Annals of Nuclear Energy xxx (2014) xxx–xxx

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

Overview of the MCU Monte Carlo software package

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ARTICLE INFO

Article history:
Received 10 April 2014
Accepted 14 August 2014
Available online xxxx

Keywords:
Transport equations
Monte Carlo method
Evaluated nuclear data
Nuclear reactors

ABSTRACT

MCU (Monte Carlo Universal) is a project on development and practical use of a universal computer code for simulation of particle transport (neutrons, photons, electrons, positrons) in three-dimensional systems by means of the Monte Carlo method. This paper provides the information on the current state of the project. The developed libraries of constants are briefly described, and the potentialities of the MCU-5 package modules and the executable codes compiled from them are characterized. Examples of important problems of reactor physics solved with the code are presented.

1. Introduction

MCU (Monte Carlo Universal) is a project on development and practical use of a universal computer code for simulation of particle transport (neutrons, photons, electrons, positrons) in three-dimensional systems by means of the Monte Carlo method. The project started in 1982 at Kurchatov Institute. The founder of the project was L.V. Mayorov.

This paper reviews the modern MCU-5 (Alekseev et al., 2012) software package that has been developed within the framework of the MCU project. The package is used to compile different versions of the codes of the MCU-5 family. Besides modules required for Monte Carlo calculations MCU-5 includes modules for depletion and thermal analysis.

The MCU-5 software package is continuation of the MCU-4 (Gomin, 2006) one which development was finished in 2006. Since then the software package was largely rewritten and many important capabilities and improvements were included: dynamic memory, parallel calculation, translation from Fortran-77 standard to Fortran-90/95 one, nuclear data updating, new modules were developed (photon and electron–positron transport, uncertainty analysis, feedback), existing modules were rewritten and expanded, and etc. All of those features allow simulating particles transport in the large models like 3D reactor core with detailed power distribution.

Now MCU-6 software package is under development.

The authors of MCU are *L.P. Abagyan*, N.I. Alekseev, A.S. Bikeev, S.N. Bolshagin, A.E. Glushkov, E.A. Gomin, S.S. Gorodkov, M.I. Gurevich, M.A. Kalugin, A.S. Kulakov, S.V. Marin, *L.V. Mayorov*, D.S. Oleynik, S.V. Ostashenko, A.V. Pryanichnikov, E.A. Sukhino-Khomenko, D.A. Shkarovsky and M.S. Yudkevich.

2. Particle transport

2.1. Criticality problem

In solving problems of criticality by means of the Monte Carlo method one usually uses generations with a fixed total weight of neutron sources in one generation. In this scheme phase coordinates of neutrons of the initial (zero) generation can be chosen arbitrarily. To calculate neutron flux tally, such as the effective multiplication factor and reaction rates in tally areas a random variable ξ is used. Its sample values are elementary estimates x_n, calculated for the so-called series, each of which includes a user-defined number of generations N_{BAT} (with $N_{BAT} = 1$ notions of series and generation coincide). This approach is realized reasoning from the idea that the correlation between series consisted of several generations is less than the correlations between generations. It provides more reliable estimates of result's uncertainty.

Each generation consists of N_{TOT} neutrons. N_{TOT} quantity and the spatial and energy distribution of the first generation neutrons are defined by the user in input data.

A history of each neutron is modeled as the sequence of collisions with nuclei from the birth point to the point of absorption or escape from the system. Phase coordinates of collision, absorption, or escape points are defined by subroutines of the geometrical and physical modules. Reaction rates and others neutron flux tally are calculated by the tally module.

For each fission point the number ν_n of the secondary fission neutrons and their energy E_n is defined. These neutrons after normalization are used to make the next generation of N_{TOT} particles.

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http://dx.doi.org/10.1016/j.anucene.2014.08.032
0306-4549/

Please cite this article in press as: Kalugin, M.A., et al. Overview of the MCU Monte Carlo software package. Ann. Nucl. Energy (2014), http://dx.doi.org/10.1016/j.anucene.2014.08.032

Secondary photons, electrons and positron are also taken into account, if it is required. Simulation of those particles is carried out at the end of each generation.

2.2. Fixed source problem

Formally, there are still such notions as series and generations, but this is only for the unification of the code's work. User may set one generation consisting of a single particle per one series.

In the beginning the source module provides N_{TOT} particles for each generation. It can be a generation of any type of particles that is supported by MCU-5 or even a mixed one. These particles create a queue in the bank, the so-called main line.

Further, a trajectory is modeled for every such particle. Secondary particles appearing as a result of the modeling are placed at the end of the same queue. After the main line is finished the code starts working with the secondary particles. This may cause additional particles to be placed into at end of the main queue.

