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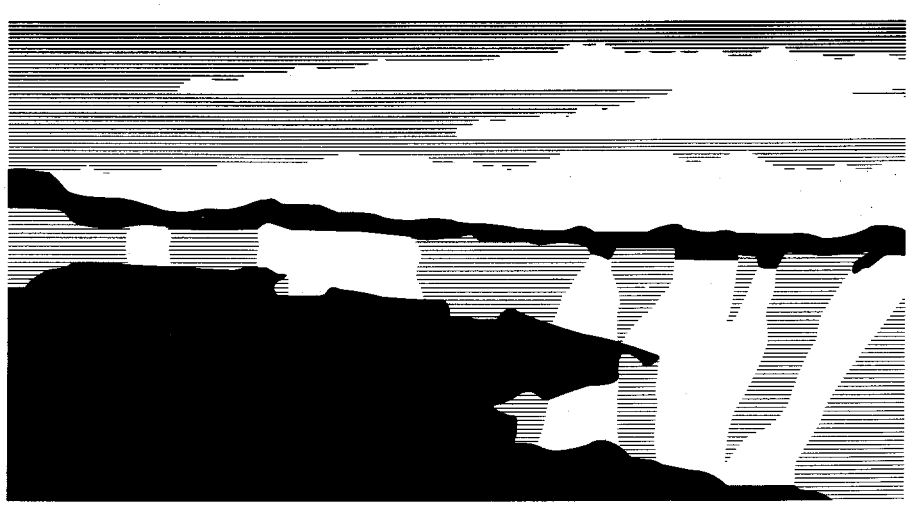

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MCNP^{TM} Monte Carlo: A Precis of MCNP

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ABSTRACT

MCNP^{TM*} is a general purpose three-dimensional time-dependent neutron, photon, and electron transport code. It is highly portable and user-oriented, and backed by stringent software quality assurance practices and extensive experimental benchmarks. The cross section database is based upon the best evaluations available. MCNP incorporates state-of-the-art analog and adaptive Monte Carlo techniques. The code is documented in a 600 page manual[1] which is augmented by numerous Los Alamos technical reports which detail various aspects of the code. MCNP represents over a megahour of development and refinement over the past 50 years and an ongoing commitment to excellence.

1. INTRODUCTION

MCNP is a general time-dependent neutron, photon, electron Monte Carlo transport code system. The code system can transport these particles in an arbitrary 3D geometry constructed of intersections and unions of regions of space bounded by 1st, 2nd and up to 4th order surfaces. Sources can be arbitrarily specified for neutrons, photons, or electrons as well as selected from a robust library of typical neutronic sources. Criticality eigenvalue, k_{eff}, problems can also be solved. The results of a calculation are scored in user specified tallies with statistical estimates of convergence and confidence automatically given. MCNP is capable of running on almost any platform, from vectorized/parallelized Cray mainframes to 386 PCs.

MCNP is distributed for Los Alamos by the Radiation Shielding and Information Center (RSIC) in Oak Ridge, Tennessee, and OECD/Nuclear Energy Agency (NEA) in Paris, France. There are approximately 3000 users world-wide.

This paper will first give a short review of the historical background of MCNP and some of its current industrial applications. The broad use of MCNP in industry shows that the code system is very flexible and can be readily adapted to a myriad of applications. Next, a few of the current features of MCNP4B, the soon-to-be released code update, will be presented. This paper concentrates on those features that are attractive for industrial applications. One of the most important, though not strictly an MCNP feature, is the general release of ENDF/B-VI cross sections for use in the code. Other noteworthy features, include cross section plotting which can be used to help qualitatively assess the results of calculations, differential operator perturbation technique applied to the transport data (cross sections, geometry, etc.) to assess the impact of small variations or the intrinsic uncertainties in these components, and an improved electron transport algorithm for more accurate transport results. Another class of new features is the software side which includes fault tolerant PVM, enhanced Xwindow graphics, and postscript output, to mention just a few. Finally, a brief review of the World Wide Web support for MCNP will be presented.

