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Intended for: MCNP6 Beta 3 Release to RSICC

# INITIAL MCNP6 RELEASE OVERVIEW - MCNP6 BETA 3

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**(This document is an update to the *Nuclear Technology* article “Initial MCNP6 Overview”, published in December 2012, which focuses on MCNP6 Beta 2)**

*MCNP6 is simply and accurately described as the merger of MCNP5 and MCNPX capabilities, but it is much more than the sum of these two computer codes. MCNP6 is the result of five years of effort by the MCNP5 and MCNPX code development teams. These groups of people, residing in Los Alamos National Laboratory’s (LANL) X Computational Physics Division, Monte Carlo Codes Group (XCP-3) and Decision Applications Division, Radiation Transport & Applications*

*Team (D-5) respectively, have combined their code development efforts to produce the next evolution of MCNP. While maintenance and bug fixes will continue for MCNP5 1.60 and MCNPX 2.7.0 for upcoming years, new code development capabilities only will be developed and released in MCNP6. In fact, the initial release of MCNP6 contains 16 new features not previously found in either code. These new features include the abilities to import unstructured mesh geometries from the finite element code Abaqus, to transport photons down to 1.0 eV, to transport electrons down to 10.0 eV, to model complete atomic relaxation emissions, and to generate or read mesh geometries for use with the LANL discrete ordinates code Partisn. This document discusses the second release of MCNP6 through RSICC, MCNP6 Beta 3. It is our expectation that Beta 3 will have very nearly the same capabilities as the upcoming production release. The production release will also contain bug fixes for issues discovered in the Beta 3, so user feedback (to mcnp6@lanl.gov) is very important to us. High confidence in the MCNP6 code is based on its performance with the verification and validation test suites, comparisons to its predecessor codes, the regression test suite, its code development process, and the underlying high quality nuclear and atomic databases.*

## I. INTRODUCTION

The particle radiation transport code MCNP, which stands for Monte Carlo N-Particle, is a general purpose three dimensional simulation tool that transports 37 different particle types for criticality, shielding, dosimetry, detector response, and many other applications.

Monte Carlo particle radiation transport methods have had an extensive history at Los Alamos National Laboratory (LANL) dating from the 1940s. Early creators of these methods include Drs. Stanislaw Ulam, John von Neumann, Robert Richtmyer, Nicholas Metropolis, and others, who investigated neutron transport issues on the first generation of computers. On March 11, 1947, John von Neumann sent a letter to Robert Richtmyer, leader of the Theoretical Division at Los Alamos, proposing the use of the statistical method to solve neutron diffusion and multiplication problems in fission devices. His letter was the first formulation of a Monte Carlo computation for an electronic computing machine.[1] In 1947, while at Los Alamos, Fermi invented a mechanical device called FERMIAC11 to trace neutron movements through fissionable materials by the Monte Carlo Method.[2] During the 1950s - 1960s, a number of special-purpose Monte Carlo codes were developed at LANL, including MCS, MCN, MCP, and MCG. These methods eventually found their way into a code called MCNG, which was first created in 1973 by merging a three dimensional neutron transport code MCN[3], with the gamma transport code MCG.[4] In 1977 MCNG was merged with MCP, a Monte Carlo photon code with detailed physics treatment down to 1 keV, to more accurately model neutron-photon interactions. The resulting code, MCNP, originally stood for Monte Carlo Neutron Photon. In 1983, MCNP3 was released for public distribution to the Radiation Safety Information Computational Center (RSICC).

The meaning of MCNP changed to Monte Carlo N-Particle when electron transport, from Sandia National Laboratory's Integrated TIGER Series (ITS),[5] was added in 1990. MCNP has been expanded ever since to include more and more particle types. In 1996, the LANL code LAHET to was added to MCNP4B, creating a "Many-Particle MCNP Patch".[6,7] Although initially developed for the Accelerator Production of Tritium (APT) program, the utility of many-particle transport has found many applications and sponsors, and continued to grow as a separate code, MCNPX.[8] In 2001-2002 MCNP4C was completely rewritten in modern Fortran 90, and was enhanced to support large scale parallelism using combined MPI message passing and OpenMP threading, resulting in MCNP5.

In July 2006, a merger effort was started, taking MCNPX 2.6.B and adding it to a LANL version of MCNP5. The resulting code, MCNP6, took more than twelve man-years to create from the two parent codes. Table I summarizes all MCNP public releases with significant developments. For a more complete description, see the history section of the MCNP and MCNPX manuals[9] and each version's release notes. Tables II A-D summarizes the 37 particle types that MCNP6 now transports, along with a brief summary of interaction physics available to each particle. These particle tables are broken up into elementary particles, composite particles and composite antiparticles, and nuclei, respectively. A description of the models used to simulate interactions is in the next paragraph. Furthermore, neutron, proton, electron and photon transport below a certain energy are based on data libraries by default, and is discussed in subsequent paragraphs. This energy regime, which varies according to particle type, is referred to as the data table range. It is shown in blue in Fig. 1. For a few particle types, the model and data table energy regimes overlap.

To address various needs of our sponsors and for some historical reasons, MCNP6 considers several nuclear reaction models, sometimes incorporated in separate modules we refer to as "event-generators". The first model of intermediate- and high-energy nuclear reactions used initially in LAHET[10] was the Bertini INC,[11] followed (by default, but not required) by the Multistage Preequilibrium Model (MPM),[12] followed by the Dostrovsky et al. evaporation model[13] as implemented in the code EVAP by Dresner.[14] If the compound nuclei produced after the INC and MPM stages of reactions are heavy enough to fission, the fission process is simulated either with the semi-phenomenological Atchison fission model, often referred in the literature at the Rutherford Appleton Laboratory (RAL) fission model, which is where Atchison developed it,[15] or with the Fong statistical model of fission as implemented in the ORNL code HETFIS,[16] often referred in the literature as the ORNL fission model. Bertini INC, MPM, EVAP, RAL, and HETFIS migrated from LAHET to MCNPX and later, to MCNP6. Bertini INC is the default option of MCNP6 for reactions induced by nucleons and pions at energies up to 3.5 GeV and it is always used to calculate such reactions on the light d, t, $^{3}$He and $^{4}$He target-nuclei, independently of the model chosen in the MCNP6 input file.

The second model, from historical point of view, migrated to MCNP6 via MCNPX from LAHET is the ISABEL INC.[17] ISABEL is the default option in MCNP6 for reactions induced by d, t, $^{3}$He, $^{4}$He, and antinucleons at energies up to 1

GeV per nucleon. If specified in the MCNP6 input file, ISABEL can be used to also simulate reactions induced by nucleons, pions, kaons, and heavy-ions at energies below 1 GeV/nucleon. Just like Bertini INC, ISABEL can be used with or without taking into account the preequilibrium reactions as described by MPM and it can describe the evaporation and fission reactions with EVAP, RAL, and HETFIS.

A newer and recently improved model used by MCNP6 is the Cascade-Exciton Model (CEM) of nuclear reactions as implemented in the event-generator CEM03.03.[18,19] CEM03.03 is used in MCNP6 as a default choice to calculate photonuclear reactions at energies up to 1.2 GeV and is the only model adopted by MCNP6 to simulate absorption of stopped muons. If selected by input, CEM03.03 can also simulate successfully reactions induced by nucleons and pions at energies up to several GeV. We recommend using it up to about 1 GeV for light targets like C and up to about 5 GeV for heavy targets like U. CEM03.03 uses its own models to describe the preequilibrium, evaporation, and fission reactions. It considers also coalescence of nucleons into complex particles up to $^{4}$He and Fermi break-up of excited or unstable nuclei with mass numbers up to A = 12 (see details in Refs. 18 and 19).

Another new and recently improved model used by MCNP6 is the Intra Nuclear Cascade model developed at Liege (INCL) by Joseph Cugnon in collaboration with colleagues from CEA Saclay, France and GSI, Germany.[20] The version of INCL implemented in MCNP6 Beta 2 can describe successfully reactions induced by nucleons, pions, and complex particles d, t, $^{3}$He, and $^{4}$He at energies up to several GeV. INCL always uses only the ABLA code developed at GSI[21,22] to describe the evaporation and fission stages of reactions, independently of what MCNP6 users would chose for evaporation/fission models; INCL does not consider preequilibrium reactions. Newer and better versions of INCL and ABLA are planned for incorporating in a future version of MCNP6.

