eolus ASCI project includes parallel, 3-D transport simulation for various nuclear applications. The codes developed within this project provide neutral and charged particle transport, detailed interaction physics, numerous source and tally capabilities, and general geometry packages. One such code is MCNP™ which is a general purpose, 3-dimensional, time-dependent, continuous-energy Monte Carlo fully-coupled N-Particle transport code.

The major new capabilities recently added to MCNP4C are:

(1) Macrobodies: a geometry simplification similar to combinatorial geometry;
(2) Unresolved resonance range probability table neutron physics;
(3) New ENDF/B-VI data library sampling schemes;
(4) Delayed neutrons;
(5) Significant electron physics enhancements;
(6) Enhancements for PC computing platforms;
(7) Extension of the perturbation capability to criticality calculations and cross-section dependent tallies;
(8) Superimposed importance meshes so that geometries no longer need be subdivided for variance reduction;
(9) Alpha eigenvalue search;
(10) Parallel computing enhancements.

Significant advances are also being made in the areas of modern software engineering and parallel computing. These advances are described in detail.

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## 1. INTRODUCTION

The Eolus ASCI project is situated in the Diagnostic Applications Group (X–5) of the Applied Physics Division at Los Alamos National Laboratory. The charter for this project includes parallel, 3-D transport simulation for various nuclear applications. The codes developed within this project provide neutral and charged particle transport, detailed interaction physics, numerous source and tally capabilities, and general geometry packages. One such code is MCNP[1] which is a general purpose, 3-dimensional, time-dependent, continuous-energy Monte Carlo fully-coupled N-Particle transport code. Neutrons are modeled from 0-20 MeV; photons and electrons are modeled from 1 keV to 100 GeV. In these ranges, MCNP provides a nearly-predictive capability of how radiation interacts with matter.

Summarized here are the major capabilities that have been recently added to MCNP version 4C and projects underway in the areas of modern software engineering and parallel computing.

## 2. NEW CAPABILITIES IN MCNP4C

MCNP and its predecessors have existed at Los Alamos since 1963. Every few years a new version is released with sufficient quality that it can stand for a few years without modification. MCNP4C[2] was released in January 2000 along with a comprehensive user manual.[1]

Three-dimensional modeling is a major objective of the ASCI program. MCNP has always had a fully 3-dimensional surface-sense geometry capable of modeling any space bounded by 1st and 2nd degree surfaces (conic sections) and 4th-degree elliptical tori. These geometries are general and flexible, but also can be complex and difficult to describe. In MCNP4C macrobodies are added. Macrobodies in MCNP4C are surfaces that mimic combinatorial geometry bodies like those used in the Integrated Tiger Series[3] (ACCEPT) and other 3-dimensional Monte Carlo codes. The MCNP4C macrobodies are BOX, RPP (right parallelepiped), SPH (sphere), RCC (right circular cylinder), and RHP or HEX (right hexaganol prism.) These macrobodies can be used in combination with all the former MCNP surfaces. Table I illustrates how the new macrobodies greatly simplify the input for an MCNP geometry. The geometry is an hexagonal prism within another hexagonal prism. Section A of Table I shows the old MCNP4B specification, and Section B of Table I shows the new, simpler, MCNP4C specification.

Predictive physics models are another objective of the ASCI program. MCNP4C improves upon the already first-rate continuous-energy neutron physics package by adding unresolved resonance range probability tables.[4-5] The statistical treatment of unresolved resonances can improve hard spectrum neutron problems whenever neutron resonance self-shielding is important. In particular, it can make significant differences in the calculation of the criticality eigenvalue, $k_{eff}$, for plutonium critical assemblies with intermediate spectra and substantial increases in reactivity for systems with a large amount of $^{238}U$ and intermediate spectra.