2. MCNP BACKGROUND AND OVERVIEW

As mentioned earlier, MCNP represents about a megahour of development effort, benchmarking, and quality assurance. (To put this new unit of effort in perspective, a person year is typically 2000 hours or 2 khours. So the megahour represents several hundred person years.) This development work began during the Manhattan project and used at that time the most advanced computing capabilities available (fly wheels, mechanical adding machines, decks of cards,

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etc...)[1,2] During the intervening years, the code has followed and sometimes nurtured the development of computing technology. Briefly, the first multipurpose code version, MCS, was written in 1963.[3] The first public release of the neutron photon code, MCNP was in the mid-70's.[4,5,6] The 1980's saw the release of MCNP3, MCNP3A, and MCNP3B which brought the code into standard Fortran and incorporated features such as generalized sources, repeated structures, criticality, multigroup option, and tally plotting. The 90's are the decade of version 4. MCNP4 was released in 1990 (MCNP4.2 was distributed from RSIC in 1991) and was specifically designed for UNIX operating systems. MCNP4 also included electron transport based upon the Integrated Tiger Series (ITS),[26] shared memory multitasking, thick target bremsstrahlung, and better random number control. MCNP4A was released in 1993 and included such features as dynamic memory allocation, X-window graphics, and distributed processor multiprocessing[35]. MCNP4B is expected to be released in about one year's time, 1997, and a few of its features will be presented later.

During the years of development the code system has been at the forefront of Monte Carlo methods and techniques, of experimental benchmarking and comparison, and of computer innovations and applications. Many innovations have been incorporated into the code after undergoing a thorough validation program; some, like those mentioned above, have withstood the test of time while others have not and have been eliminated (such as the ablility to run in obsolete operating systems or once more collided flux estimators.) Similarly, specific capabilities, such as importance sampling or weight window generation, have been implemented in such a way as to allow the skilled user to take advantage of them while not penalizing the neophyte. This constant improvement is a reflection of the MCNP philosophy of "Quality, Value and New Features" in action. The issue of quality is of paramount importance and will be discussed later with respect to software quality assurance. Put simply, quality means that the code and models are the best and most accurate available. Coupled closely to the quality component is the value component which is exemplified by extensive documentation and portability; the value is the usability of the code. Finally, we need new features to keep the code robust but new features never take precedence over quality or value.

Let me discuss quality assurance in more detail. The most important aspect of the MCNP code development effort is software quality assurance(SQA)[7]. This is evidenced in many ways but I will focus on a few which illustrate how features are incorporated in the code. First there is the validation of the capability or feature. Does the enhancement improve the code performance in actual problems while not conflicting with other existing capabilities? The validation effort requires an extensive set of code runs to be done and compared to experimental data or other independent runs to demonstrate that the feature is performing as expected. A typical suite of runs is illustrated by the validation of the differential operator technique reported by G. McKinney and J. Iverson in LA-13098[8,9] where over a hundred independent code runs were done to show that this new feature performed as expected and was consistent with previous results. Typically, this benchmarking effort is documented internally to Los Alamos with several detailed technical memoranda and a final Los Alamos technical report. Once documented, the feature undergoes multiple reviews before incorporation in the code. This evolutionary process reflects how the physics models have improved or numerical techniques have advanced, and we expect to see MCNP to continue to improve along these lines in the future.

Another important aspect of SQA is that the lines of codes are indeed performing as expected on any platform. This involves the test suite[10] which comes with the code and is derived from the validation runs and related experience. When the code is installed on any platform, it is required to give the same answers on a set of test problems; deviations indicate that there is an error in the installed code and it should be reinstalled or that there is another hardware/ software problem. Hardware problems may have no significant impact on code accuracy but the test set usually catches most of these problems. Thus we require passing of all test problems for a successful installation. In point of fact this may sound pretty easy, but it actually has many subtleties. This subtlety is illustrated by a recent installation of MCNP on a 64-bit workstation with multiple processors.[11] Much of the hardware/software architecture was peculiar to that workstation, and was different from the 64 bit architecture of Cray mainframes. Moreover, the results from the test problems were not tracking. This problem uncovered a bug in the C code which impacted only the installation on these platforms and was corrected.

Finally, a $4 reward is offered for any bug found by a user. Since the release of MCNP4A in October 1993, there have been 81 bugs found, 25 of which have merited $4. None of the bugs was significant enough to warrant recall or replacement of the code and most have been there for ages and have only been discovered because of our stricter SQA. This SQA procedure has been documented in LA-13138,[7] and as the code continues to evolve we are adhering to the practices and the procedures presented in that report.

