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DEVELOPMENT OF MONTE CARLO CODE FOR THE ASSESMENT OF CRITICALITY OF FISSILE SYSTEMS

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Abstract

An Indigenous Monte Carlo code, MCkeff, for solving the steady-state neutron transport equation is currently under development at the Manipal Centre for Natural Sciences to estimate the neutron multiplication factor (k_{eff}) of systems containing fissile materials such as U-235 and Pu-239. Any arbitrary configuration of materials contained in cells can be described by its bounding signed analytical linear or quadratic surfaces (half-spaces) combined with Boolean operators of intersection and union. In the present code, the events simulated are elastic scattering, fission, inelastic scattering, (n, xn) and several other absorption reactions (n, c) given in any particular ENDF evaluation. For reactions which results with one or more secondary neutrons, energy and angles are sampled as per the laws prescribed in the ENDF 6 file. Special treatment is employed in the code for thermal neutrons (<4eV) using S (α, β) cross-sections (for light nuclides) and for intermediate energy neutrons (few keV to tens of keV) in heavy elements to account for self-shielding effects on cross-sections using probability tables of cross-sections. At the end of the simulation, the neutron multiplication factor (k_{eff}) of a system is estimated.

1. Introduction

Safety in the Nuclear industry is of utmost importance as it involves handling large quantities of fissile isotopes of uranium and plutonium. Some places where a large amount of fissile material is involved are fuel storage, fuel reprocessing, fuel fabrication, etc. The crucial parameter in handling fissile materials is the neutron multiplication factor (k_{eff}) of the system. A precise estimate of this parameter is essential to avoid criticality accidents [1]. Monte Carlo Codes are preferred due to flexibility in handling complicated geometrical arrangements of materials, ease of incorporating detailed physical processes, and simplicity in estimating errors associated with the results. The theory behind this method is described in detail in the references [2-4]. Several Monte Carlo codes [5-8] exists to estimate the k_{eff} of a system. An overview of general-purpose Monte Carlo radiation transport codes existing in the ORNL/RSICC library is published by Kirk [9]. It is known that the Monte Carlo methods consume a lot of computer resources and computation (CPU) time to get the result of a problem with a desirable precision. This prohibits the usage of few of the previously available codes for computation as they are obsolete due to sea changes in the hardware and software of the computer industry besides the development of new algorithms. A new Monte Carlo code MCkeff has been written from scratch, keeping in mind the advances made over time.

2. Method of solution

For criticality problems, a steady-state neutron transport equation, which is in the Eigen value-form, is solved [10-11]. The eigenvalue equation(ref [12] eq. 1) is:

$$[\Omega \cdot \nabla + \Sigma_t(\vec{r}, E)]\, \Psi(\vec{r}, E, \Omega) = \iint \Psi(\vec{r}, E', \Omega')\, \Sigma_s(\vec{r}, E' \rightarrow E, \Omega \cdot \Omega')\, \mathrm{d}\Omega'\, \mathrm{d}E'$$

$$+ \frac{1}{k_{eff}} \frac{\chi(E)}{4\pi} \iint \nu \ \Sigma_f(\vec{r}, E') \ \Psi(\vec{r}, E', \Omega') \ dE' \ d\Omega'$$

Where,

$\Psi(\vec{r}, E, \Omega)$	- neutron angular flux
$\Sigma_t(\vec{r}, E)$	- total cross section
$\Sigma_f(\vec{r}, E')$	- fission cross-section
ν	- the average number of neutrons emitted per fission
(r, E′ → E, Ω′ → Ω)	- the probability of transfer from (E′, Ω′) to (E, Ω)
k_{eff}	- is the neutron multiplication of the system.

The left-hand terms represent the neutron leakage and absorption and the first term on the right-hand side is the scattering term, and the second term describes the neutron production term due to fission. The constant k_{eff} is an eigenvalue included in the above equation to match both sides of the equation. The Monte Carlo method proceeds for the solution by the methods of successive generations or power iteration method [13] to estimate the largest eigenvalue of the system. This calculation scheme is employed in MCkeff. The definition of k_{eff} is given as

$$k_{eff} = \frac{\text{fission neutrons produced in the current generation}}{\text{fission neutrons started in the previous generation}}.$$

In Monte Carlo simulations, generation means tracking neutron events from the birth of a neutron (site of fission) to its death (parasitic absorption or escape from the system) over a batch of neutrons. Any individual history (sequence of recorded events) from the batch may not have any physical meaning. However, an average of histories over a large number contains the physical characteristics of the medium. The required parameter can be deduced from the histories. At the end of tracking neutrons, the predetermined number of neutrons, k_{eff} is estimated, and fission sites are stored for subsequent iterations. The iterations are stopped when the value of k_{eff} of a system converges. At the end of the simulation, the code estimates from the recorded histories the neutron multiplication factor (k_{eff}) of a system

