RTS&T MONTE CARLO CODE (FACILITIES AND COMPUTATION METHODS)

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Abstract

The paper describes facilities and computation methods of the RTS&T new Monte Carlo code. This code performs simulations of three dimensional electromagnetic showers development and low energy neutron production and transport in accelerator and in shielding components with a calculation of the isotopes transmutation problem. RTS&T is based on the compilations from ENDF/B-VI, JENDL-3, EAF, FENDL and EPNDL evaluated data libraries to detailed physical processes simulation, and only a few approximations are made. It is possible to use RTS&T complex to solve the critical reactor problem. Combinatorial method of the geometry definition is provided with the program. Recently RTS&T code interface to the ANSYS 4.4 code system has been developed and tested.

1 RTS&T MAIN FEATURES

The code RTS&T (Radiation Transport Simulation and Isotopes Transmutation calculation) was assigned for Monte Carlo simulation of many particle types transport in complex 3D geometries with composite materials and calculation particles fluences and functionals of radiation fields and isotopes transmutation problem as well.

The specific features of RTS&T Code are: basic processes of particles interactions during their passage through the matter are taken into account for the energy range about

1. 10 eV to 10 TeV for photons
2. 0.01 MeV to 10 TeV for leptons
3. 1 MeV to 25 GeV for charged hadrons
4. Thermal region to 25 GeV for neutral hadrons

In RTS&T Code 3D geometry definition is provided with combinatorial (recursivial) method. Complex 3D geometries can be defined to a combination of boxes, cylinders, spheres and etc. More then 15 standard or user–written base shapes and 10 types of the initial radiation source distributions may be defined in this code version.

The secondary particles transport parameters are retained in stack which can be organized according to lexicographical or direct method.

RTS&T Code can be successfully used for verification of non-grouping constant systems was recorded in ENDF-VI format.

2 ELEMENTARY PROCESSES SIMULATION

2.1 Photonic processes

In the current version of RTS&T Code the following photonic processes types are simulated: Photoelectric effect (from K, L_I, L_{II}, L_{III} atomic shells), Rayleigh scattering,Compton scattering, pair production by photons, hadronic interactions of photons (photonuclear effect).

The EPDL evaluated data library[2] of photon-interaction total cross sections, coherent and incoherent scattering form-factors are used in photon transport simulation for the energy range about 10 eV to 100 GeV.

2.2 Charged particles ionization processes

To simulate the ionization processes induced by the charged particles two different models are provided:

1. Continuous energy loss model with δ-ray generation.
2. Continuous energy loss model without δ-ray production and full Landau - Vavilov fluctuations. The density effect correction to the stopping power of matter has been taken account.

Multiple scattering of charged particles was simulated according to Moliere theory. Direct pair production by charged hadrons is included in the calculations as well.

2.3 $e^{\pm}$ discrete bremsstrahlung process

The discrete bremsstrahlung photon energy is sampled from a Seltzer and Berger[4] differential cross section for electron kinetic energy below 10 GeV and Bethe-Heitler cross section above this value. The angular distribution of the emitted photon is sampled according to facilitated form of the double differential cross section[5–6].

2.4 Hadronic processes

2.4.1 High energy hadronic interactions

To simulate the interactions of hadrons and charged pions with the nuclei in kinetic energy range about 20 MeV to 25 GeV intranuclear cascade-evaporation model (Dubna version) was provided. To calculate the distance to the interaction point and simulation of hadronic process type the Barashenkov total cross sections compilation[7] was used. π^0-mesons decay into two photons is simulated according to decay kinematical scheme.

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2.4.2 Low-energy neutrons transport

In practice of low-energy neutrons transport calculation the files of evaluated nuclear data present the original constant information, however, they are used not directly but after treatment to multi-group constant systems. In this approach comparison of calculation results with benchmark-experiments allows to test only information obtained after treatment. Then the system mistake supplemented by treatment itself cannot be estimated in principle, since it is indivisible from the system errors of the evaluated data file itself[8].