Variance Reduction and Convergence Assessment[12,13]

Most Monte Carlo codes provide the mean of some requested quantity and usually an estimate of the standard deviation of the scored tallies about that mean. Then using the central limit theorem, one usually extrapolates this mean to the true mean and uses the standard deviation as an estimator of the confidence interval on that value for the mean. The MCNP code has taken this usual interpretation a major step further with the incorporation of the ten statistical tests of convergence. The critical point is that the tests for convergence check to see if the underlying distribution has been sampled enough and that anomalous scores are not biasing the answers. These tests were developed because certain problems are so difficult that intuitive notions of whether the results are converged or reasonable are almost impossible to obtain. In such cases, one can only rely on the numerical diagnostics which the code provides.

Applications, Applications, Applications

The MCNP code has an extensive base of users worldwide with about 3000 users at about 300 installations. The applications span aeronautics, neutronics, medicine, electronics, and even more. Having so many users and such a variety of applications has served us in many ways. First, users may find bugs (and become $4 richer) but more importantly may suggest improvements or novel applications of capabilities. Users are always trying new ways to use the code or adapt a capability; such a resource is really hard to assess but has usually been beneficial for the code. Another major benefit from the large application base is the ever-widening body of validating, benchmarking, and corroborating results. LANL cannot perform every possible experiment, and having users out there using our codes and databases to predict and evaluate (or post-dict) their experiments is invaluable. Finally, there is the healthy competition with other codes and databases which helps us (and them) achieve better transport models and capabilities.

3. MCNP4B CURRENT FEATURES

In this section, I will illustrate a few of the most significant recent features of the code. This list is by no means an exhaustive and is by necessity abbreviated. However, it shows how the code is evolving and improving.

ENDF/B-VI cross sections

A radiation transport code is really only as good as the cross sections (the fundamental transport data) it has. We recognize this and strive to keep the physics models and cross sections libraries provided with the code as current and detailed as possible. This effort is illustrated by the recent inclusion of the ENDF/B-VI evaluations into our cross section libraries and their ongoing enhancements.[14,15,16,17,18] A highlight of this is effort is the inclusion of more isotopic evaluations to get, for example, a better resolution of the resonance regions in different isotopes of iron or uranium. A comparison of the total cross for U235 is shown in Fig. 1 for the ENDF/B-VI (92235.60c) and ENDF/B-V (92235.50c) evaluations where the more recent evaluation has a much more detailed resonance cross section description above a few keV but is otherwise quite close to the previous one. Of course, these new releases are not made glibly and are supported by extensive benchmarking and documentation. Further, we retain several previous cross section libraries for backward compatibility or for cases in which the previous libraries may be deemed more accurate.

Cross Section (XS) plotter

A recent addition to the MCNP code is a cross section plotter. This capability has been included primarily to assist users in qualitatively assessing their transport results. With this capability, the user can plot most of the cross sections used by the code in performing a calculation for the three major particle types, neutron, photon, and electron. Of particular note is that the plotter will display cross sections for a material as mixed by the code as instructed on the material card. Thus the user does not have to mix the cross sections by hand and can see the material cross sections used by the code. Individual isotopes are also available for plotting. Fig. 2 shows the total and absorption neutron cross sections for a more fully described isotopic concrete and a simpler version containing only the three major isotopes. There are few differences in the total cross sections for the different concrete descriptions but the absorption cross sections do show some differences which may have an impact on certain shielding considerations.

The cross section plotter will also plot most neutron reaction cross sections available in the evaluation unless they have been expunged by the code (in which case they will not be used in the calculation). Another neutron feature that is not available with any other code, is the ability to plot $S(\alpha,\beta)$ total, elastic, and inelastic cross sections. For photons, the total, coherent, incoherent, photoelectric, and pair production cross sections can be plotted for materials and individual isotopes. The heating numbers for photons are also available. Finally, the electron stopping power and range can be displayed for materials. Multigroup cross sections can be plotted, and some of their edit cross sections can also be plotted.

Differential Operator Perturbation Technique[8,9]

In many problems, precise chemical or geometrical descriptions of the problem are unknown. Major features are known, and allowed variations around those means are also known, but the impact of these perturbations on final results could only be determined by performing many independent code runs for problems that spanned the expected variations. To address such problems, a differential operator perturbation technique has been introduced in the code and will be incorporated with the next release version. This technique is based on a mathematical representation of the tally as a functional of the transport data. Variations of the functional can be cast in a form that are similar to the already tallied quantities for first and second order perturbations. Thus, as the unperturbed tally is being scored, the effects of perturbations to first and second order can also be tallied with little increase in the effort. At the end of a calculation the unperturbed tally and perturbations can be displayed and assessed. Figure 3 shows the results of several perturbation calculations with the exact calculation. The exact calculation is one that was run for the material composition described by the perturbation. The increase in efficiency for such a trade-study is proportional to the number of excursions one desires.