Finally, MCNP6 uses the Los Alamos version of the Quark-Gluon String Model (LAQGSM) as implemented in the event-generator LAQGSM03.03.[19,23] LAQGSM03.03 is the default option to describe in MCNP6 reactions induced by heavy-ions, by photons at energies above 1.2 GeV, particle-nucleon interactions, as well as reactions induced by projectiles not considered by other models. LAQGSM was developed to describe reactions induced by almost all types of elementary particles and by nuclei at energies up to about 1 TeV/nucleon. LAQGSM uses its own models to describe the preequilibrium, evaporation, and fission reactions; it considers also coalescence of nucleons into complex particles up to $^{4}$He` and Fermi break-up of excited or unstable nuclei with mass numbers up to A = 12 (these are the same models used by CEM, but adjusted to LAQGSM; see details in Refs. 19 and 23). For lower energy neutrons, photons and electrons, nuclear data can also be used to sample nuclear and atomic interactions.

The MCNP6 code represents one of a set of synergistic capabilities developed at Los Alamos that also includes the evaluated nuclear data files (ENDF), and the data processing code NJOY. The ENDF project is a collaboration among many US National Laboratories and universities, coordinated by the Cross Section Evaluation Working Group (CSEWG) and Brookhaven National Laboratory (BNL). LANL plays a leadership role in the evaluation and integral data testing CSEWG committees, and leads the theory, modeling, experiment, and evaluation work cross sections for actinides and light nuclei. The ENDF/B-VII.0 database was released in 2006,[24] and the latest version of the database was released in December 2011.[25] The NJOY code developed by R.E. MacFarlane, and more recently Skip Kahler, takes the ENDF files and makes application data files for transport codes such as MCNP. It is used widely in the nuclear technology community for this purpose, as well as for computing certain quantities such as radiation heating and damage.[26] MCNP has played a central role in the Validation and Verification (V&V) of these ENDF data.[27]

The ENDF/B-VII nuclear data consists of interaction and secondary particle production data for a variety of particles and energies. Depending on the nuclear data being used, neutron interaction data is available up to 20, or more recently, 150 MeV. Thermal neutron scattering, $S(\alpha,\beta)$, data is available for 20 different materials. Proton interaction data is available for 48 isotopes, up to proton energies of 150 MeV. Photoatomic data is available for photon and electron transport up to 100 GeV and 1 GeV, respectively. Photonuclear data, including Nuclear Resonance Fluorescence (NRF), is available for 157 specific isotopes up to 150 MeV, but is not active in calculations by default. Above the respective energy, and for all the hadrons, interactions are based on theoretical models with empirical corrections. There are no nuclear interactions for leptons based on models, with the exception of negative muon at-rest nuclear capture, which uses data for X-ray emissions and CEM to simulate the effects of de-excitation on the nucleus. While MCNP6 will allow particles up to 100 TeV in energy, only particle energies up to 1 TeV have been reviewed for accuracy.

While the merged code has taken approximately twelve man-years of effort to develop, both the LANL code teams and their management believe that maintaining and developing a merged code is best for the developers themselves and the extensive user community. A single merged code eliminates the duplicate development costs incurred when each code team implements a particular feature in each parent code. The combined code also allows many of the independent capabilities developed in each of the parent codes to be used together. The DOE's Advanced Simulation and Computing (ASC) program's national code strategy has a goal of increasing code development efficiencies and reducing long-term maintenance costs;[28] they have wholly funded this merger effort, recognizing the importance of the combined code.

In August 2011, forty-five advanced users were invited to beta test MCNP6_Beta1, providing valuable feedback relevant to a wide range of applications. In late 2011, MCNP6 source and executables have been made available and may be requested through RSICC (http://rsicc.ornl.gov/). The MCNP6 distribution package is on three DVDs. The first DVD includes the MCNP5 1.60, MCNPX 2.7.0 and MCNP6 codes, with executables pre-built for Windows, Linux, and MacOSX platforms (pre-built MCNPX 2.7.0 executables for the MacOSX are not provided). The second DVD includes the nuclear and atomic data, including the ENDF/B-VII release. The third DVD includes a collection of more than 1 gigabyte of PDF references: most of the documents are from Los Alamos, but a few are from other DOE laboratories. For FY12, the DOE ASC program has agreed to underwrite the distribution fees for MCNP6, making it free to the requestor.

For at least the next several years, MCNP6 will be distributed with MCNP5 1.60 and MCNPX 2.7.0. Users are encouraged to run their particular problems with MCNP6 and their previous code of choice. MCNP6 is a new code and is not expected to track (produce exactly the same random number and particle interaction sequence) either of its parent codes. Significant differences from either MCNP5 or MCNPX should have some explanation, such as the inclusion of new physics, different default behavior, new or improved data, even bug fixes. A document will be provided with MCNP6 listing known reasons for expected differences from MCNP5 or MCNPX. Any other differences should be discussed with the MCNP6 development team by sending an email to mcnp6@lanl.gov.

MCNP is one of the world's leading particle radiation transport codes, with an estimated user base of more than ten thousand users. In fact, in fiscal years 2009 and 2010, RSICC distributed 1514 and 1512 copies, respectively, of the MCNP5 & MCNPX package, to users in US government institutions, academia, and private companies worldwide.[29] In the time between January, 2001 and October, 2011, there were 11,586 requests for MCNP, but it is not known how many of these requests are from the same user asking for a newer version of the code.[29] MCNP is RSICC's most widely requested and distributed computer code.

MCNP6 user support is provided in several different ways. The MCNP6 reference DVD contains several user manuals, hundreds of specific LANL MCNP publications, and discussions on Monte Carlo theory. A few other resources are provided, such as a database of MCNP input files of medical physics human phantoms, which includes the ICRP 110 phantoms. The mcnp6-forum@lanl.gov has been created to allow users to post questions to users and developers. MCNP6 developers will provide limited feedback to this forum. The MCNP6 development team provides week long classes for MCNP beginners, and separate advanced classes in criticality, variance reduction, and sometimes other specific topics.

## II. MCNP6 MERGER PROCESS

MCNP6 was created by merging lines of coding from MCNPX into a LANL version of MCNP5 which had already been upgraded to use more Fortran 90 features and adapted to transport protons. As the lines of Fortran were taken from MCNPX, conflicts in variable names, array dimensionality and lengths, common blocks, subroutine calling logic, hardwired parameters, default parameter settings, transported particles, input card processing, compilation and build mechanics, and output file formats were resolved. When a conflict was severe enough to cause lengthy delays in the merger progress or when both codes had independently developed different algorithms for the same capability, those lines of code were identified and wrapped with a flag to preserve each of the parent code's methods. This flag could be set in the MCNP input file, and was the data card *dbcn 28j x*. If *x=0* (or omitted), then the MCNP5 algorithms are used; if *x=1*, then MCNPX algorithms were selected. Unfortunately for the initial MCNP6_Beta1 testers, there was only one global flag to perform this "switch", and thus it was not possible to run with certain combinations of features, such as explicit magnetic field tracking with heavy charged particles ($Li^+$ and above), or invoking delayed particle emissions and a MCNP5-style *fmesh* tally. While these two particular issues were resolved in

MCNP6 Beta 2, the *dbcn 28j x* flag still existed for that release. For the MCNP6 Beta 3 release, however, all occurrences of *dbcn 28j x* have been removed. During merger efforts, several routines were made more modular and multi-particle overhead was reduced by changing array dimensions from the product of number of particles that could be transported in MCNPX times the number of cells or surfaces to the product of the number of particles actually transported in a particular simulation times the number of cells or surfaces.

Extensive efforts to remove the more than 200 individual conflicts have been the focus of the most recent six months of merger efforts. Most of the merged capabilities needed by users were achieved in the merging of the eight MCNP5 and MCNPX particle history and transport routines to create new combined routines. In other parts of the code, individual conflicts were resolved by simply choosing an appropriate default method, and providing some backwards capability with a new option on a specific card. In a few specific cases in which independent development had occurred in both codes, and one code had all the capabilities of the other, then one algorithm was deprecated. Input parsing for either method, however, was mostly kept in place, again to allow for backward compatibility. Much care was also taken to preserve as much backward compatibility for input files as possible. The document MCNPX to MCNP6 Migration Notes[30] addresses more of the details of running MCNPX input files with MCNP6. Backward compatibility is not maintained for the binary files created during execution (*runtpe, srctp, htape*, etc), nor have previous releases of MCNP maintained backwards compatibility with these files.