Table I. Specification of an Hexagonal Prism Within Another Hexagonal Prism

A. MCNP4B Geometry Specification Without Macrobodies

```
MCNP4B hex in hex
1 100 .01    -11 12 -13 14 -15 16 -17 18
2 200 .01    -21 22 -23 24 -25 26 -27 28
             (11:-12:13:-14:15:-16:17:-18)
3 0          21:-22:23:-24:25:-26:27:-28

11  py    2.
12  py   -2.
13  p    -8.6602540E-01    .5     0.   2.
14  p    -8.6602540E-01    .5     0.  -2.
15  p    -8.6602540E-01   -.5     0.   2.
16  p    -8.6602540E-01   -.5     0.  -2.
17  pz    4.
18  pz   -4.
21  py    3.
22  py   -3.
23  p    -8.6602540E-01    .5     0.   3.
24  p    -8.6602540E-01    .5     0.  -3.
25  p    -8.6602540E-01   -.5     0.   3.
26  p    -8.6602540E-01   -.5     0.  -3.
27  pz    5.
28  pz   -5.
```

B. MCNP4C geometry specification with macrobodies

```
MCNP4C hex in hex
1 100 .01    -10
2 200 .01     10 -20
3 0               20

10   rhp  0 0 -4   0 0 8    0 2 0
20   rhp  0 0 -5   0 0 10   0 3 0
```

Neutron physics has also been improved by adding new ENDF/B data library sampling schemes in anticipation of new ENDF/B-VI rev. 5 data. Tabular-angular sampling distributions are added to the MCNP ACE (A Compact ENDF) format for representing angular information in finer detail than through the 32 equi-probable bin distribution. Neutrons and photons are now handled consistently within the energy-sampling portion of ENDF laws 4, 44, and 61, which use emission-energy tables.

A time-dependent delayed neutron treatment now produces a more accurate fission model in fixed-source and criticality calculations. A natural sampling of prompt and delayed neutrons is now the default. An additional delayed neutron biasing scheme is available because of the low probability of a delayed neutron occurrence.

Electron physics enhancements were made to make MCNP4C more current with the Integrated Tiger Series (ITS) version 3.0.[3] Improvements have been made to:

1. Density effect calculation for stopping power;

2. Radiative stopping power upgraded to the ITS3.0 Seltzer model;

3. Bremsstrahlung production (intensity and angular distribution);

3. Impact ionization.

Variance reduction has been enhanced to improve the sampling of the photons produced from a bremsstrahlung event. The fluorescence and k-xray relaxation models in MCNP have been made more consistent with each other. A new electron library, EL3, has also been prepared with better data.

A number of improvements have been added for PCs, including the ability to compile on PCs with FORTRAN 90 using either Lahey (Version 5.50) or Digital Visual Fortran (Version 6.0) compilers. Plotting is with an X-window interface using either compiler, or one can opt for Windows graphics (98 or NT) using the Lahey Winteracter library or the DVF QuickWin library.

The differential operator perturbation technique has been upgraded to enable perturbations of tallies with cross-section dependent tallies.[6-7] Previously,[8] a laborious correction had to be made for determining perturbations to criticality ($k_{eff}$) and reaction rate tallies involving cross sections. Now the perturbed values of $k_{eff}$ are automatically printed for each perturbation along with the proper standard deviations in criticality problems. Cross-section dependent tallies, particularly heating tallies, work with perturbations without further adjustment.

A major advance has been made in MCNP variance reduction with the new superimposed importance mesh and weight window enhancements.[9-11] Before MCNP4C, users had to subdivide geometries sufficiently well to specify importance functions for variance reduction. Simple problems which should be described with a few dozen geometric cells often required hundreds of cells to specify smoothly changing importances. Now the simple geometry can be specified with an importance mesh superimposed in either rectangular or cylindrical geometry. Further, the weight window generator technique of MCNP may be used so that the code will determine the optimum importance function for the superimposed mesh. An assessment of the revised weight window capabilities added in MCNP4C indicated that (1) MCNP4C utilized weight windows comparably to MCNP4B, but (2) generated cell-based weight windows 50% better than MCNP4B and (3) that superimposed mesh windows could be superior to cell-based windows and eliminate the need to subdivide geometries for importances. The superimposed mesh windows and their assessment are described more fully in another paper in this meeting.[12]