RTS&T code is based on the *direct* use of ENDF/B-VI[1] evaluated data library to detailed low-energy neutron interactions simulation. The partial neutron-interactions processes simulation is performed according to ENDF/B laws. During constants preparation process linearization and restoration of resolved resonances of neutron cross sections with LINEAR and RECENT ENDF-utilities is made. Data reading and constants preparation procedure was written in the ANSI "C" language.

3 ISOTOPES TRANSMUTATION CALCULATION METHOD

The isotopes transmutation process is described by a system of balance ordinary differential equations. For the isotopes concentration N_i, where $i = 1, M$ (M is the total number of nuclides which to participate in connected transitions) the given system of equations is the following:

$$\frac{dN_i(t)}{dt} = -N_i \cdot \left(\lambda_i + \sum_k \int_0^{E_0^k} \sigma_i^k(E) \cdot \phi^k(E,t) dE \right) + \quad (1)$$

$$+ \sum_{j \neq i} N_j \cdot \left(\lambda_{ji} + \sum_k \int_0^{E_0^k} \sigma_{ji}^k(E) \cdot \phi^k(E,t) dE \right)$$

$$N_i(0) = N_i^0,$$

Where $\sigma_i^k(E)$ - summary cross section of reactions presenting the change of i-th nucleus structure, $\sigma_{ji}^k(E)$ is the partial cross sections of i-th isotopes formation reactions from j-th mother nucleuses under action of particles of grade k with the energy E, λ_i - disintegration constant of the i-th isotopes, λ_{ji} - disintegration constant of the j-th isotopes on the channels were presented to i-th nuclide formation; $\phi^k(E,t)$ is the particles of grade k with the energy E total flux, maximum significance of which is E_0^k. Breaking a period of exposition of a material on a number of temporary sessions with $\phi^k(E,t \cong \phi^k(E)$, we receive from (1) the independent system of equations with constant factors, the analytical decision of which is recorded in a matrix kind:

$$N(t) = N_0 \exp(Ct), C_{ij} = \begin{cases} -(\lambda_i + \sum_k \int_0^{E_0^k} \sigma_i^k(E) \cdot \phi^k(E) dE) \\ \text{if } i = j \\ \lambda_{ij} + \sum_k \int_0^{E_0^k} \sigma_{ij}^k(E) \cdot \phi^k(E) dE \\ otherwise \end{cases} \quad (2)$$

where $\exp(Ct)$ is matrix exhibitor:

$$\exp(Ct) = \sum_{s=0}^{\infty} \frac{C^s t^s}{s!}, C^0 = E. \quad (3)$$

We shall note a number of the equation system (1) features:

- Practically at any modes of exposition or endurance of any material the isotopes transmutation process contains both fast and slow making, and the distinction between them can reach 20 and more orders. Such spread of significances of elements of a matrix results to its bad conditionality [$cond(C) \gg 1$] and allows to assume, that a system of equations (1) is "stiff". Correctly the definition of "stiffness" of the equations system requires the calculation of own significances λ of matrix C, that reasonably is a difficult problem for large-size matrixes. Usually for these purposes a ODE system use the following criterion — the system is "stiff" if inequalities are executed:

  $$\|C\|_1^{-1} \ll H, \quad |Sp(C)|^{-1} \ll H \quad (4)$$

  Where H is the duration of exposition session or endurance, $\|C\|_1$ and $Sp(C)$ is the norm and trace of matrix C respectively:

  $$\|C\|_1 = \max_{1 \leq i \leq n} \sum_{j=1}^{n} |c_{ij}|, \quad Sp(C) = \sum_{i=1}^{n} c_{ii} = \sum_{i=1}^{n} \lambda_i.$$

  Numerical integration of "stiff" systems any obvious discrete methods (Runge-Kutta, Adams and etc.) results in effect "error explosion" at the chosen step $h \geq \max(\|C\|_1^{-1}, |Sp(C)|^{-1})$.