Fault tolerant and Load balanced PVM[19]

Version 4A of MCNP supports distributed-memory multiprocessing through the parallel virtual machine (PVM) software package, version 3.1.4.[20] Using PVM for interprocessor communication, MCNP can simultaneously execute a single problem on a cluster of UNIX-based workstations. This capability can provide an increase in efficiency approximately proportional to the number of workstations or CPUs available.[21,22] However, for heterogeneous systems, efficiency could be degraded by a particularly slow or overworked processor. Similarly, a crash or interruption in one of the workers would effectively curtail the whole calculation. To address these problems, load balanced and fault tolerant processing has been introduced into the PVM architecture MCNP uses. The major benefit here relates to clusters of heterogeneous and non-dedicated processors where these improvements could enhance throughput; on dedicated systems the previous PVM paradigm can still be used to increase throughput by a factor nearly equal to the number of processors.

Improved electron physics models[23]

The electron physics model in MCNP is based upon the condensed history algorithm of Berger and Seltzer[24,25] and the various improvements and enhancements to it that have been distributed in the ITS (Integrated Tiger Series) code package.[26] In this model, the numerous interactions an electron has are averaged over a step to obtain a composite result at the end of the step. This model is implemented in a two tier process. First, there is a major step over which the electron will lose on the average a specific fraction of its kinetic energy (default is $1\text{-}2^{-1/8}$). This step is further divided into several equally spaced substeps over which the multiple scattering deflections are applied.

Over each major step, the pathlength is calculated by integrating the total stopping power over the energy grid boundaries. Radiative losses are accounted for explicitly from the emission of bremsstrahlung photons. The energy loss straggling and multiple scattering deflections are also calculated on this grid. The multiple scattering deflection is sampled from the Goudsmidt-Saunderson theory applied to a combination of the analytical Mott and Rutherford cross sections with Moliere screening and the numerical distributions of Riley (cf. ref. 23 for these citations). The energy loss straggling model has been significantly enhanced to improve the large energy loss portion of the distribution and improve the sampling resolution of the full distribution. A comparison of the collisional energy loss spectrum calculated from the two straggling models is shown in Fig. 4 for 10 MeV electrons in Silicon.

This improvement to the energy loss straggling model was originally discovered in the comparison of electron energy deposition calculations in water. The fact that the large energy losses were not being sampled skewed the distribution away from the measurements, allowing for more deposition deeper in the water. When the straggling model was improved, the profiles moved nearer the measurements. However, another set of data are also very sensitive to the details of the energy loss model: electron albedoes from thick slabs of material. Figure 5 shows the results of several calculations of the backscatter fraction from mono-energetic normally incident electrons on thick slabs of gold and aluminum. The improved straggling model shifts the curves into much closer agreement with the measurements of Darlington[27] and Neubert.[28] However, the agreement is still not as good as we would like, and there is ongoing research into how the energy grid and sampling schemes may effect these results.

Multigroup Boltzmann-Fokker-Planck Transport (MGBFP)

A little know feature of MCNP is the capability to perform coupled charged neutral particle transport using a special multi-group Boltzmann Fokker Planck algorithm[29]. This algorithm is set up to use the standard multi-group transport capability of MCNP with a few modifications to allow for the modeling of energy loss with no significant angular deflection. As with any multigroup calculation, the user must supply a cross section library. For electron/photon problems, a special procedure has been developed which uses the CEPXS[30] code to generate the Legendre moments of the multigroup electron/photon cross sections. These are processed by CRSRD into a suitable set for use in a Monte Carlo code. Once these cross sections are available, MCNP can run with them quite easily.[31] It should be noted that energy loss straggling is included in this model.

Figure 5 also shows the multigroup results for the electron albedoes mentioned above. The agreement is quite good. Note that the multigroup calculation uses a different physics model (mgbfp is based upon the CEPXS code) than MCNP and hence is not expected to agree with MCNP exactly. The discrepancies are pointing to several improvements in the energy grid sampling schemes.

