SIMULATION OF RELATIVISTIC HADRONIC INTERACTIONS IN THE FRAMEWORK OF THE RTS&T-2004 CODE

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Abstract

The paper describes the current status of general-purpose RTS&T (Radiation Transport Simulation and Isotopes Transmutation) multi-particles Monte Carlo radiation transport code [1]. New developments in modelling of discrete hadronic interactions (implementation of improved version for hA-interaction models and modern evaluated nuclear data libraries) are described. A comparison of the recent experimental data on double differential and total yields of diffractive, s, g and b-particles resulting from the high-energy hN- , hA- and AA-interactions is made with different semi-empirical and theoretical models of direct hadron production: data-driven model, parametrization-driven model, intranuclear cascade model, quark-gluon string model, parton cascade model and quantum molecular dynamic model combined with generalized exciton-evaporation (Fermi break-up)-fission model to describe of slow particles and residual nuclei emission. The geometry presentation system and enhanced RTS&T-CAD-interface are described also.

PARTICLE PRODUCTION MODELS

Inelastic hadronic and photonic interactions are simulated within RTS&T code by several energy-dependent models based on the different microscopic and macroscopic approaches (Fig. 1).

ENDF-data-driven Model of Low-energy h(γ)-interactions and Transport

The RTS&T uses continuous-energy nuclear and atomic evaluated data files to simulate of radiation transport and discrete interactions of the particles in the energy range from thermal energy up to 150 MeV. In contrast with the MCNP and GEANT4 the ENDF-data driven model of the RTS&T code has access evaluated data directly. A first model version was originally develoved in 1997 to simulate of low-energy (up to 20 MeV) neutron transport using the neutronic part of the ENDF/B-VI evaluated data library. In current model development all data types provided by ENDF-6 format are takes account due to coupled multy-particle radiation transport modelling. Universal data reading and preparation procedure allows to use various data library written in the ENDF-6 format (JENDL, FENDL, CENDL, JEF, BROND, LA150, ENDF-HE/VI, IAEA Photonuclear Data Library etc.). The ENDF data pre-processing (linearization, restoration of the resolved resonances, temperature dependent Doppler broadening of the cross sections and checking and correcting of angular distributions and Legendre coefficients for negative values are produced automatically with the Cullen's ENDF pre-processing codes LINEAR, RECENT (RECEN-DD for Reich-Moore parameters of several isotopes of JENDL library only), SIGMA1 and LEGEND rewritten in ANSI standard FORTRAN-90. ENDF-recommended interpolation laws are used to minimize the amount of data. For data storage in memory and their further use the dynamically allocated tree of objects is organized. All types of reactions provided by ENDF-6 format are taken into account due to particle transport modelling: elastic scattering, radiative capture and production of one neutron in the exit channel, absorption with production of other type particles (with division on excited states of the residual nucleus), the fission with separate yields of prompt and delayed neutrons and residual nucleus simulation by MF=8 data, etc. The energies and angles of emitted particles are simulated according to the distributions from MF=4, 5, 6, 12, 13, 14 and 15 files. For example, the following representations of outgoing energy-angle distributions for secondary particle can be used: tabular energy distributions, angular distributions via equally-probable cosine bins, Kalbach-Mann systematics for continuum energy-angle distributions (44 ENDF law), discrete two-body scattering, N-body phase-space energy distributions.

Theory-driven (microscopic) Models

In the RTS&T-2004 microscopic model the $h(\gamma)$-induced nuclear reaction is assumed to be three-step process: direct-stage, pre-equilibrium emissions and decay of the equilibrated system (evaporation / binary fission processes competition).

The intra-nuclear cascade model is one of the most popular to simulate of the secondary particle parameters for the $h(\gamma)A$-inelastic scattering in the intermediate energy region. It allows one to reproduce the experimental observations up to energies about 0.1 to several-tens GeV. The isobar production channels covered by the INC model are presented in Table 1. The strange channels like $\gamma p \rightarrow \Sigma K^+, \Lambda K^+, \Lambda K^0 \pi^+$ and non-strange pseudoscalar and vector meson photoproduction channels $\gamma N \rightarrow [\rho/\omega/\eta]N$ are included also. For multi-particle final states we adopt

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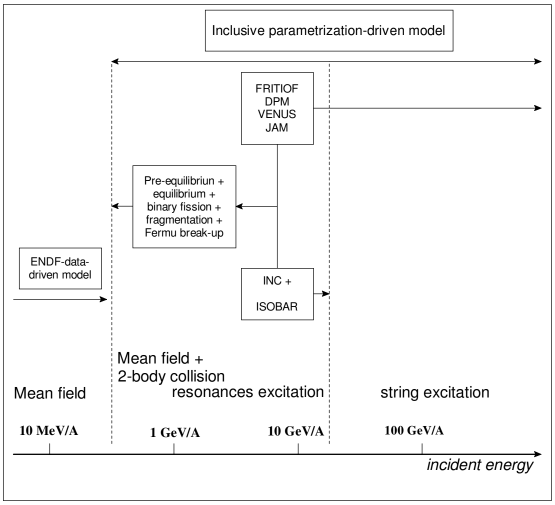

Figure 1: Particle production models implemented in the RTS&T-2004 code.

