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MCNP Accomplishments for the Nuclear Criticality Safety Program

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INTRODUCTION

MCNP is a mature and robust continuous-energy Monte Carlo code. It has been used to perform high-fidelity benchmark calculations for cross sections, calculations for critical experiment design, analyses for criticality safety problems, and many other applications since the 1970s. For the past decade, the production release of the code has been MCNP5 [1], with over 10,000 copies distributed throughout the world. The next major version of the code, MCNP6.1 [2], is, as of the time of this writing, being finalized for release and distribution by RSICC. This paper summarizes progress during FY 2013 in the development and support of MCNP for the US DOE Nuclear Criticality Safety Program (NCSP). Activities and accomplishments are summarized for the following: MCNP6.1 capabilities and status, verification and validation testing at LANL, user support and training for NCSP, current methods research and development efforts, progress on sensitivities and uncertainty analysis capabilities, and the future issues with MCNP.

MCNP6.1 RELEASE

MCNP6.1 is the next major release of MCNP, scheduled to be released in the summer of 2013. For the past few years, the production version of MCNP has been MCNP5-1.60 [3], which was released in October 2010. The production of MCNP6.1 is a major, multi-year code development effort at LANL, largely focused on the merger of MCNP5 and MCNPX [4]. During the time between MCNP5-1.60 and MCNP6.1, new capabilities relevant to criticality have been developed: the fission matrix, a fast method of Doppler broadening as needed (the "On-the-Fly" or OTF Method), and continuous-energy sensitivity profiles for k_{eff}. MCNP6.1 also distributes the ENDF/B-VII.1 nuclear data libraries as the default cross sections, while still including all the nuclear data from previous releases.

An important aspect of MCNP6.1 for criticality safety practitioners is that the results for k_{eff} problems are unchanged [5], which should make migration not too onerous. MCNP5 development has completely ceased, and in a few years the MCNP Development Team at LANL will only be providing support for MCNP6. Therefore, managers of criticality safety groups at DOE/NNSA sites should plan on migrating to MCNP6 in the next few years.

VERIFICATION & VALIDATION

Throughout the over 35 year history of MCNP, ongoing, serious effort has been devoted to ensuring that MCNP provides reliable, accurate results for criticality safety applications with the best available cross-section data. The MCNP website (mcnp.lanl.gov) provides over 50 verification/validation reports for criticality safety and cross-section data evaluation. The current MCNP code distributions from RSICC include over a hundred ICSBEP Handbook problems used in the routine evaluation of MCNP [6], numerous verification problems to test the underlying algorithms in MCNP, and hundreds of other test problems to diagnose the code.

The MCNP Development Team does nightly testing of the code to ensure results have not changed unintentionally as part of development. Annually as part of NCSP support, the Development Team performs a detailed assessment of the impact of changes to the code, new compilers, new platforms, and new nuclear data on criticality calculations. A publicly available technical report [5] that shows results have not changed as a consequence of coding changes between MCNP5-1.60 and MCNP6.1. Some results may not match exactly, but should agree within statistics, because of numerical roundoff as a result of switching from the Intel-10 compiler to Intel-11 or Intel-12. The Development Team has analyzed these results and confirmed that this is not an issue with the code; it still gives the same results. Additionally, testing was done with the ENDF/B-VII.1 nuclear data libraries and compared results from ENDF/B-VII.0, the last major nuclear data release. Overall, the results differ slightly with some minor improvements for specific cases. Based on this testing and additional testing by the nuclear data team [7], it appears that MCNP6.1 is correctly handling the new nuclear data, and users should feel confident in switching to the newest libraries should they choose.

USER SUPPORT & TRAINING

The MCNP development team continues to provide a high level of user support, including 3-4 one week long introductory classes on MCNP each year at LANL and several on-site classes at other DOE/NNSA Laboratories targeted toward criticality safety specialists. In the last two years, on-site classes have been held at Hanford, Idaho National Laboratory, and Sandia National Laboratory. In early

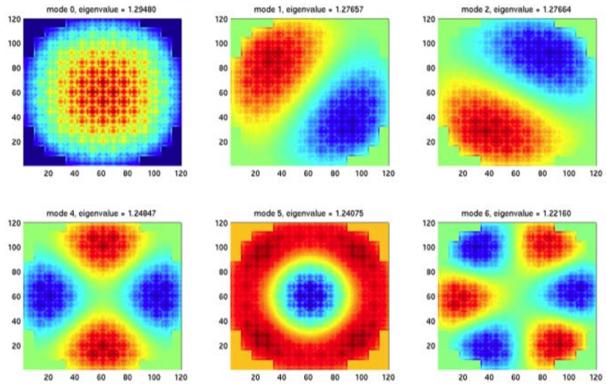

Fig. 1. Some eigenmodes for a 2-D PWR.

2013, the Development Team taught a special class exclusively for the Criticality Safety group at LANL.