AVATAR[32]

The subtlety of choosing weight windows and other biasing options is more of an art than a science because problems of sufficient complexity typically overwhelm intuitive guidance in selecting effective variance reduction schemes. Too many regions of phase space have conflicting importances making it very difficult to figure out which is really the most important; biasing is usually done by guessing or trial-and-error. A more scientific solution is AVATAR, MCNP's automatic variance reduction method. The trick here is to use a deterministic code to generate approximate values of the adjoint flux within a grid representation of the geometry. The adjoint flux values are then used as the importances in a grid of weight windows superimposed over the geometry to greatly enhance convergence.

Graphics support

MCNP4B for the first time enables the generation of postscript files from the display of the geometry, tally, and cross section plots. (The cross section plots appearing in Figs. 1 and 2 were made this way.) There is also an effort to develop a graphical user interface (GUI) for our transport codes called JUSTINE. Among the features of JUSTINE will be the 3D display of the problem geometry, the ability to construct the geometry in 3D, display of particle tracks, the ability to read and write code input files and to launch a calculation.

Web support

The transport methods group (XTM) of the Applied Theoretical & Computational Physics Division (X Division) has an ongoing project to make our transport code information available on the World Wide Web. The MCNP home page is at URL: http://www-xdiv.lanl.gov/XTM/mcnp/mcnp.html. One can find documentation on the code and benchmarks, an MCNP users group forum, a command summary (both in plain text and HTML versions,) and "who we are" amongst other things. Please feel free to visit and comment.

4. FUTURE ENHANCEMENTS

More particles (LAHET code merger)[33]

Currently, the MCNP code system can transport neutrons, photons, electrons, and positrons. Complementing this capability is the LAHET code system,[34] which is described in the XTM home page, that is the transport package for high energy and particle physics. LAHET was primarily developed as a code system supplement to MCNP to transport protons with particular emphasis on the energy range above 1 GeV. The procedure was to run LAHET separately for the hadrons and then write a source file for neutrons and photons generated in the cascade to be transported in MCNP.

A current effort is merging the two code systems so that MCNP will be able to transport protons, mesons, and several other hadrons. A major portion of this effort is in the merging of the LAHET physics package into MCNP and the development of suitable cross section libraries for use in the transport of these particles. The outcome of this effort will be a version of MCNP which will be able to rigorously transport a large class of hadronic particles. The energy range will span 1 keV to 1 TeV with cascades being modeled either from cross section libraries or the LAHET physics package.

Exponential convergence and Adaptive Monte Carlo for the 21st Century
A major internally funded research effort called "Monte Carlo for the 21st Century" is currently underway at LANL. The overall objective of this effort is to develop new Monte Carlo techniques that will advance the calculational capability by over an order of magnitude over today's standards. This objective is grandiose but it has a solid basis in past demonstrations. For example, one of the major thrusts is into the area of adaptive Monte Carlo, where the biasing, to put it loosely, is done as the calculation proceeds. That is, the mean value of a tally is scored and the contributions from all tracks are remembered. This information will then be used in the code to bias the tracking to give the desired mean value. In other words, the tracks will be biased to give a zero variance faster since most of the contributions will be near the mean. The gains in efficiency have been shown to have an exponential dependence on the number of histories. However, the research problems are still prodigious. There is the problem of false convergence. Moreover, the speed-up is usually for one tally and may adversely effect other tallies. For more details and interaction with this project see the Webpage: http://www-xdiv.lanl.gov/XTM/projects/mc21/mc21.html.

Radiography
A final enhancement to MCNP is the ability to generate synthetic radiographs. This capability is very attractive to the medical community since a virtual experiment can be done to determine optimal detector or source parameters for a variety of situations. Essentially, the technique generates a grid of point detectors (tally 5) and tallies each grid point as a distinct detector. Thus each collision within the problem geometry generates a score for each detector. The resulting images are qualitatively similar to the photographic images typically obtained in diagnostic radiographs (X-rays in more prosaic terms.) Ongoing efforts are examining the accuracy of the method both from the validity of the physics models and numerical techniques.

5. CONCLUSIONS

As can be seen, the MCNP code is alive and thriving after 50 years. The rigorous SQA protocol will ensure that MCNP will live up to the code philosophy of "Quality, Value, New Features." Several new features have been described which illustrate this philosophy in action. The future work shows some of the directions the MCNP code system will be heading toward.