Table 1: Baryon Resonance Production Channels

Entrance channel	Exit channel
pp	$p\Delta^+$, $n\Delta^{++}$, $\Delta^+\Delta^+$, $\Delta^0\Delta^{++}$
pn	$n\Delta^+$, $p\Delta^0$, $\Delta^0\Delta^+$, $\Delta^-\Delta^{++}$
γp	$\Delta^{++}\pi^-$, $\Delta^{++}\pi^0$, $\Delta^0\pi^+$
γn	$\Delta^+\pi^-$, $\Delta^0\pi^0$, $\Delta^-\pi^+$

the CERN library GENBOD (W515) routine. The DPMJET II, FRITIOF 7.02, VENUS 5.21 and JAM models were implemented into the 2004 version of the RTS&T code for particle and heavy ion projectiles at 10 GeV/A.

The *pre-equilibrium* stage of the reaction is simulation in the frame of exciton model. The initial exciton configuration for pre-equilibrium decay formed in cascade stage of the reaction or postulated in general input ($2p1h$ configuration for incoming particle or $1p0h$ for incoming photon).

The *equilibrium* stage of reaction (evaporation/fission processes) is performed according to the Weisskopf-Ewing statistical theory of particle emission and Bohr and Wheeler theory of fission. Double-humped fission barrier parameters for $Z > 90$ taken from the data set obtained in Obninsk and recommended by IAEA Reference Input Parameter Library (RIPL). Experimental single-humped fission barrier heights are incorporated in the RTS&T model as proposed in RIPL, or can be calculated according to any phenomenological or theoretical models: Barashenkov et al. phenomenological approach; Barashenkov and Gereghi semi-phenomenological approach; liquid drop model (LDM) with Myers and Swiatecki parameters; LDM with Pauli and Ledergerber parameters; Krappe and Nix single-Yukawa modified LDM; Krappe, Nix and Sierk Yukawa-plus-exponential modified LDM; Yukawa-plus-exponential modified LDM.

The ratio of neutron emission to fission widths is taken in form proposed by Kupriyanov et al.: $\Gamma_n/\Gamma_f = \frac{\tilde{\Gamma}_n}{\tilde{\Gamma}_f} \exp\{-\frac{\delta W_g^{N-1}}{\tilde{T}_n} \exp(-\lambda U_n) + \frac{\delta W_f}{\tilde{T}_f} \exp(-\lambda U_f)\}$, where $\frac{\tilde{\Gamma}_n}{\tilde{\Gamma}_f}$ is Vandenbosch and Huizenga form of Fermi-gas model (asymptotic value occurring at high energies),δW is the shell correction term, $\lambda = 0.05$ MeV. The post-fission parameters of the fragments are taken from the systematics by Adeev (A_f, Z_f) and Zhao et al. (TKE). The inverse reaction cross section is calculated in form $\sigma_{inv}(T) = \sigma_{geom} T_b(T)$ with $\sigma_{geom} = \pi[R + R_b + \lambda/2\pi]^2$ where σ_{geom}, R, R_b, λ and T_b are the geometric cross section, radii of the potential residual nucleus and particle, the non-relativistic reduced channel wavelength and the non-relativistic s-wave Coulomb barrier transmission probability, respectively. The s-wave transmission factor is given by expression $T_b(\rho, \eta) = [F_0^2(\rho, \eta) + G_0^2(\rho, \eta)]^{-2}$, where F_0 and G_0 are the non-relativistic zero-order regular and irregular Coulomb wave-functions of variables $\rho = \hbar^{-1}(R_a + R_b)(2\mu T_{cms})^{1/2}$, $\eta = \hbar^{-1} Z_a Z_b (m/2T_{cms})^{1/2}$, where Z_a, Z_b, R_a and R_b are the charge and radii of two particles, respectively, μ is the reduced mass of the two particle system, T_{cms} is the kinetic energy in cms. In the current version of RTS&T code the Fermi breakup model for disintegrating of light nuclei has replaced the evaporation model for nuclei with a mass number between 2 to 16. The evaporation of fragments with a mass number $A > 4$ does not included in current version RTS&T. The RIPL recommended Audi and Wapstra experimental compilation of atomic masses and binding energies is used in the RTS&T model. The level density parameter derived from the RIPL-systematics for any level density models: Gilbert-Cameron, back-shifted Fermi-gas model, Ignatyuk form of Fermi-gas model, generalized superfluid model (GSM), microscopic GSM, shell depended model proposed by Kataria and Ramamurthy, Mughabghab and Dunford systematic determined from the neutron resonance data. To estimate of the averaged squared matrix element two different models can be used: estimation in approximation of quasi-free scattering of a nucleon above the Fermi level on a nucleon of the target nucleus or by using a set of semi-empirical parametrizations. The RTS&T-2004 has three different models to simulate the gamma-ray emission in pre-equilibrium and equilibrium stages: the Weisskopf single-particle model, the Brink-Axel GDR model, and the Kopecky-Uhl generalized Lorentzian model. To calculate the partial level densities for pre-equilibrium emission simulation the Avrigeanu systematic is used. Composite formulas include the advanced pairing and shell correction in addition to the Pauli blocking effect, and average energy-depended single-particle level densities for the excited particles and holes.