During the merger process, meticulous care was taken to maintain the confidence in the code's calculated results. Throughout the merger process, MCNP6 (with *dbcn 28j 1* and separately with *dbcn 28j 0*) was frequently run before and after each specific set of changes (occasionally even single-line changes) to isolate and understand the specific effect of what was added to MCNP6. Because the *dbcn 28j x* flag has been removed in MCNP6 Beta 3, it is not possible to perform these tests in that version. Even changes as simple as converting 4-byte real parameters to 8-byte real parameters can be detected in the regression test suite and were identified and isolated from other changes. Occasionally unique versions of MCNPX were generated by including MCNP5 methods and running the MCNPX test suites. By looking at the changes in the MCNPX test suites, the code developers verified that the effect of particular change in MCNP6 was completely understood. A description of the MCNP6 and MCNPX test suites is presented in the **MCNP6 VERIFICATION, VALIDATION AND REGRESSION TEST SUITES** Section of this paper.

The intent of the merger was to create a new code with the existing capabilities of both codes; while that was successfully completed, there only has been modest effort to make all capabilities of each code fully compatible with every other capability. In fact, this effort would constitute new development and likely will be proposed to sponsors in the future. An example of this new development would be the expansion of MCNP5's OpenMP shared memory threading. MCNP6's OpenMP capability will work with all the MCNP5 capabilities, but there is no expectation that it will work with MCNPX capabilities, especially those that utilize other code packages, such as the high energy models (CEM, LAQGSM, INCL, ABLA) or the delayed particle emissions (Lawrence Livermore National Laboratory's photon multiplicity or LANL's CINDER).

Because MCNP6 contains both MCNP5 and MCNPX capabilities, we hope that MCNP6 will be used by both sets of user communities. We have tried to predict what some of these communities would expect from the merged code and anticipate conflicts. For example, the default in MCNP5 is to use *totnu*, the sum of prompt and delayed fission neutron emissions, for criticality (*kcode*), and *totnu no* (prompt emissions only) for fixed source problems. The default in MCNPX is to use *totnu* for both. MCNP6 will use *totnu* for both calculations by default.

As several of the new capabilities were created or incorporated into MCNP6, new data files of physical data were created. Examples include characteristic gamma emission lines from radioisotope decays, improved form factors, low energy atomic cross sections, and muonic X-ray emissions. These new data files should also reside in the same directory as the usual nuclear data files, specified with the environmental variable DATAPATH. These new data files were created by and are the responsibility of the MCNP code development team, not the T & X division nuclear and atomic data team, which has historically produced and maintained the ENDF nuclear data used by MCNP. More details of each of these capabilities should be found in the draft MCNP6 manual, which is also released with MCNP6 Beta 3.

## III. MCNP6 NEW FEATURES

In addition to the code capabilities of MCNP5 and MCNPX, MCNP6 includes several significant new capabilities not found in either of the parent codes. These capabilities are described below.

**1) Adjoint-based sensitivity coefficients**

MCNP6 contains the first implementation of adjoint-weighted tallies for perturbation theory in continuous-energy Monte Carlo. The adjoint-weighted tallies are implemented using the integrated fission probability,[31] similar to the MCNP5-1.60 approach to determining adjoint-weighted reactor kinetics parameters. MCNP6 can compute sensitivity coefficients of *k* with respect to some cross sections. This capability was first available in MCNP6 Beta 2 and is utilized through the use of the *kpert* and *ksen* cards.

**2) Geometry mesh file creation (Ref. 32)**

MCNP6 provides the initial file-based link to the LANL discrete ordinates neutron and photon code Partisn[33], separately distributed by RSICC. The initial intent is to provide an easy way to perform Monte Carlo vs. SN comparisons, separating geometry, multigroup data, and methodology effects. The longer-range goal is to take the adjoint flux weights from Partisn to use within MCNP for weight windows. The initial capability takes MCNP's constructive solid geometry (CSG), creates a regular mesh of homogenized materials in 1D (r), 2D (rz, xy), or 3D (xyz), and writes a Partisn-style geometry file in the LNK3DNT file format using the , as well as reads a Partisn-style geometry for continuous energy neutron transport. This capability was first available in MCNP6 Beta 2 and is utilized through the *mesh* and *dawwg* cards.

### 3) Unstructured mesh geometry

MCNP6 now includes the capability to track and tally neutrons and photons on an unstructured mesh embedded as a mesh universe within MCNP's constructive solid geometry. The unstructured mesh geometry can be created with Abaqus/CAE.[34] First and second order mesh element types with four, five, and six sides are supported; all six element types may exist simultaneously in a model. When geometry models are assembled from parts, gap and overlap regions may exist, giving rise to undefined and over-defined phase space; the unstructured mesh tracking algorithms successfully address these conditions. Results collected on the mesh are written to special output file that can be imported by Abaqus/CAE for visualization or thermo-mechanical analysis. Tracking through the unstructured mesh geometry can be competitive in run times with constructive solid geometries, but varies greatly with the geometry complexity.[35] (This publication appears in this issue of *Nuclear Technology*.) Reference 35 work shows that when performance from a mesh model with a moderate element count is compared to performance from a traditional model with few surfaces, the traditional model wins every time. However, our unpublished results indicate that this is not always the case when the models are put on equal footing; there are situations where tracking on the mesh is faster and when the geometry detail is significant, setup times for the mesh models are much shorter. Dose calculations of human phantoms using the unstructured mesh geometry are typically an order of magnitude slower in run time when compared to an identical voxel lattice geometry. Unstructured mesh memory usage is also typically several times larger than a comparable human phantom lattice geometry, but is lower for simplistic cases.[36] Complex models are much quicker and easier to construct with a tool such as Abaqus/CAE plus the visualization of results is superior; to many users these capabilities are more important. When it comes to multi-physics integration, the unstructured mesh is the hands down winner in terms of meeting requirements. The unstructured mesh capabaility is fully compatible with MPI, shared memory threading, or hybrid methods utilizing both, parallelism. This capability was first available in MCNP6 Beta 2 and utilizes the *embed* and related cards. New in MCNP6 Beta 3 is the ability to do parallel setup and initialization of the unstructured mesh by decomposing individual Abaqus “parts” onto separate MPI processes. Also new in MCNP6 Beta 3 is that these unstructured mesh geometries can be plotted in the MCNP plotter.

**4) Low energy photon and electron transport for atomic cross sections**

MCNP6 has extended the minimum energy cutoff for photon transport down to 1 eV. The necessary photo-atomic cross sections from ENDF/B-VI release 8 are included in the interim photo-atomic library mcplib09, selected by requesting .09p photon transport tables. The default photon energy cutoff remains 1 keV, so the user must explicitly request a lower cutoff on the *cut:p* card, for example *cut:p j 1.0e-06* for the lowest possible cutoff. These lower energies can be specified on *sdef, de/df*, and energy bin cards. While they are likely compatible with other energy-specific cards, not all possible combinations have been tested. This new feature is closely coupled with the following new capabilities in atomic relaxation. Users are cautioned that at very low energies, molecular and other effects become important for scattering and absorption, and these more complex effects are not yet included in the photon transport methods, with the exception of the molecular cross sections for $N_2$ and $O_2$. In addition, electron transport has been extended down to 10 eV. This feature was first available in MCNP6 Beta 2.

**5) Complete photon-induced atomic relaxation**

Complete element-specific relaxation processes, with the emission of fluorescent photons and Auger and Coster-Kronig electrons, can now be modeled in MCNP6. The necessary data (from ENDF/B-VI.8) are included in the interim library mcplib09, in .09p photon tables. Going beyond previous MCNP treatments, which considered only K-shell and average L-shell transitions, the new treatment addresses the full detailed relaxation cascade, sampling all allowed transitions down to the photon and electron energy cutoffs, and providing a much more detailed prediction of the relaxation spectra. It should be noted that higher-order effects in which early transitions change the probabilities of later transitions in the same cascade are not modeled, and that relaxation from electron-induced atomic vacancies has not been implemented yet. This feature was first available in MCNP6 Beta 2.

**6) Explicit tracking of all charged particles in magnetic fields (Ref. 37)**

MCNP6 can model magnetic fields in two different ways. The card *bfld* can be used to model constant (dipole), square edge quadrupole, and quadrupole magnets with a fringe-field kick, magnetic fields that co-exist with low density materials, such as air. This new capability is an alternative to the existing MCNPX COSY maps,[38] which is a direct correlation of entry and exit particle states in a magnetic field, which can only be applied in a vacuum, i.e. a void cell. COSY maps are also specific to one particle type, and only one COSY map can exist at a spatial location, while the *bfld* capability correctly treats all charged particle types passing through a particular cell. This feature was first available in MCNP6 Beta 2.