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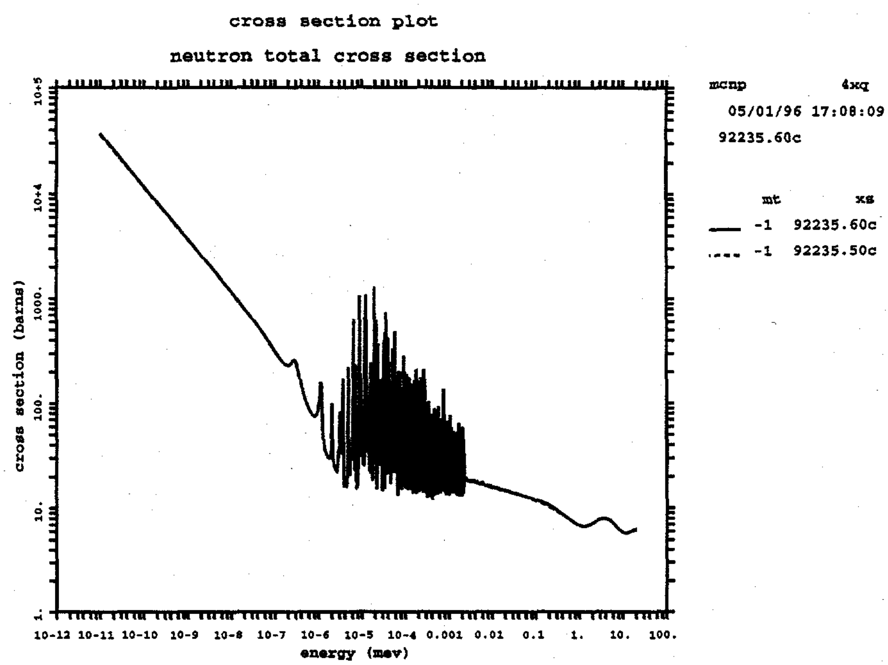

Figure 1: The total cross sections for U235 using the cross section plotting capability of MCNP4B. 92235.60c is based upon ENDF/B-VI and 92235.50c is based upon ENDF/B-V.

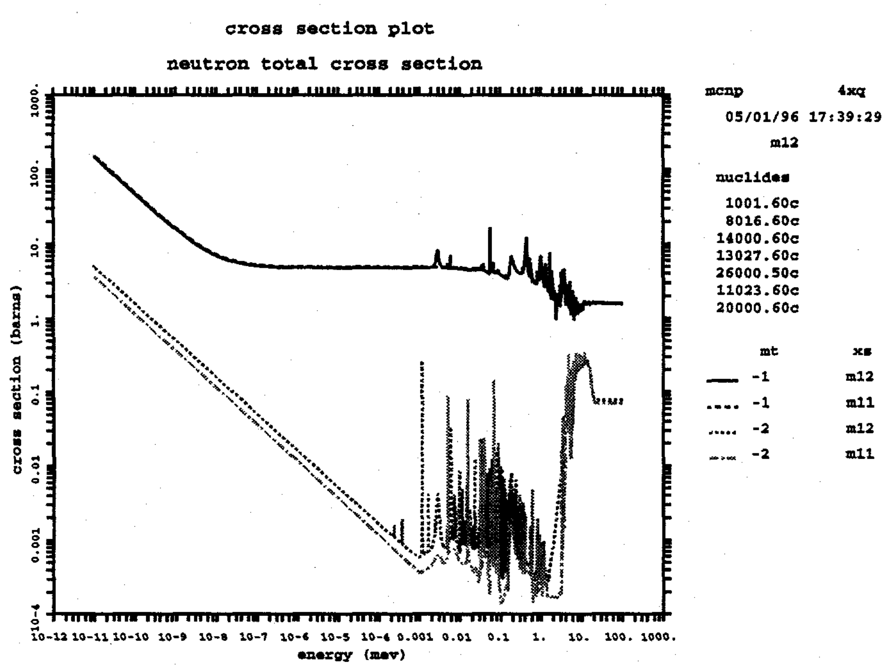

Figure 2: The total (mt=-1) and absorption (mt=-2) cross sections for two isotopic mixtures of concrete. Material m11 is the more detailed one using the isotopes listed above. Material m12 uses only the first three isotopes.