The MCNP website has recently been modernized and should be far more navigable and useful to users. Perhaps the most important development is the MCNP reference collection, containing over 600 documents with over 1 GB of content. The publicly available PDF files are reports and papers covering all aspects of MCNP – theory, practice, verification and validation, parallel computing, etc. The Development Team hosts a mailing list (the "MCNP Forum") consisting of over 1000 members where users can ask questions and get support from developers or other MCNP users. Additionally, the Development Team assists users with the installation and use of MCNP on a large number of different computer platforms: Windows, Macs, Linux, Unix, threaded parallelism on laptops and desktops, MPI parallel use on clusters, various Fortran compilers, etc.

METHODS RESEARCH & DEVELOPMENT

In addition to supporting the existing code capabilities and its users, the MCNP developers also perform research on new methods pertaining to criticality. Notable developments in this area have been the fission matrix, the OTF Doppler broadening, and continuous-energy sensitivity analysis capabilities.

Fission Matrix

Conceptually, the fission matrix [8] gives information about how fission neutrons emitted in one region of the problem "communicate" with other regions of the problem by causing fission. Using linear algebra packages, the eigenvalues and eigenvectors of this matrix can be solved to obtain information about the fundamental mode (k_{eff} and the steady fission source distribution in the system) as well as higher modes (see Fig. 1 for an example). This information is useful for accelerating fission source convergence, correcting the non-conservative bias in the uncertainty estimates in Monte Carlo eigenvalue calculations, computing the dominance ratio for noise and stability analysis, and doing perturbations, xenon oscillations, etc.

A developmental version of the capability to compute a fission matrix is available in MCNP6.1 for interested users to try for specific applications. Future plans for this capability involve applying the fission matrix in a more automatic way, e.g., for convergence acceleration and detection. Also, development is underway to more elegantly handle the memory requirements of storing the matrix, allowing for unprecedented resolution of the eigenmodes, which may lead to new possibilities for neutronic analysis.

OTF Doppler Broadening

For select applications in criticality, understanding the effect of temperature variations throughout an assembly is important. Historically, there have been a few approaches to handle this. All of these methods are labor intensive and not practical to scale up to high-fidelity analysis requiring hundreds of temperatures. A solution called the OTF method was developed that can efficiently calculate the Doppler broadened cross sections as needed. The idea is to construct special data libraries containing polynomial fits of the cross section as a function of temperature for each isotope, reaction, and incident neutron energy. This typically requires a few GB of storage, but allows for an arbitrary number of temperatures to be represented with minimal user input. This method is attractive because the slowdowns observed in the calculation are empirically small, a few tens of a percent on average.

The OTF method has been implemented in MCNP6.1 [9]. Currently, however, the data libraries needed to use the OTF method are not provided with the distribution, but a script for generating them is, and interested uses may generate their own libraries. In the future, the hope is to have official distributions prepared and distributed with MCNP.

Continuous-Energy Sensitivities

MCNP6.1 is the first version of MCNP that has the ability to generate sensitivity profiles for k_{eff} from continuous-energy ENDF data [10]. This new capability is meant to provide criticality safety analysts and integral experiment designers with estimates of how important specific nuclear data are to the overall multiplication of a given system. This is the second such capability funded by the NCSP, with TSUNMAI from Oak Ridge National Laboratory (ORNL) being the historic mainstay for this purpose. MCNP sensitivities have been shown to largely agree with those produced by TSUNAMI, and criticality safety practitioners may use either or both for their validation exercises. The advantages of the MCNP capability versus the

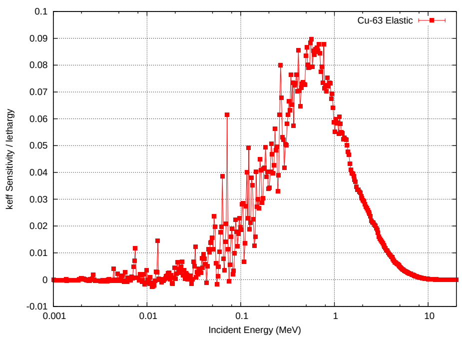

Fig. 2. Elastic scatter sensitivity of ^{63}Cu in Zeus.

elastic	elastic	462.1
elastic	inelastic	-867.5
elastic	n,2n	-3.4
elastic	fission	-82.2
elastic	n,gamma	36.0
inelastic	inelastic	859.0
inelastic	fission	1.3
n,2n	n,2n	11.1
fission	fission	331.0
fission	n,gamma	0.3
n,gamma	n,gamma	72.4
total nu	total nu	81.6
fission chi	fission chi	174.1
		587.6

Fig. 3. Uncertainty in k_{eff} (pcm) from ^{239}Pu in Jezebel.

current version of TSUNAMI (ORNL is currently working on equivalent capabilities) is that the sensitivities are generated with a single continuous-energy calculation (as opposed to multigroup) and that there is no required discretization in space or energy. See Fig. 2 for an example of sensitivities of a recent NCERC experiment.