The salient features of the MCkeff code are:

- Written from scratch incorporating FORTRAN 2008 features for Windows and Linux Operating systems.
- The input file is a filed free text file. The structure and format followed are the same as that of other Monte Carlo codes.
- Input checking is done extensively to detect all possible errors, and messages of fatal errors and warnings are displayed on the screen.
- It allows building a complex configuration of materials in geometric regions (cells) bounded by linear and/or quadratic surfaces combined with Boolean operators of intersection and union. Besides, it allows urinary complement operator of a cell.
- It has provision for specifying universes and lattices, enabling built of complex repeated structures with ease
- Interactive debug features of 2D geometry plotting. Attempts are being made to run on Parallel computers.

3. Results

The newly developed code testing and validation of the results are carried out by the Validation of full core problem and other criticality benchmark problems.

Validation of full core problem and other criticality benchmark problems

Hoogenboom et al. [16] had proposed a criticality Benchmark problem of a typical reactor core to test the efficacy of newly developed Monte Carlo codes. Fig. 1 shows the layout of the (A) ¼th of the core, (B) fuel assembly within a core, including guide tubes and (C) the fuel pin. MCkeff and OpenMC were run with 100,000 particles per cycle, 150 inactive batches, and 4000 active batches. These two codes do not use any biasing techniques or convergence acceleration techniques, using the same ENDF/B-VII.1 libraries. Table 1 shows the k_{eff} results with their standard deviations.

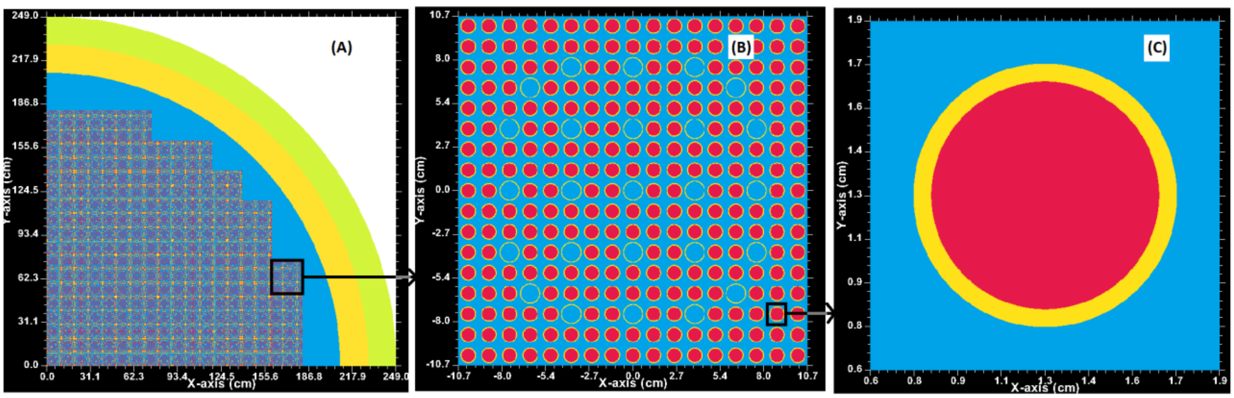

Fig. 1. shows the layout of (A) the ¼ th core, (B) fuel assembly within a core including guide tubes and (C) the fuel pin.

Table 1. Comparison of k_{eff} values for performance Benchmark problem with 2 different codes

Performance benchmark	$k_{eff} \pm 1\sigma$
MCkeff	1.00088 ± 0.00004
OpenMC	1.00105 ± 0.00004

From the above table, it is clear that the k_{eff} value of MCkeff is in good agreement with OpenMC with a minimal difference of less than 100 pcm in reactivity.

Conclusions

A new Monte Carlo neutron transport code, called MCkeff, has been developed to estimate the neutron multiplication factor of fissile systems. The code is developed in Fortran language using GNU compiler and is compatible with both Windows and Linux based operating systems. A point-wise, continuous energy ACE format cross-section was used to treat neutron-nuclei collision physics accurately (without approximations). For constructing geometrical shapes containing homogenous material regions, first and second degree signed surfaces along with intersection and union operators are permitted. Since MCkeff is developed from scratch, it will be rather easy to incorporate advances happening in the computer industry as well as in the physics models.

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