Parametrization-driven Model

The existing rigorous theoretical approaches and models allow estimate of various characteristics of secondary particle emission due to nuclear inelastic interactions, but they have uncertainly in choice of free parameters and the calculations are time-consuming. The RTS&T parametrization-driven model (PDM) is based on the set of semi-phenomenological systematics of particle production parameters.

RTS&T GEOMETRY PRESENTATION SYSTEM

The RTS&T-2004 code includes an effective geometry definition system provided with a combinatorial method. Universal geometry module GEOMETRY [3] basically was intended for the performing of two functions: detailed description of the spatial geometry and material composition of considered system and localization of the site of transported particle in this system. In the framework of the combinatorial approach the geometry of any physical object can be extremely precisely approximated by set of geometrical regions limited by closed surfaces, filled by homogeneous material and having the constant reflection coefficient. The representation of geometry of a system as combination of geometrical regions is generally ambiguous and it is a problem of combinatorial topology solved in this case by a method of covering of investigated object's space by a system of subsets of Euclidean space.

Shapes Definition

The surface form of each region must correspond to one of the primitives from an available set. More than 30 primitive shapes are defined in the current code version. The recursivial coordinate surface method is used in effective algorithms for analysis whether the considered point is into the region limited by the given surface form. This method allows to define the shape surface by set of equations of the type $u = f(\vec{r})$, where u is one of coordinate variables and $\vec{r} = (x, y, z)$ is a considered point (generally in arbitrary coordinate system).

Hierarchical Embedding Tree

The complex 3D geometry can be constructed with Boolean algebra operations (union, intersection, substraction) on the primitive shapes with arbitrary position and rotations. Let the considered system be defined by set of geometrical regions S_n, $n = 1, 2, \ldots, N$. The region S_{n_1} will be embedded in S_{n_2}: $S_{n_1} \subset S_{n_2}$, if S_{n_1} is wholly in S_{n_2} and these regions don't coincide: $S_{n_1} \in S_{n_2} = \vec{r}/\forall\vec{r} : (\vec{r} \in S_{n_1} \Rightarrow \vec{r} \in S_{n_2}) \wedge (\exists\vec{r} : (\vec{r} \in S_{n_2}) \wedge \vec{r} \notin S_{n_1})$, where $\vec{r} = (x, y, z)$ is a point in a cartesian coordinate system. We shall name the embedded region S_{n_1} the daughter region in relation to the mother region S_{n_2}. In addition it is supposed, that the transitivity property is not saved and each region has only one mother: $S_{n_1} \subset S_{n_2} \subset S_{n_3} \Rightarrow S_{n_1} \not\subset S_{n_3}$. All geometrical regions are numbered in any order by numbers from 1 to N, where N is the total number of regions, and the mother region number of each region is specified in an explicit form. If it is necessary, some regions with a homogeneous material can be united and get a common number. The optimization algorithms for hierarchical embedding tree analysis use the information about a previous particle history.

Region Positioning

The beginning of a local coordinate system serves an origin point. The positioning of the region in the space is defined by position and rotation of local coordinate system in relation a coordinate system of the mother region. Position and rotation of a coordinate system of the most external region are arbitrary in relation to some global coordinate system. The special service routines form geometry input files for often-used configurations (e.g. periodical structures, core cells, mathematical phantoms, etc.) automatically.

Boundary Localization

The GEOMETRY module includes two alternative boundary localization packages based on the different approaches. In the first case the coordinates of the boundary intersection point can be found by iterative way. The second approach requires the alternative definition of each primitive shape by the combination of surfaces bound it (quadric method). The boundary intersection point is calculated analytically as the result of the simultaneous solution of the system of equations describing the surfaces bound the region and the particle trajectory. On the base of the unified input data format the combined algorithm which is taking into account a features of reviewed localization methods has been developed and tested.

RTS&T-CAD-INTERFACE

The role of graphical supporting tools for geometry verification and output analysis is indisputable. There are two basical approaches to the solution of the problem of visual presentation of investigated object's geometry:

- creating the own graphic application interpreting the geometry input language;
- using of a program interface to widely used graphical complexes, predominantly to CAD/CAM/CAE-systems.

The RTS&T geometry input data transform into the format ASCII DXF (Drawing Interchange Format), designed by the Autodesk company as a standard for exchange by graphic information between AutoCAD and other applications.

REFERENCES

[1] A.I. Blokhin, I.I. Degtyarev et al., Proc. of the SARE-3 Workshop, KEK, 1997.