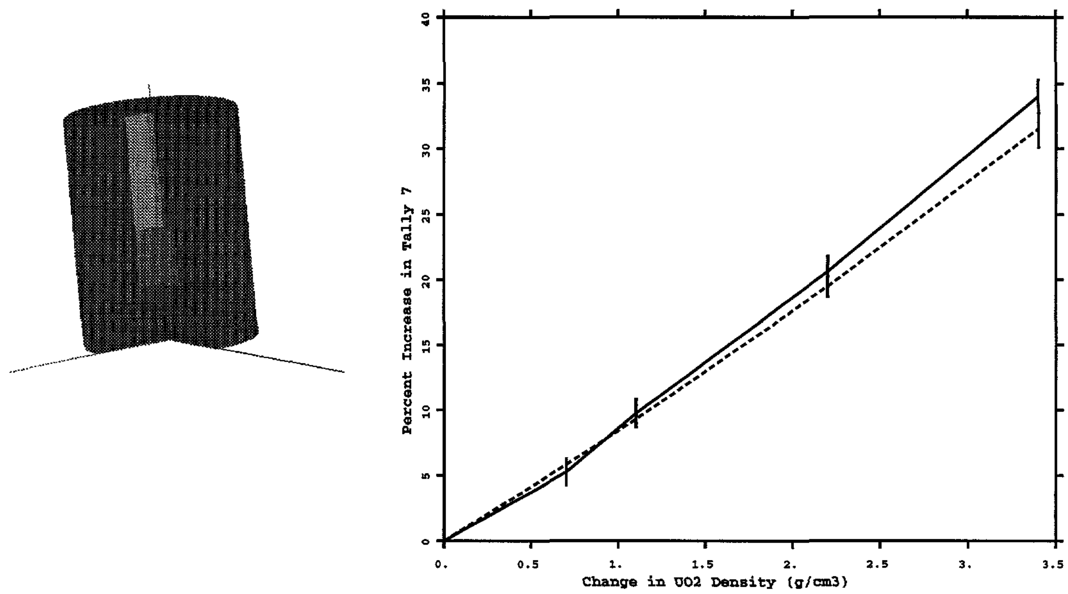

Figure 3: The results of perturbation calculations showing the variation in the fission heating from increasing the density of UO_2 (red region) from 8.1 g/cm^3 to 8.8, 9.2, 10.3,and 11.5 g/cm^3; based upon inp07 of the MCNP4A test set and shown in a JUSTINE rendition in the upper left corner. Solid is actual and dashed is perturbation calculation.

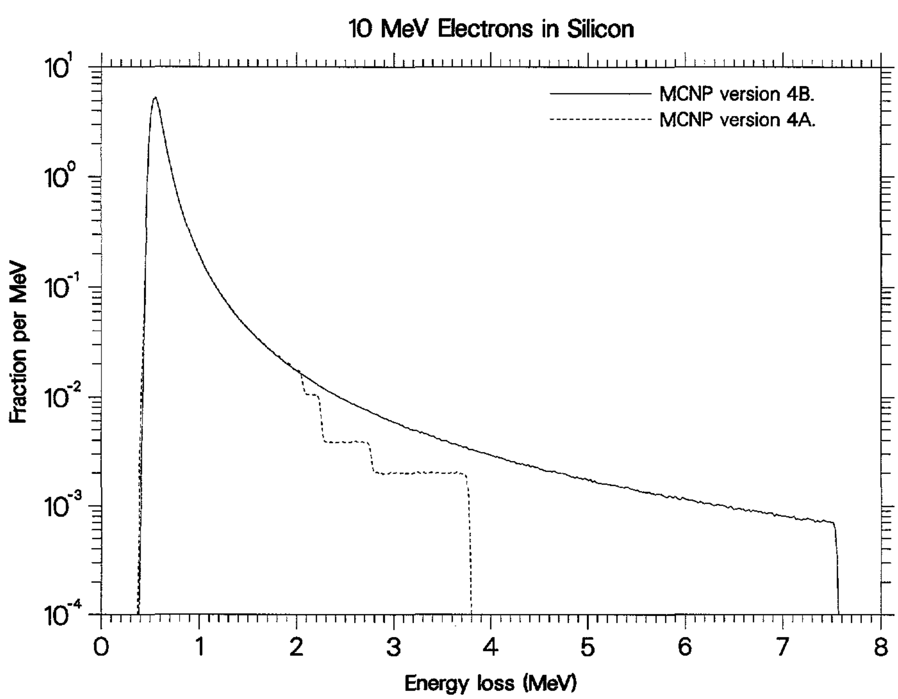

Figure 4: The energy loss spectrum for 10 MeV electrons in Silicon calculated using the improved energy loss model in MCNP4B and the previous less detailed model.