### 7) Nested *dxtran* spheres

*dxtran* spheres, a form of variance reduction and population control, can now be nested inside of each other. More than one *dxtran* sphere may be nested inside a larger *dxtran* sphere and the nested *dxtran* spheres need not be concentric. The primary restriction is that the spherical surfaces must not intersect. This nesting allows *dxtran* particles to be directed to one or more regions of interest. This feature was first available in MCNP6 Beta 2.

### 8) Uncollided secondaries

An uncollided particle in MCNP was historically defined to be any particle that had not undergone a collision since its creation as a source particle or as a secondary particle. This definition, in which secondary particles are created as uncollided particles, makes separation of the contribution from the direct source and contribution from secondary particles difficult for the user. This is especially true when users employ track-length tallies in radiography applications instead of next-event estimators. A new cell card, *unc*, has been added to MCNP6 that allows the user to control if secondaries are born as uncollided or collided particles. This feature was first available in MCNP6 Beta 2.

**9) Time bins for mesh tallies**

Time bins have been added for the MCNP5-style mesh tallies. Users can specify time bin boundaries in units of shakes (1 shake is $10^{-8}$ sec) on the *fmesh* card. The tally results can be obtained as integrated over the time bin (units of $cm^{-2}$), as an average rate (tally per unit shake), or as a tally per unit energy (tally per MeV per shake). Specific *fmesh* time bins can also be plotted in the mesh tally plotter. MCNPX-style mesh tallies previously had the ability to have time bins. These time bins are added with the *tint* and *tbin* keywords on the *fmesh* card. This feature was first available in MCNP6 Beta 2.

**10) Enhanced photon form factors**

New form-factor data from ENDF/B-VI.8 for coherent and incoherent photon scattering are available in the interim photoatomic transport library mcplib09, which is selected by requesting .09p photon transport tables. These data extend the treatment of coherent and incoherent scattering to higher energies and/or larger scattering angles. The interpolation algorithms for the form-factor data have also been corrected for validity over the enhanced energy/angle range.[39] These improvements provide a more complete representation of photon scattering, and are especially important for backscattering of coherent photons. This feature was first available in MCNP6 Beta 2.

**11) Surface and cell flagging are now possible with MCNP5-style mesh tallies**

Mesh tallies can be used in combination with the surface (*sf*) and cell (*cf*) flagging tally cards. However, unlike the regular tallies, only one mesh tally, the flagged tally, is created. A separate mesh tally will need to be provided for unflagged tally results. This feature was first available in MCNP6 Beta 2.

**12) Upgrade to CEM03.03 and LAQGSM03.03**

The LANL high-energy physics models have now been updated to their most recent releases. The stand-alone versions of CEM03.03 and LAQGSM03.03 are not available yet from RSICC. In comparison with the versions used by MCNPX 2.7.0, MCNP6 uses an upgrade of CEM03.03 allowing us to calculate much better fission cross section and fission fragment yields from $^{181}$Ta and the nearby target-nuclei; several other unobserved bugs in CEM and LAQGSM were also fixed. These updates were included in MCNP6 Beta 2.

**13) Generation of gamma rays from muonic atoms**

When a negative muon survives to reach its lower energy cutoff, it attaches to an atom to form a negatively charged "muonic atom." The muon then relaxes by a series of transitions toward the most tightly bound shell, emitting fluorescent gamma rays, in analogy to the electronic transitions characterizing ordinary atomic relaxation. Both MCNPX and MCNP6 contain a programmed library for muonic gamma-production for a variety of isotopes of interest. A new feature of MCNP6 is the ability to read and sample from new data in independent data files. This capability is a work in progress, since an ACE-like format for such data files has not yet been developed. By default, this capability is on, and users should specify both photons and muons on the mode card. The current data files are available for 71 isotopes. This feature was first available in MCNP6 Beta 2.

### 14) Pre-collision next event estimator (Ref. 40)

A pre-collision next-event estimator for point detectors has been developed for MCNP6. This pre-collision estimator augments the post-collision next-event estimator that has historically been used for point flux estimation in MCNP. The pre-collision next-event estimator includes the contribution of all possible reactions before the collision isotope and resulting reaction are sampled. This procedure provides an improved expected estimate per collision, but with a significant increase in computational costs per collision. This improved sampling technique removes the requirement to suppress coherent scattering for photon transport problems that include photon next-event estimators. The sampling of all possible scattering reactions generally provides an increase in the Figure of Merit (FOM) for most photon problems. This increase in the FOM can be significant when the contribution to a photon next-event estimator is primarily from forward coherent scattering. For most neutron problems there is typically not a large increase in the FOM. However, for both photons and neutrons the pre-collision next-event estimator increases the convergence rate as measured by the time to pass MCNP's 10 statistical checks. This option is enabled by the FTn command and the new keyword PDS (for point detector sampling) with a single value to select the desired pre-collision option. This feature was first available in MCNP6 Beta 2.

**15) Double differential particle interaction cross section generator (Ref. 41)**

The GENXS option on the *tropt* card in MCNP6 allows the application of high-energy nuclear interaction models in a cross section generation mode, without particle transport. A source may be specified inside a medium; each history will consist only of the interaction of the source particle at the source energy with the components of the medium. The tallied outcome from the event consists of the energies and direction cosines of the secondary particles and the recoil nuclei (in the laboratory system). Although one expects that, in normal applications, the material composition will be a single isotope, averaged results may be obtained for a natural multi-isotopic element or a complex composition. This feature was first available in MCNP6 Beta 2.

**16) New MCNP6 Depletion Capability**

MCNP6 depletion enables complete, relatively easy-to-use depletion calculations in a single Monte Carlo code. The enhancements described here help provide a powerful capability as well as dictate a path forward for future development to improve the usefulness of the technology. The MCNP6 depletion capability enhancements beyond MCNPX 2.6.0 include: (1) new performance enhancing parallel architecture that implements both shared and distributed memory constructs; (2) enhanced memory management that maximizes calculation fidelity; and (3) improved burnup physics for better nuclide prediction; (4) added *swapb* keyword on the *burn* card, which allows universe swapping at each time step during the burn to mimic fuel shuffling at the assembly and pin levels. These improvements, as well as their performance in the H. B. Robinson fuel assembly benchmark, are detailed in the reference (The New MCNP6 Depletion Capability, by M. Fensin, M. James, J. Hendricks, and T. Goorley, LA-UR-11-07032)

**17) Cosmic Ray sources**

The GENXS option on the *tropt* card in MCNP6 allows the application of high-

## IV. MCNP6 BUG FIXES

While there were many bugs (which will not be listed here) that have been identified as a part of the merger and corrected, there are several bugs that were identified and corrected in MCNPX 2.7.0 but were not corrected in MCNP6 Beta 2. These bugs have been fixed in MCNP6 Beta 3 and are identified below:

**1) Muonic Photons in Pulse-Height Tallies**

Muons disintegrating into photons (actually, x rays from (Z,A)+u => (Z-1,A) reactions) did not add the photon energy to pulse-height tallies. (The energy of the photons exiting a pulse height cell was still subtracted from the pulse-height tally.)

Consequently muon disintegrations in pulse-height tally cells in problems transporting muons could incorrectly reduce the score to those pulse height tallies.

**2) Muon-induced K-shell photon production control**

The probability of emitting a K-shell photon from muon disintegration (Pb and higher) is controlled by the 8th entry on the PHYS:| card:

PHYS:| 7J *xmugam*

If random number, $\xi$ > *xmugam* then a K-shell photon is emitted from muon disintegration for nuclides with Z>81. (The MCNPX 2.7.0 fixed value was *xmugam* = .92 for Z>81) The value should be different for each nuclide, but until a good set of values is provided, the single value of *xmugam* is used for Z>81. *Default: xmugam=.65*

**3) Array Overflows Caused by User Errors**

An improper initialization caused an array overflow in the geometry plotter. The overflow occurs only when there is a user error. The user error only occurs in the PLOT prompt command mode when the LABEL command is given an invalid cell parameter entry. Another array overflow occurs when the user improperly specifies an input card name of longer than five characters in the INPUT file.

**4) Incorrect Directions Possible**

After the photons from neutron-induced photon production (ACEGAM) are banked, the neutron direction was restored only for the universe level of the neutron. In repeated structures the higher level universe directions were not restored. Consequently, a call to UPLEV has been added after the GETPAR call at the end of ACEGAM. Perhaps this affects modified versions of MCNPX270, but it does not affect the 500+ problem test suite. Possibly the higher level directions are reset later before they are needed again.

