

MCNPX Delayed-Gamma Feature Enhancements

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INTRODUCTION

The MCNPX[1] delayed-gamma (DG) feature enables automated radiation transport simulations of DG emission created by the products of neutron fission, photofission, and activation for either low- (basic signal detection) or high-fidelity (signature recognition at discrete line energies) studies[2]. However, the sheer quantity of DG emission data causes severe strains on computational performance. We report on important upgrades that significantly improve execution speed, improve the accuracy of the calculated DG emission spectra, and provide the user with some latitude in controlling aspects of the DG simulations.

DG SPEEDUP METHODOLOGY

The MCNPX DG emission procedure begins by determining the nuclear-reaction byproducts (residual nuclides “RNs”) for each fission or activation event. For each unstable RN, the atom densities of their decay progeny are then determined using CINDER’90[3]. Next, the atom densities, radioactive decay constants, and photon-emission probabilities of each unstable RN are used to calculate cumulative distribution functions (CDFs). Finally, the CDFs are sampled for DG emission as a function of energy and time (intra-cell densities are treated as constants, and isotropic DG emission is presumed). This procedure is executed repeatedly until a sufficient number of histories has been executed to give statistically adequate results (“tallies”).

CINDER’90 treats 3400 nuclides. The emission-probability dataset consists of ENDF/B-VI line data for 979 nuclides and 25-group data for the remainder of the 3400 nuclides. CDFs for RN decay chains are created using line data, 25-group data, or a combination thereof depending on the emission-data type for each nuclide in each chain.

The CDFs are time consuming to calculate. It is preferable to calculate the CDFs once and store them for reuse to reduce CPU time. However, even on modern computers memory limitations are encountered. Thus, CDF traits must be examined and coding created that balances the competing issues of speedy execution and storage constraints.

We have implemented new CDF calculation and storage algorithms for the two MCNPX DG execution modes. For 25-group-mode execution (“DG=mg”), the

CDFs are now calculated once and stored for reuse for all 3400 nuclides. For line-mode execution (“DG=lines”), where there can be hundreds of lines per CDF, the CDFs are made and saved for the most frequently sampled fission (FPs) and activation products (APs). For line-mode fission, because many users are interested in ^{235}U and ^{239}Pu , CDFs are stored for the most frequently sampled pre-calculated list of FPs. For line-mode activation, a list of frequently sampled APs is dynamically updated to accommodate the wide range of materials that may interest users.

DG ACCURACY IMPROVEMENT

The CDF calculation involves integral evaluation in energy and time. Until now, MCNPX has utilized the trapezoidal rule to do the time integration. In general, a numerical scheme must be used to treat lengthy decay chains. For the important case of a single RN decaying to a stable product, we have installed analytic evaluation. As such, emission for nuclides such as ^{60}Co now has analytic accuracy.

ADDITIONAL DG USER CONTROLS

New switches have been implemented on the DG “ACT” input-file card to permit improved user control of DG simulations. The CUT card time cutoff can now be used to limit the maximum time for DG emission, thereby reducing the CPU time. The “THRESH” parameter can be used to do a-priori elimination of weak lines from a simulation. Other switches provide additional flexibility.

RESULTS

Test results for the DG AP speedup upgrades are given here for three models: a) ^{60}Ni bombarded by 15-MeV neutrons, b) natural copper impacted by 800-MeV protons, and c) HEU (92.4/7.6 wt% $^{235}\text{U}/^{238}\text{U}$) struck by 800-MeV protons. Model a) results in the production of ^{60}Co , whereas large numbers of APs are created for models b) and c). Simulations were done using 25-group and line execution modes.

We report percentage CPU-time reduction for the upgrades vs the base MCNPX v27c. For 25-group execution, 99, 98, and 97 percent reductions were obtained for the three models. For line-mode execution,

99, 86, and 88 percent reductions were observed. As the number of line data increases, the speedup limit for line-mode execution diminishes due to the handling of line data (sorting and sampling). Thus, the speedup for simulations involving APs is problem dependent, yet appreciable. These speedups are observed using a single-processor desktop PC and parallel MPI execution on clusters.

The model a) ^{60}Co emission is calculated to be 1.99882 photons per decay at 10^{10} s using THRESH=95, which is in analytic agreement with the CINDER'90 emission data.

The upgrades reported here will enable MCNPX users to conduct DG simulations in a much more expeditious manner with improved accuracy and flexibility.

ACKNOWLEDGMENT

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