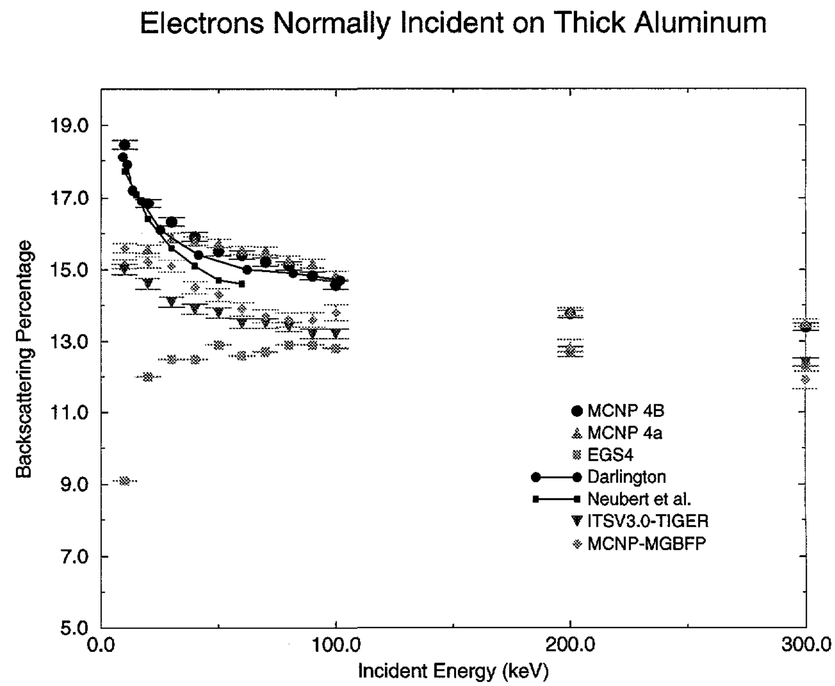

Figure 5a: The calculated and measured electron albedoes from mono-energetic normally incident electrons on Aluminum. All code comparisons were done using default settings. The impact of the improved energy loss straggling model brings MCNP4B in closer agreement with measurement at low energies.

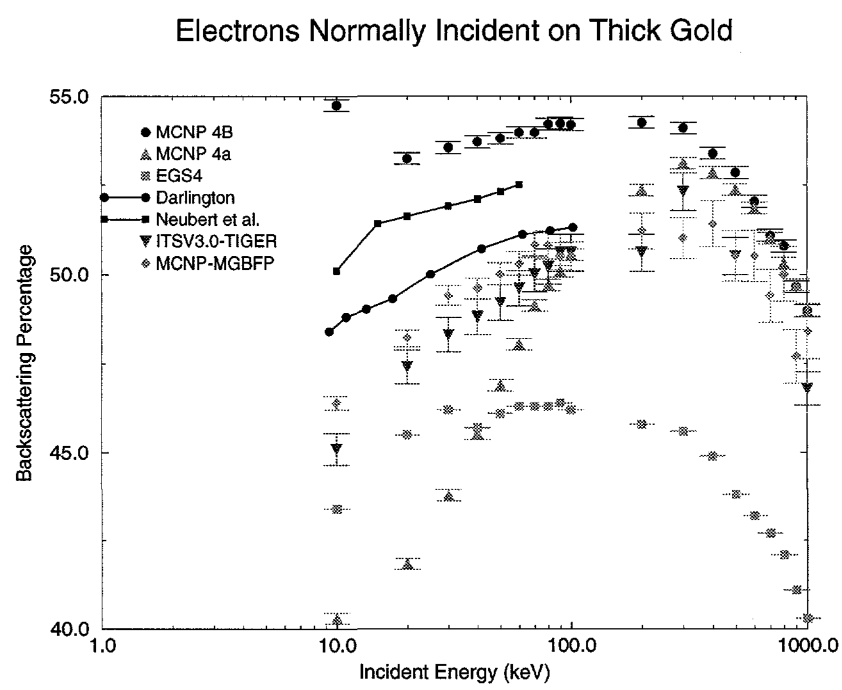

Figure 5b: The calculated and measured electron albedoes from mono-energetic normally incident electrons on Gold. All code comparisons were done using default settings. The impact of the improved energy loss straggling model brings MCNP4B in closer agreement with measurement at low energies though slightly higher in value.