**5) Photofission Errors**

A zero divide causing a crash was possible for photonuclear reactions at energies for which the ACE photonuclear data libraries had photofission and no other reactions.

*Affects photofission problems (MODE n p) using photonuclear data for fissionable nuclides in rare cases.*

LLNL photofission (PHYS:P 6J 1) failed when the photonuclear cross section was zero. The fatal error, "*photonuclear reaction type not found,*" was issued when a 12.8346241514980 MeV photon tried to interact with 8016.70u. LLNL photofission should be bypassed when the photonuclear cross section is zero.

## V. MCNP6 CODE DEVELOPMENT PROCESSES

MCNP6 is considered risk level two, the second highest category of four levels. Risk level two software is treated as if failure of the software could result in temporary injury or illness to workers or the public. MCNP6 is not considered a risk level one, i.e. failure of the software would result in death, loss of life or limb, or permanent illness in the public or workers (i.e. one definition of risk level one software), because MCNP was not developed expressly for nuclear safety calculations, an explicit criterion for risk level one software.

The MCNP6 team uses TeamForge® software for source code and document version control and for tracking code defects and new features. TeamForge uses the concurrent version system (cvs) for version control. Each code developer has the ability to check-out the source code, make modifications, and check-in improvements. Each check-in must also reference a TeamForge artifact, which is a description of the background and intent of a particular new feature or defect fix. Artifacts query the developer regarding the status, category, priority, platform, and version of defects. Emails, input files, other documentation, and other artifacts can also be associated with each artifact. Artifacts also contain information about which developer owns the artifact and which developer is the artifact reviewer. Through this process, each line change in the source code has an associated artifact and developer. A web-based user interface allows developers to easily search by developer, artifact name or containing text, or subroutine. Changes in MCNP6 are required to be peer reviewed within the MCNP6 development team. Prior to check-in, each developer is required to ensure that his modifications pass the regression test suites on at least one computing platform with at least one compiler. Thirty minutes after the check-in, the automated continuous build and test system (CTBS) builds MCNP on several platforms with different compilers and runs several of the test suites, described below (Ref. 42).

The development history of each MCNP5 subroutine change has been maintained and updated this way since 2005, when the team switched from different version control software. MCNP6 changes associated with the merger were associated with an overarching merger artifact, not individual features or defect corrections associated with the merger process. New features created in MCNP6 during the merger process, however, are identified by their own separate artifacts and check-ins.

## VI. MCNP6 VERIFICATION, VALIDATION AND REGRESSION TEST SUITES

The MCNP6 development team strives to deliver a high quality production code that works on many compilers and platforms. The confidence behind MCNP6 is supported by its favorable comparisons with benchmark experiments and, in some cases, analytical results. To a lesser degree, an extensive level of regression test processes and our code development process add to that confidence. Comparisons for the verification and validation (V&V) tests are automated, and html tables or plots of code results compared to experimental data or analytical results are created each week. These comparisons are available to the MCNP code developers and form the basis for the MCNP6 V&V documents.

MCNP6 has 22 test directories containing several hundred specific problems testing that MCNP6 is running as expected. These tests span regression, verification and validation problems and are detailed by directory below. Each of these test suites has expected Linux and Windows Templates, for regression tests, or a set of analytical or benchmark values for V&V tests. The MCNP6 team strives to make the calculated results of the test suites independent of computer platform, compiler and serial or parallel execution, where possible. For more information, see the “About_the_tests” or README file in many of the subdirectories in the MCNP6 distribution. Users are cautioned that regression test problems intentionally create fatal errors or otherwise exhibit poor geometry, source, tally or physics input practices. Regression tests are not to be imitated in production calculations.

## VI.A. ELECTRONS

This test suite contains 54 test problems that exercise various aspects of electron and coupled photon/electron transport. An important subset of these problems explore three different algorithms for the application of the Landau straggling theory for electron collisional energy loss. These are the "bin-centered" method, the ITS-style "nearest-group-boundary" method, and the more recently developed (and preferred) "energy and step specific" method.[43] These tests show that the recommended algorithm (which is now the default in MCNP6) greatly reduces the occurrence of step-size-related artifacts in the energy-loss sampling for electrons.

## VI.B. FEATURES

Recognizing that regression tests should be more appropriately ordered by what features they test, this directory is broken into regression tests for four new features. DAWWG tests the ability for MCNP6 to create a mesh of constructive solid geometries and write the appropriate LNK3DNT files. The FMESH_INC directory contains five tests of the interaction of the *fmesh* card and the *unc* card. The UNC directory contains eleven tests for the collided or uncollided secondary particle production features. The POINT_DETECTORS directory contains twenty tests analyzing the effects of different photon and electron transport options on point detectors.

## VI.C. KOBAYASHI

The “Kobayashi Benchmarks” are added to the MCNP6 test suites. This set of 3D benchmark problems consists of simple geometries that contain at least one void region and one monoenergetic isotopic, cubic source region.[44] Each configuration is simulated first with a purely absorbing and then with a fifty-percent scattering medium. Fluxes are calculated at various points throughout the geometries using point detector tallies. For the purely absorbing cases, there are exact solutions obtained using numerical integration. For the cases with scattering, reference solutions were computed by very long runs with the MVP Monte Carlo code.[45] Overall, for two cases of each of the three problems, 136 different fluxes are compared between computed MCNP6 results and the reference.

### VI.D. LONG_INTEGER

MCNP6 contains more than fifty integer variables that are always stored as 8-byte integers. This allows users to run more than 2.1 billion source particles on 32-bit operating system, for example. These six test problems help test that these large integer values can be read in the input parser, and that these variables do not overflow (i.e. become large negative integers) during execution of MCNP. Some of these tests may require hours or days to execute on some powerful LANL supercomputers.

### VI.E. MAG_FIELDS

These six input tests exercise the magnetic field transport in air and down a proton radiography beam line. Constant and quadruple magnetic fields are modeled.

### VI.F. MCNPX_65

This is the set of seventy five MCNPX regression test problems. Several of these test problems include continue runs, surface sources, ptrac file production, weight-window file creation and usage, and mixing nuclear data tables and models during neutron transport.

### VI.G. MCNPX_EXTENDED

This set of directories includes the MCNPX test problems from later MCNPX releases. They are divided into subdirectories based on the feature being exercised. See Table 3 for a more detailed listing of these inputs. In each of these directories, the file TheCount is a listing of the total number of output files created. Currently these tests are considered regression checks, but several of these problems exercise two different ways of doing the same thing. For example, the macrobody test problems mimic the same geometry as the conventional CGS.

### VI.H. MUONS

These nineteen test problems exercise the creation of characteristic muonic X-rays using older and newer methods. This suite is mostly used by the developers to probe the effects of changing particular muon physics options.

### VI.I. PERFORMANCE

These four tests are used to evaluate runtime performance for a variety of features. They are intended to be run repeatedly to collect an average execution time. The input files include cases representing criticality, pulse height tally variance reduction, photon transport through a lattice representation of a human head, and a generic porosity tool used in nuclear oil well logging.

**VI.J. PHOTONS**

This test suite of fifty three tests was used by the developers as they extended photon transport down to 1 eV to investigate certain physics effects.

**VI.K. PHTVR**

This set of 209 problems test the pulse height tallies with several combinations of variance-reduction methods.

**VI.L. REGRESSION**

The standard MCNP6 Regression Test Suite comprises one hundred and thirty four problems, with new tests added to cover code features or to explicitly confirm that particular bugs are fixed. The regression tests do not verify code correctness; they are used only for the purpose of detecting unintended changes to the code and for installation testing. This directory also contains eleven regression tests of transport through unstructured meshes.

**VI.M. VALIDATION_CEM**

These benchmarks exercise the ability to create and transport high energy particles using CEM.[46,47] Tests, and their experimental comparisons to data, are of the following categories: isotope production by bremsstrahlug photons of energies from 30 MeV to 4.5 GeV impacting a thin $^{93}$Nb target and double-differential spectra of protons spectra at several angles produced by bremsstrahlug photons of energies from 30 MeV to 4.5 GeV on a thin $^{12}C$ target; delayed neutron emitters production from a thin $^{238}U$ target bombarded with 1 GeV protons; neutron and gamma spectra resulting from 18 MeV protons on water containing $^{18}O$; backward and off-axis angle spectra of neutrons resulting from 1200 MeV protons on thick Fe cylinders; proton and complex particles spectra (gas production) from thin $^{238}U$, $^{197}Au$, and $^{209}Bi$ thin targets bombarded with nucleons of energies below 1 GeV, to name just a few.