It is possible to turn off modeling of the secondary particles and only do the transport of the main line.

2.3. Variance reduction techniques

Nonanalog Monte Carlo or variance reduction techniques allow to focus the particles in regions of interest (e.g. with a small volume) that substantially decreases the number of histories that is necessary to achieve required statistics.

Traditional variance reduction techniques such as a weight window, energy cutoff, energy and geometry splitting with Russian roulette, ring and point detectors are implemented in the transport module of MCU-5.

3. Particle physics treatment

3.1. Neutron physics treatment

When simulating collisions of neutrons with nuclei in different energy regions, it is possible to combine data libraries listed in Table 1 by applying the corresponding submodules of the physical module. In other words it is possible to build physical model from pure multigroup to pure point-wise approximation. Intermediate models are also allowed.

In the fast energy region it is possible to use either the constants of the point-wise ACE/MCU library or the 26-group BNAB/MCU library.

In the unresolved resonance region the cross-sections are calculated using subgroup parameters, Bondarenko's f-factors or probability tables.

In the region of the fully resolved resonances both subgroup and point-wise representation of the cross-sections may be used. If point-wise representation is used, the cross-sections of the most important nuclides are described by "infinite" number of points, because they are calculated using resonance parameters in each energy point during simulation. Such scheme allows calculation using the data on resonance parameters without preliminary preparation of tables of cross-sections and to evaluate temperature effects through analytical dependences of cross-sections on temperature.

Modeling of collisions in the thermal area is carried out either in multigroup transport approximation, or using the model of continuous change of energy considering correlations between changes of energy and scattering angles. In both cases chemical bounds, thermal movement of nucleus and coherent effects for elastic scattering are taken into account.

It is possible to take into account both prompt and delayed neutrons in the fission spectrum.

Generation of photons in the result of neutron reactions is simulated using multigroup approximation.

3.2. Photon physics treatment

The interaction of photons with matter can be simulated using both multigroup and point-wise representations of the cross-sections. The following processes are simulated: coherent and incoherent scattering, photoelectric effect and production of electron–positron pairs with the possibility of generation of secondary photons, electrons and positrons.

The cross-sections and the spectra for photoneutron generation are obtained from the analytical dependences for two isotopes characterized by low reaction thresholds and important for reactor applications, namely, deuterium and beryllium.

Table 1
Composition of the MCUDB50 data bank.

Library	Description
ACE/MCU	Library of cross-sections of neutron interaction with nuclei in the epithermal energy region in a point-wise representation obtained from ENDF/B-VII.0 files and other source
BNAB/MCU	Expanded and modified version of the BNAB-93 26-group system of constants
LIPAR	Parameters of nuclide cross-sections in the region of resolved resonances
MULTIC	301-Group library containing the data on the temperature dependence of subgroup parameters of nuclides in the region of unresolved resonances
KORT	Library of neutron physical constants in a point-wise representation for the energy range from 10^{-5} to 5 eV
TEPCON	Library of 40-group cross-sections for the thermalization region (up to 1 eV)
VESTA	Library for simulating neutron collisions with the nuclei of moderators taking continuous variations in the neutron energy in the thermalization region into account; it is represented in the form of probabilistic tables obtained from the $S(\alpha, \beta)$ scattering laws
BOFS	Library of generalized phonon spectra of moderators
DOSIM	Library of activation cross-sections in a point-wise representation
ABBNL	Library of 63-group cross-sections used for obtaining "summarized isotope" cross-sections
PHOTONS	Library of multigroup cross-sections of photon generation in neutron interaction with matter based on the data of DLC-41/VITAMIN-C and DLC-184/VITAMIN-B6 libraries
PHOTONT	Multigroup cross section of the photon interaction with matter based on the data of DLC-41/VITAMIN-C and DLC-184/VITAMIN-B6 libraries
BURN5	Data for depletion calculation: half-lives of nuclei, yields of fission fragments, chains of transformations, etc.
SHELLDATA	Library of atomic transitions (LLNL EADL)
PHOTDATA	Library of point-wise cross-sections of photon interaction with matter in the energy range from 100 eV to 100 MeV (LLNL EPDL)
ELECDATA	Library of point-wise cross-sections of electron interaction with matter in a point-wise representation for the energy range from 100 eV to 100 MeV (LLNL EEDL)
POSIDATA	Library of point-wise cross-sections of positron interaction with matter in a point-wise representation for the energy range from 100 eV to 100 MeV (LLNL EEDL)
NEUTRONK	Library of neutron heating cross sections in a point-wise representation for the energy range from 10^{-5} eV to 20 MeV
PHOTONK	Library of photon heating cross sections in a point-wise representation for the energy range from 10^{-5} eV to 20 MeV

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