MCNP4C also has added an alpha eigenvalue search in addition to the $k_{eff}$ criticality eigenvalue.[13] The alpha eigenvalue is

$$N = N_O \, e^{\alpha t} \qquad (1)$$

where N is the neutron population at some time t that builds up from some initial population $N_o$. Alpha is of interest for comparison to benchmark calculations and comparison to deterministic transport codes such as DANTSYS.[14] The alpha capability allows positive and negative alpha searches and a fixed positive or negative alpha value to be used in a $k_{eff}$ eigenvalue calculation. Negative values of alpha can result in a time creation (n,2n) delta scattering reaction. Positive alpha is treated as time absorption.

There are many more smaller enhancements in MCNP4C including cumulative tallies, improved coincident surface treatments, pause and universe level geometry plotter commands, and more. The MCNP manual has been significantly rewritten and translated from TeX to FrameMaker.

## 3. MODERNIZED SOFTWARE ENGINEERING PRACTICES

A major thrust of the MCNP ASCI program effort is in the area of software engineering practices. Although the above list of new features is impressive, the top priority for MCNP is not new capabilities, but rather quality.

Major components of the MCNP quality program are building upon the past (rather than constantly starting over) and widespread distribution of the code for maximum peer review. Over 1000 person years have been invested in the Monte Carlo methods and the code itself. Cash rewards are issued for any bug found in the code. MCNP is distributed for Los Alamos by the Radiation Safety Information Computational Center (RSICC) in Oak Ridge, TN, pdc@ornl.gov, and is used by an estimated 3000 individuals worldwide. An internet user forum is sponsored by Los Alamos, mcnp-forum@lanl.gov.

Another component of the MCNP quality program is the MCNP Software Quality Assurance (SQA) Plan[15] which is consistent with the requirements of IEEE-730.1[16] and the guiding principles of ISO 9000.[17] This SQA Plan is presently being rewritten to reflect a modernization in software engineering procedures. The Eolus code development team is currently implementing the RAZOR software package for configuration management, regression testing, and bug tracking. Once implemented, this package will formalize the process of code modifications and documentation, automatically generating required SQA reports for the release of new code versions. In the 1999 ASCI software engineering assessment of the Eolus project, our SQA process received an average SEI rating of 4 on level 2 and 3 key process areas. This rating puts Eolus in the 80-90 percentile of code development projects.

## 4. PARALLEL ENHANCEMENTS

The ability to efficiently utilize the massively parallel ASCI hardware, such as the Los Alamos Blue Mountain Silicon Graphics (SGI) computers, is another major ASCI thrust area. In MCNP4C the ability to compute on massively parallel platforms has been enhanced. Distributed memory multiprocessing (DMMP) and shared memory multiprocessing (SMMP) methods are both supported— separately or in combination.

DMMP is supported through either PVM[18] or MPI.[19] The DMMP communication pattern has been reworked to be fully compatible with either PVM or MPI. The necessary calls to the low-level libraries are isolated to a single module of the code.

SMMP is supported through OpenMP™.[20] The addition of threading allows efficient computation on shared-memory platforms such as SGI Origin2000 (ASCI Blue Mountain) hardware. The SMMP communication has been somewhat hardwired for OpenMP, but is encapsulated into only a few routines to allow localized modification for other shared memory paradigms.

By combining shared memory threading with distributed memory multiprocessing, most MCNP calculations can be run efficiently on large numbers of processors for high throughput. Clusters of multi-processor computers can be linked together to do a single calculation. Calculation of memory intensive problems is also enhanced by the use of read-only shared memory; only that which each thread needs to change need be duplicated.

Care has been taken to ensure that the same answer will be obtained from any processor configuration for almost all problem types. Extensive testing has been done on 2000+ processors with some calculations run on all 6144 processors of the ASCI Blue Mountain machine.

## 5. SUMMARY

MCNP provides important modeling and simulation capabilities in the DOE/ASCI program. Many significant code enhancements have been added, software engineering practices are being modernized, and massively parallel capabilities are being developed.

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