## VI.N. VALIDATION_CRITICALITY

The criticality validation suite[48] consists of thirty-one problems from the International Handbook of Evaluated Criticality Benchmark Experiments.[49] It contains cases for a variety of fuels, including $^{233}U$, highly enriched uranium (HEU), intermediate-enriched uranium (IEU), low-enriched uranium (LEU), and plutonium in configurations that produce fast, intermediate, and thermal spectra. For each type of fuel, there are cases with a selection of moderators, reflectors, spectra, and geometries. The cases in the suite were chosen to include a broad range of configurations. The suite was modified to permit running with either ENDF/B-VI data libraries or the newer ENDF/B-VII.0 data libraries.

## VI.O. VALIDATION_CRIT_EXPANDED

This directory contains one hundred nineteen problems from the International Handbook of Evaluated Criticality Benchmark Experiments and is an extension of the VALIDATION_CRITICALITY suite.[50,51]

## VI.P. VALIDATION_LAQGSM

It is similar to the VALIDATION_CEM suite, but intended to test the high-energy event generator LAQGSM03.03.[46,52] LAQGSM is the only model used by MCNP6 allowing simulated interactions with heavy-ions and with almost all types on elementary particles at energies up to about 1 TeV/nucleon. This directory contains eighteen comparisons of resulting neutrons, protons, deuterons, tritons, $^{3}$He, $^{4}$He, pion, and kaon double-differential spectra from various reactions induced by protons, photons, and heavy-ions with incident energies up to 400 GeV. Additionally, several comparisons are made of the production of radioisotope fragments from thin gold, silver, copper, and silicon targets bombarded with protons and heavy-ions with energies up to 800 GeV. Neutron spectra from a thin carbon target bombarded with a 290 MeV/nucleon $^{12}$C beam, of interest to cancer treatment with a carbon-beam, are also investigated.

## VI.Q. VALIDATION_ROSSI_ALPHA

MCNP6 has the capability to compute the point-kinetics parameter Rossi-Alpha for a system at delayed critical. For such a system, Rossi-alpha is minus the ratio of the effective delayed neutron fraction to the effective neutron generation time. Here the term "effective" implies that the quantities are importance or adjoint weighted. The Rossi-Alpha validation suite includes thirteen criticality benchmarks and assesses how well MCNP6 and associated nuclear data (e.g., ENDF/B-VII.0) can match experimentally measured values.[53]

## VI.R. VALIDATION_SHIELDING

The radiation shielding validation suite contains thirty seven inputs in three subcategories: time–of-flight neutron spectra from pulsed spheres,[54] neutron and photon spectra at shield walls within a simulated fusion reactor, and photon dose rates from shielded sources and skyshine. Two of the cases are coupled neutron-photon calculations, while the others are exclusively neutron or photon calculations. This suite was overhauled to generate plots comparing calculated results against experimental data.

## VI.S. VERIFICATION_KEFF

Reference provides a set of seventy-five criticality problems found in the literature for which exact analytical solutions are known.[55] Number densities, geometry, and cross section data are specified exactly for these problems. As a part of MCNP6 verification, ten of these analytical benchmark problems are run to high precision.

A small addition to the overall confidence of MCNP6 is its use of automated regression testing suites. MCNP6's ~900 problem test suites are run nightly on Windows 64, Linux 32, and Linux 64 bit computers, with Intel 10, Intel 11, Intel 12, Portland, Absoft, and GFortran compilers; but, each compiler is not tested on each operating system. By compiling with this variety of compilers, the development team is more likely to find and correct coding defects. To exercise parallel capability, the regression suite is run nightly in serial, openmpi, omp, and openmpi+omp modes with the Intel 10 compiler on Linux 64. The serial tests are also compiled with array overflow and use of uninitialized variable debugging checks. When the Intel test coverage tool is applied to parallel execution of the ELECTRONS, FEATURES, MAG_FIELDS, MCNPX_65, MCNPX_EXTENDED, MUONS PHOTONS, PHTVR, POINT_KINETICS, and REGRESSION suites, we found that 91% of the files are tested, as are 79% of the functions, and 65% of the blocks. In this context, a block is defined as portion of code for which the instructions are executed exactly once, in order, with one entry and exit point. A large fraction of the remaining files and functions are associated with plotting. The results of these tests (more than 20,000 tests) are displayed on a large video screen in the XCP-3 lounge area. Our experience is that this highly visible status report results in faster identification of code compile failures and unintended impacts on regression suites, and therefore faster resolution of these issues. This test system was created by Charles Zeeb in the scripting language Perl, and is tightly integrated with the SQL database PostgreSQL. Additional parallel and compiler tests are performed on versions prior to a release.

## VII. FUTURE MCNP6 DEVELOPMENT

MCNP6 continues development in several widely disparate fields of Monte Carlo particle transport. We continue to improve its physics, either by improving our own transport algorithms or incorporating those developed by others. We are currently interested in lowering electron transport to about 100 eV, adding molecular interaction cross sections for both photons and electrons, and improving the optical light transport with reflection and refraction. Improving the energy and time signatures of delayed particle emissions also continues to be a focus area.

Most of the interaction physics today in MCNP assumes that average quantities (number and energies of products) are correct. While necessary a decade ago to fit within computer hardware requirements, this limitation is no longer necessary and many users are now interested in correlations of emitted neutrons and gammas.

MCNP6 will continue to merge the unstructured mesh capability with the other features, especially the plotting, variance reduction and volume source rejection features. Improvements to the temperature effects on neutron interactions are under development.

We attempt to anticipate what the next generation of supercomputers will look like, and how to exploit their massive number of processors, and possibly even their hardware acceleration. We are in the process of investigating Fortran 2003 features, specifically the co-array capabilities, for advanced parallelism with lower communication overhead.

It is the intent of the MCNP developers to produce publically available MCNP6 updates every six months. Although the MCNP source and executables are only available through RSICC, source code patches will be posted to the MCNP6 website, mcnp6.lanl.gov. Users who have the ability to compile (which is not limited by cost since GFortran and gcc are free) and who possess the source from RSICC can produce their own executables; other users will need to request a new executable from RSICC.

## VIII. CONCLUSIONS

MCNP6 is now available from RSICC and we encourage MCNP5 and MCNPX users to migrate to this code. MCNP6 will not exactly recreate the particle tracks of either MCNP5 nor MCNPX because several default options have been changed. This first release is not considered a full and robust "production" release for one main reason. Although full inter-operability MCNP5 and MCNPX features exist (i.e., there are no more remaining *dbcn 29* flags), this large combination of features has not been extensively tested. While there has been a significant amount of V&V behind MCNP6 already, and this V&V is made available with the MCNP6 distribution, users have been cautioned and continue to be cautioned that they are responsible for V&V for their own particular application of the code. It is expected that users of this initial release apply MCNP6 to the problems that they know well and have some intuition about, and report back to the MCNP6 team (email mcnp6@lanl.gov) their findings, either pro or con. Evidence for appropriate performance of MCNP6 should be added to the MCNP6 documentation and verification test suites, and evidence of discrepancies, especially discrepancies with MCNP5 1.60 or MCNPX 2.7.0, should be submitted for investigation.

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The MCNP6 code developers thank the authors of the other codes, modules and libraries who have allowed their algorithms to be incorporated into and distributed with MCNP6. Although typically developed at other DOE national laboratories, several algorithms were developed at other international institutes. The high-energy (typically 100s of MeV to 10s of GeV or higher) nuclear reaction models (event-generators) CEM and LAQGSM were initially proposed at the Joint Institute for Nuclear Research (JINR), Dubna, Russia, and developed, improved, and maintained thereafter at LANL; INCL + ABLA was developed initially at the Liege University, Belgium, and GSI, Darmstadt, Germany, with important contributions from researchers of CEA/Saclay, France. Lower energy physics contributions include the Sandia National Lab code ITS 3.0 for electron transport and LLNL's fission multiplicity model for both photon and neutron induced fissions. The LANL CINDER team and other T Division contributors are responsible for the radioactive isotope cross sections (for production and depletion) as well as the decay emission data. We also would like to thank the RSICC for their many years of distributing MCNP.

Finally, we also thank our users, especially those users who provide us with insight into what is not working as expected, what features would be more useful, and the code's performance against experiments. Those users who take the time to create small test problems and fully describe suspected code defects are extremely valuable to us, and they will be acknowledged with individual certificates and listed on the MCNP6 website, mcnp6.lanl.gov. Many other users make the effort to provide detailed feedback to those who post questions to the mcnp email forums.