SENSITIVITY/UNCERTAINTY DEVELOPMENTS

For FY 2013, the NCSP is funding the development of uncertainty analysis capabilities with MCNP, similar to those found in SCALE. The long term goal is to have MCNP generate estimates of uncertainty for various responses with minimal effort by the user. The current vision is with one option in the MCNP input, to have the code read in covariance data from its data files, create the energy-resolved sensitivity profiles, run the transport calculation, and convolve the computed sensitivities with the covariances to provide uncertainty estimates. Also funded under this effort are necessary enhancements and user support for the new sensitivity capability.

Progress for FY 2013 involves the development of a format for covariance data in the MCNP data (ACE) file. The format uses principal eigenvectors, which allows for compact storage of the large amount of information normally required to represent covariance matrices. Empirically, accurate uncertainty estimates on critical assemblies is possible with a memory savings of often times over 50% [11]. The format specification is currently available on the MCNP website [12]. Modifications to NJOY are currently underway to allow for the incorporation of the new format into existing ACE files.

A prototype capability in MCNP has been prepared that reads the new covariance format and generates uncertainty estimates by way of automatically generated sensitivity profiles. Results for ^{239}Pu uncertainties of k_{eff} of the Jezebel critical experiment using ENDF/B-VII.1 nuclear data are given in Fig. 3.

For user support, a user's guide [13] for the new k_{eff} sensitivity capability is available on the MCNP website. Under development in this area is a capability to convert MCNP sensitivity formats into SCALE formats and vice versa, allowing users of either MCNP or SCALE to more easily compare results. Also in development related to this is a capability to calculate sensitivities for fixed-source subcriticality measurements as well as other responses than k in eigenvalue problems.

FUTURE OF MCNP

Between MCNP5-1.60 and MCNP6.1, the codebase has increased from about 100 thousand lines of code to nearly half a million. This growth is largely from the merger of MCNP5 and MCNPX, which were two divergent branches of a version of MCNP from the 1990's. MCNP5 originally focused on code modernization in the early 2000's and since then has largely been supported by the Advanced Scientific Computing (ASC) program and the NCSP, and focused on specific application relevant to those two sponsors. MCNPX had a myriad of sponsors and incorporated a much wider variety of capabilities: high-energy physics, Monte Carlo depletion with CINDER90, radiation detection features, etc.

As exposed by the difficulty with releasing MCNP6.1 as a quality product, this large expansion of the codebase introduces new challenges going forward. The current core transport routines in MCNP were designed with assumptions about software design that are acceptable for smaller software, but do not scale well into the regime of a code with many hundreds of thousands of lines. The consequence is that future development and maintenance of new capability becomes more difficult and therefore expensive unless steps are taken to increase the flexibility of the codebase.

Also making this more urgent is the imminent coming of new computing architectures (e.g., GPUs, the Xeon Phi, etc.). The last decade and a half of computing has largely been quite stable and MCNP has been able to adapt without serious rethinking of software design. With the coming constraints of the new hardware (e.g., many more cores but less memory per core), the time for this is in the near future as waiting too long will likely lead MCNP into obsolescence.

As the release of MCNP6.1 nears completion, the MCNP Development Team is discussing the path forward. One probable option is an aggressive modernization effort that will incrementally revitalize the core transport routines in MCNP, optimizing them for flexibility and adaptability going forward. For better and worse, this is an issue spanning all of scientific computing within and far beyond the DOE, so MCNP will not be alone in this effort and will most likely be able to take advantage of developments elsewhere. Nonetheless, some investment will be required from all MCNP's stakeholders to keep the software going strong into the 2020's.

CONCLUSIONS

MCNP6.1 is about ready for release and will be available to general criticality safety analysts summer of 2013. The code has been extensively verified and validated with nightly testing, validation to ICSBEP benchmark results, verification to analytic solutions, etc. and the results show that there are no significant differences in results of MCNP5-1.60 and MCNP6.1. The MCNP Development Team will be dropping support for old version of MCNP, and therefore criticality safety managers should plan on migrating to MCNP6 in the next few years. The Development Team supports, and plans to continue to support, NCSP users through on-site and LANL classes, online resources, one-on-one installation support, etc.

The NCSP also funds development of new capability in MCNP related to criticality calculations. Recent accomplishments are the implementation of the fission matrix, the OTF Doppler broadening, and the continuous-energy sensitivity capabilities in MCNP6.1. NCSP has also funded the development of new uncertainty analysis tools for MCNP. For this, a new covariance format for the ACE data has been developed and proposed, a prototype capability in MCNP for convolving sensitivities and covariances to provide uncertainty estimates of k_{eff} has been developed, and NJOY modifications to produce the new format are currently under development.

The rapid expansion of the codebase from the merger of MCNP5 and MCNPX and coming new computer hardware introduce challenges for the longevity of MCNP. A rethinking of the core design of MCNP is required, and the MCNP Development Team is currently deciding on a path forward and will make proposals to the MCNP stakeholders in the next year.

ACKNOWLEDGMENTS

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