  Given restriction from above on a integration step can result in unreal times of account when connected transitions (chains combined with nuclear reactions of radiation disintegration) contain nuclides with strongly distinguished life-times. Hence, application of standard methods of numerical integration non-stiff systems in an isotopes transmutation problem unacceptably.

- The majority of specialized methods of numerical integration of "stiff" systems of equations are based on implicit discrete methods (Rosenbrok, Kollahan and etc.), which in case of a system with constant factors

require calculations of a return matrix $(E + hC)^{-1}$, where h is the integration step, E – unit matrix. As the overwhelming majority of matrix C elements is considerably less than 1, reference (manipulation) of a given matrix is made with a large error, which grows with an increase of its size and with a reduction of the integration step. Use of arithmetics with a floating point of double accuracy to isotopes transmutation problem solution does not remove this problem (for example, at radioactive disintegration of U^{235} nuclei, $C_{ii} = 3 \cdot 10^{-17}$ and, in case of small h, even the operation of summation the diagonal elements of matrices E and hC already passes on limit of allowable accuracy by use of the 64 bits computers).

The marked specific of an isotopes transmutation problem limits the applicability discrete methods of numerical integration of ODE systems, that makes the their universal settlement circuit unsuitable for construction.

Direct use of the analytical decision (2) at large times and bad conditionality of the matrix C results in unjustified quantity terms at calculation exhibitor and high error. For the decision of a system of equations (1) in RTS&T code the circuit of calculation $\exp(Ct)$ was applied recurrent, which gives satisfactory results even in case of brightly expressed "stiffness" of a equations system (1) in a wide range of intervals of time h.

To construct recurrent of the calculation circuit $\exp(CH)$, where H is the duration of the exposition session, the interval H is broken into a number of any uniform sections h. Then isotopes concentration in each discrete moment of time $t_n = nh$, $n = 0,\ 1,\ ...$ are defined by the formula:

$$N_{n+1} = N_n\ \exp(Ch),\ n = 0,\ 1,\ ... \qquad (5)$$

To the exponential ($\exp(Ch)$) calculating the additional recurrent matrix equation construction is required. Such step h' is chosen, which satisfied to following conditions:

$$h' = \frac{h}{2^K}, \qquad h" \ll \min(\|C\|^{-1}, |Sp(C)|^{-1})$$

where K is any integer value. Having calculated on (3) $\exp(Ch')$, we can find $\exp(Ch)$, applying consistently formulas:

$$\exp(2Ch') = \exp(Ch')\exp(Ch'),$$

$$\ldots.$$

$$\exp(2^K Ch') = \exp(2^{K-1}Ch')\exp(2^{K-1}Ch').$$

We shall record these equations as the recurrent matrix equation:

$$\phi_{k+1} = \phi_k^2, \text{ where } \phi_k = \exp(2^k Ch'), \quad k = 0, 1, ..., K-1; \qquad (6)$$

Thus, it is possible to choose so small size h', that high accuracy of representation $\exp(Ch')$ by decomposition (3) with small number of the members (s) is provided no matter how. On the other hand, the use recurrent of equations (5) and (6) for the decision of a system (1) considerably reduces number of steps of integration for the given interval H:

$$H/h = 2^{-K} \cdot H/h',$$

That removes a "large times" problem in any isotopes mixes. Valuation of a relative error of the numerical circuit of the decision of a equations system (1) to be made according to the Runge rule: i.e. results received for the steps $h'(K)$ and $h'/2(K+1)$ are compared.

4 ACKNOWLEDGEMENTS

The contribution to the RTS&T code (geometry description procedures) have been made by O. Lyashenko to whom the autors expresses his cordinal gratitude.

The autors is grateful to Yu. Fedotov for his interest to the work and R. Mukhamadeev (SRC IPPE) for the stimulating discussions.

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