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TABLE I
Summary of MCNP public releases

| MCNP Version | Release Month/ Year | Some Significant New Features (For a more detailed description, see each versions release notes). |
|---|---|---|
| MCNP3 | 1983 | First release through RSICC. Written in Fortran 77 |
| MCNP3A | 1986 | |
| MCNP3B | 1988 | Plotting graphics, generalized source, surface sources, repeated structures/lattice geometries |
| MCNP4 | 1990 | Parallel multitasking, electron transport |
| MCNP4A | 10/1993 | Enhanced statistical analysis, new photon libraries, ENDF-6, color X-Windows graphics, dynamic memory allocation |
| MCNP4B | 4/1997 | Operator perturbations, enhanced photon physics, PVM load balancing, cross-section plotting, 64-bit executables, lattice universe mapping, enhanced lifetimes |
| MCNPX 2.1.5 | 11/1999 | First public release of MCNPX, based on MCNP4B with CEM INC, HTAPE3X, mesh and radiography tallies, and an improved collisional energy loss model. |
| MCNP4C | 4/2000 | Unresolved resonance treatments, macrobodies, superimposed importance mesh, perturbation, electron transport, plotter and tally enhancements |
| MCNP4C2 | 1/2001 | Photonuclear physics, interactive plotting, plot superimposed weight-window mesh, weight-window improvements |
| MCNPX 2.3.0 | 4/ 2002 | LAHET 2.8 and some 3.0 extensions. |
| MCNPX 2.4.0 | 8/2002 | Update to MCNP4C, build system for Windows OS, support for Fortran 90. |
| MCNP5 1.14 | 11/2002 | Fortran 90, photonuclear collisions, geometry superimposed mesh tallies, time splitting, shared memory threading with OpenMP. Mac OSX support |
| MCNP5 1.20 | 10/2003 | Increased number of detectors to 100 and number of tallies to 1000. Mostly a code defect fix release. |
| MCNP5 1.30 | 8/2004 | Explicit 8-byte integers for nps > 2.1 billion, Lattice and fmesh tally enchantments. Support for MPI on Mac OSX. |
| MCNPX 2.5.0 | 4/2005 | 34 particle types, four light ions, mix and match nuclear data tables and model physics, CEM2k, INCL4/ABLA physics models, fission multiplicity, spontaneous fission sources, pulse height tallies with variance reduction, pulse height light tally, coincident capture tallies, variance reduction with model |
| MCNP5 1.40 | 11/2005 | Lethargy plots, logarithmic data interpolation, neutron multiplicity distributions, stochastic geometry, source entropy, mesh tally plots, new electron energy loss straggling |
| MCNPX 2.6.0 | 4/ 2008 | Depletion/Burnup, heavy ion transport, LAQGSM physics, CEM03 physics, delayed gamma emission, energy-time weight windows, charged ions from neutron capture, spherical mesh weight windows, spontaneous photons |
| MCNP5 1.51 | 1/2009 | Photon Doppler broadening, variance reduction with pulse height tallies, |

| | | |
|---|---|---|
| | | annihilation gamma tracking, Doppler broadening in makxsf, large lattice enhancements |
| MCNP5 1.60 | 8/2010 | Adjoint weighted tallies for point kinetics parameters, mesh tallies for isotopic reaction rates, up to 100 million cells & surfaces, up to 10 thousand tallies |
| MCNPX 2.7.0 | 4/2011 | Tally Tagging, embedded sources, cyclic time bins, focused beam sources, PTRAC coincidence, LLNL fission multiplicity, Receiver-operator characterization (ROC) tally, NRF data in ACE libraries, triple & quadruple coincidence, LAQGSM 3.03 and CEM 3.03 physics. |
| MCNP6 0.1 | 1/2012 | Unstructured mesh geometry transport, automatic weight-window generation with SN code Partisn, photon transport to 1 eV, magnetic field tracking in air |

TABLE IIA
MCNP6 elementary particle types and interactions

<table>
<tr><th>MCNP particle number, symbol</th><th>MCNP particle name</th><th>Summary of interaction physics, when appropriate particles are listed on the mode card. Negative or positive refers to electric charge.</th></tr>
<tr><td>2, p</td><td>photon</td><td>photon, common symbol: $\gamma$<br>Production from neutron and muon capture, inelastic interactions (including fission, and spallation), atomic relaxation (characteristic X-Ray production), positron annihilation, bremsstrahlung, particle and radioactive decay. No synchrotron or Chrenkov production.<br>Transport with photonuclear interactions, Raleigh scattering, Compton scattering, photoelectric effects, and pair production.</td></tr>
<tr><td>3, e</td><td>electron</td><td>electron, common symbol: $e^-$<br>Production from: High-energy inelastic interactions, particle decay, Compton scattering, photoelectric interactions, atomic relaxation (Auger electrons), pair production, electroionization (knock-on electrons), nuclear relaxation (conversion electron production), and beta decay.<br>Transport with: multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), electroionization, bremsstrahlung, and interaction with magnetic fields.</td></tr>
<tr><td>4, |</td><td>mu -</td><td>negative muon, Common Symbol: $\mu$-<br>Transport with elastic scattering, continuous slowing down approximations, energy and angle straggling, decay, magnetic field effects, and at-rest capture.</td></tr>
<tr><td>6, u</td><td>nu_e</td><td>electron neutrino, common symbol: $\nu_e$<br>Transport with in-flight decay only, no interaction mechanisms</td></tr>
<tr><td>7, v</td><td>nu_m</td><td>muon neutrino, common symbol: $\nu_m$<br>Transport with in-flight decay only, no interaction mechanisms</td></tr>
<tr><td>8, f</td><td>positron</td><td>positron, common symbol: $e^+$<br>In nuclear data based transport, treated as identical to electron except for annihilation at rest, directions in magnetic fields, and a few special tallies. For model based transport, treated as separate particle for interaction physics.</td></tr>
<tr><td>16, !</td><td>mu +</td><td>positive muon, Common Symbol: $\mu$+<br>Transport with: Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields.</td></tr>
<tr><td>17, <</td><td>anti nu_e</td><td>anti electron neutrino, common symbol: $\bar{\nu}_e$<br>Production from decay, but no interactions during transport.</td></tr>
<tr><td>18, ></td><td>anti nu_m</td><td>anti muon neutrino, common symbol: $\bar{\nu}_m$<br>Production from decay, but no interactions during transport.</td></tr>
</table>

TABLE IIB
MCNP6 composite particle types (hadrons) and interactions

| MCNP particle number, symbol | MCNP particle name | Summary of interaction physics, when appropriate particles are listed on the mode card. Negative or positive refers to electric charge. |
|---|---|---|
| 1, n | neutron | neutron, common symbol: n<br>Production from Absorption (n,2n, n,3n, etc.), fission (prompt and delayed), photonuclear interactions, high energy spallation and fragmentation.<br>Transport with capture, elastic and inelastic scattering, and some molecular scattering and temperature effects on scattering |
| 9, h | proton | proton, common symbol: $p^+$<br>Production from neutron elastic scattering off of hydrogen, and (n,p) reactions, inelastic scattering<br>Transport with elastic and inelastic nuclear scattering, Continuous slowing down approximation, energy and angle straggling, magnetic field effects |
| 10, l | lambda0 | Lambda baryon, common symbol: $\Lambda^0$<br>Transport with in-flight decay only, no interaction mechanisms |
| 11, + | sigma+ | positive sigma baryon, common symbol: $\Sigma^+$<br>Transport with:  Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields. |
| 12, - | sigma- | negative sigma baryon, common symbol: $\Sigma^-$<br>Transport with:  Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields. |
| 13, x | xi0 | Xi baryon, common symbol: $\Xi^0$<br>Transport with in-flight decay only, no interaction mechanisms |
| 14, y | xi - | negative Xi baryon, common symbol: $\Xi^-$<br>Transport with:  Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields. |
| 15, o | omega - | omega baryon, common symbol: $\Omega^-$<br>Transport with:  Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields. |
| 20, / | pi + | positive pi meson or pion, common symbol: $\pi^+$<br>Production with all physics modules from high energy interactions<br>Transport with:  Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields. |
| 21, z | pi_zero | neutral pi meson or pion, common symbol: $\pi^0$<br>Production with all physics modules from high energy interactions<br>Transport with in-flight decay only, no interaction mechanisms |
| 22, k | K + | positive K-meson or kaon, common symbol: K+<br>Transport with:  Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields. |
| 23, % | K0_short | short K-meson or kaon, common symbol: $K^0_S$<br>Transport with in-flight decay only, no interaction mechanisms |
| 24, ^ | K0_long | long K-meson or kaon, common symbol: $K^0_L$<br>Transport with in-flight decay only, no interaction mechanisms |
| 29, w | Xi+ | positive anti-Xi baryon, common symbol: $\bar{\Xi}^+$<br>Transport with:  Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields. |
| 35, * | pi - | negative pi meson or pion, common symbol: $\pi^-$<br>Production with all physics modules from high energy interactions<br>Transport with:  Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields. |
| 36, ? | K - | negative K-meson or kaon, common symbol: K-<br>Transport with:  Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields. |

TABLE IIC
MCNP6 composite anti particle types (hadrons) and interactions

| MCNP particle number, symbol | MCNP particle name | Summary of interaction physics, when appropriate particles are listed on the mode card. Negative or positive refers to electric charge. |
|---|---|---|
| 5, q | Antineutron | antineutron, common symbol: $\bar{n}$<br>Transport with in-flight capture and annihilation |
| 19, g | Antiproton | antiproton, common symbol: $\bar{p}$<br>Transport with in-flight or at-rest capture and annihilation, and interaction with magnetic fields. |
| 25, b | Anti lambda0 | antilambda baryon, common symbol: $\overline{\Lambda^0}$<br>Transport with in-flight decay only, no interaction mechanisms |
| 26, _ | Anti sigma+ | positive antisigma baryon, common symbol: $\bar{\Sigma}^+$<br>Transport with: Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields. |
| 27, ~ | Anti sigma- | negative antisigma baryon, common symbol: $\bar{\Sigma}^-$<br>Transport with: Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields. |
| 28, c | Anti Xi0 | neutral anti-Xi baryon, common symbol: $\bar{\Xi}^0$<br>Transport with in-flight decay only, no interaction mechanisms |
| 30, @ | Anti omega- | negative antiomega baryon, common symbol: $\bar{\Omega}^-$<br>Transport with: Multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), decay, and interaction with magnetic fields. |

TABLE IID
MCNP6 complex particle types (nuclei) and interactions

| MCNP particle number, symbol | MCNP particle name | Summary of interaction physics, when appropriate particles are listed on the mode card. Negative or positive refers to electric charge. |
|---|---|---|
| 31, d | deuteron | $^{2}H$ (deuterium) nucleus, common symbol: d<br>Transport with elastic and inelastic nuclear scattering, continuous slowing down approximation, multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), and interaction with magnetic fields. |
| 32, t | triton | $^{3}H$ (tritium) nucleus, common symbol: t<br>Transport with elastic and inelastic nuclear scattering, continuous slowing down approximation multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), and interaction with magnetic fields. |
| 33, s | helion | $^{3}He$ nucleus, common symbol: $^{3}He$<br>Transport with elastic and inelastic nuclear scattering, continuous slowing down approximation, multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), and interaction with magnetic fields. |
| 34, a | alpha | alpha particle (Helium-4 nucleus), common symbol: α<br>Transport with elastic and inelastic nuclear scattering, continuous slowing down approximation, multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), and interaction with magnetic fields. |
| 37, # | heavy ion | atomic nuclei with proton number from Z = 3 to Z = 100<br>Transport with elastic and inelastic nuclear scattering, continuous slowing down approximation, multiple Coulomb scattering for angular deflection and energy loss (including energy-loss straggling), and interaction with magnetic fields. |

TABLE III
Summary of MCNPX Extended Test Problems incorporated into MCNP6

| Directory | Number of test problems | Notes |
|---|---|---|
| avr | 22 | Advanced variance reduction |
| class | 25 | Simple problems used in the week-long MCNP classes |
| classgeom | 20 | Examples of more advanced geometries, including macrobody hexagonal prisms, cell based rejection, filling universes |
| classvar | 10 | Class problems on variance reduction methods |
| heavyions | 9 | Test problems focusing on heavy ion transport |
| mbody | 19 | Test reading and transporting particles through all the macrobodies |
| phys | 28 | Tests a variety of coupled particle physics interactions, data sampling routines, |
| push | 24 | Variety of simple historic tests |
| test27a | 12 | Tests the new features released in MCNPX 2.7.A: tally tagging, activation, embedded sources |
| test27b | 13 | Tests the new feature released in MCNPX 2.7.B: spontaneous fission weighting, charged ion creation from nuclear reactions, LET tallies and dose equivalent tallies, |
| test27c | 10 | Tests the new feature released in MCNPX 2.7.C: muons, new ptrac features, time dependant mesh tallies, delayed neutron treatments |
| test27d | 19 | This is a test suite to test the new feature released in MCNPX 2.7.D: improved form factors, cyclic time bins, elemental residuals, coincidence, signal to noise PDFs. |
| test27e | 21 | Tests the new feature released in MCNPX 2.7.E: fission multiplicity, photofission, background sources, nested file read statements, |
| testburn | 16 | Tests that exercise the production/depeletion features relating to the burn card. |
| testdndg | 18 | Tests relating to delayed neutron and gamma emission spectra |
| testincl | 42 | Tests relating to high energy particle transport, energy deposition, photonuclear physics |
| testmcnp | 31 | The set of regression test problems from MCNP4B |
| testmesh | 10 | Tests mesh tallies with various geometries and particles. |
| testmix | 13 | Tests of the transition between using models and data tables for transport. |
| testpht | 58 | Tests of the Pulse Height Tally with variance reduction |
| testxnew | 19 | Test of previous version of MCNPX |
| testxold | 35 | Test of even older version of MCNPX |
| zrecoil | 37 | Test of light ion recoil |

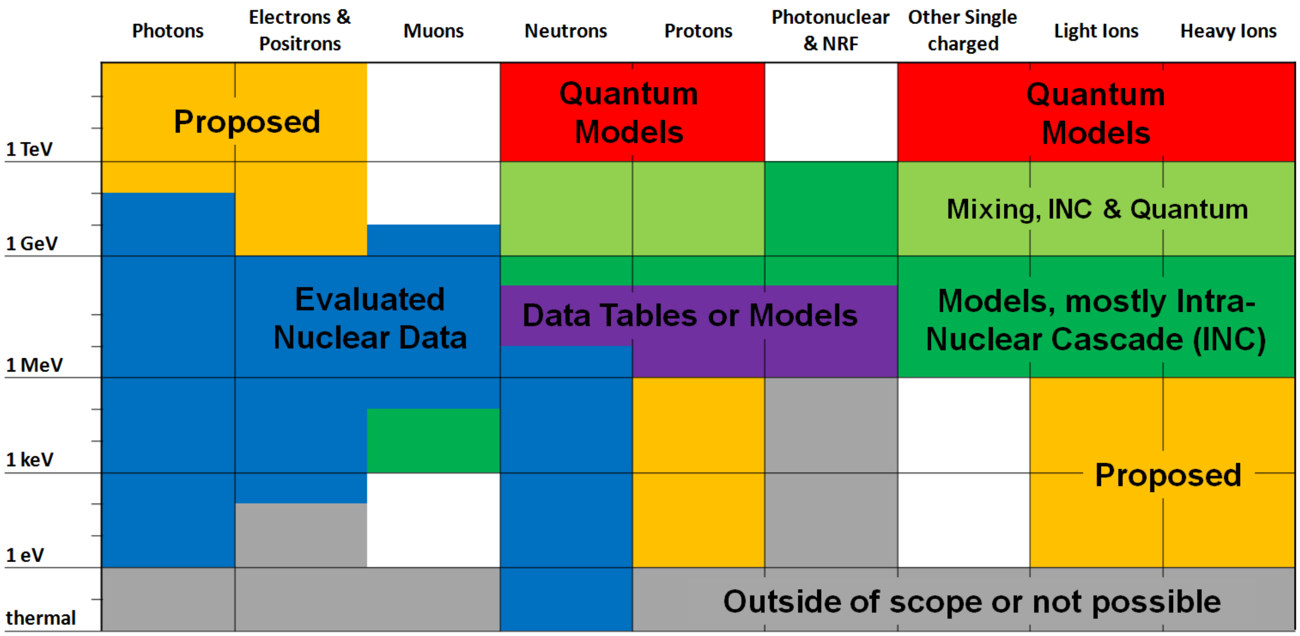


Fig. 1. Tabular representation of MCNP6 particle types, energy ranges and interaction physics. The column titled other single charged includes the charged composite particles listed in Tables 2b and 2c.