MCAPM: All Particle Method Generator and Collision Package

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MCAPM: All Particle Method Generator and Collision Package

J.A. Rathkopf (LLNL)

MCAPM (Monte Carlo All Particle Method) is a collection of subroutines that read the data necessary for and perform the physics involved in collisions of neutrons, protons, deuterons, helium-3, alphas, and gammas with background material. These subroutines are divided into two packages. The first package, *gen2000*, reads the cross sections and distributions from binary libraries that describe in-flight reactions and formats them in a form appropriate for use by the second package. Libraries are organized by incident particle type, but contain information describing the attributes of all output particles. The method of tabulating cross section data depends on the incident particle type. Neutron and charged particle cross sections are multi-group; gamma cross sections are log-log interpolated from a energy grid consistent over all target elements. The second package, *bang2000*, uses these data to perform the collision physics. Each Monte Carlo particle possesses a discrete energy value allowing the kinematics of collisions to be performed on a continuous energy basis. The result of the kinematics is the attributes (type, number, energy, and direction) of all the particles emerging from the collision. MCAPM is modular and has been ported to a variety of platforms.

Introduction

The All Particle Method (APM), a system of data and algorithms to enable the Monte Carlo simulation of many particle types, has been under development at LLNL for four years.^{1,2} Data have been developed to describe the interaction of neutrons, photons, deuterons, helium-3, alphas, gammas, x-rays, and electrons with matter. These interactions may result in the production of any of the particles considered as well as ions with specific vacancy positions. Additional data describing the relaxation of ions as a function of vacancy position and the resulting emission of x-rays or electrons through fluorescence and Auger processes are part of the All Particle Method. The All Particle Method generator and collision package, denoted MCAPM (Monte Carlo All Particle Method), enables production Monte Carlo transport codes to access a portion of the APM data and perform collision physics. MCAPM is limited to neutrons, protons, deuterons, helium-3, alphas, and gammas. It currently does not consider x-rays, electrons, or relaxation effects of ionized atoms.

Libraries are organized by incident particle type, but contain information describing the attributes of all output particles. Neutrons incident on a target may, as determined by the data, produce any of the particles treated in the library: neutrons, heavy charged particles, and gammas. Tritons, for example, may similarly produce any of these same particles. Libraries for all particles types have identical formats and use identical subroutines.

This paper describes the two subroutine packages of MCAPM and their associated data. The first package, the generator *gen2000*, reads the cross sections and distributions from binary libraries that describe in-flight reactions and formats them in a form appropriate for use by the collision package. The second package, *bang2000*, uses these data to perform the collision physics.

MCAPM Data

MCAPM's generator, *gen2000*, reads data files containing four major types of data: cross sections, projectile multiplicities, projectile characteristic distributions (angle and energy distribu-

tions), and depletion/accretion information. Projectiles are the subset of particles exiting from a reaction for which an APM data file exists (neutrons, heavy charged particles, and gammas).

Cross Section Data

The method of tabulating cross sections depends on the incident particle type. In the case of neutrons and charged particles, the tabulated cross sections have been averaged with a flat particle spectrum over energy intervals or *groups*. The value of the cross section is taken to be constant over a group. The neutron multi-group cross sections span the energy range between 1.3×10^{-3} eV to 20 MeV in 175 groups. Charged particle multi-group cross sections are tabulated over 63 groups ranging from 1.0×10^{-4} eV to 20 MeV. Although the cross sections are considered multi-group, Monte Carlo particles possess a discrete value of energy allowing kinematics to be performed on a continuous energy basis. This Plechaty Hybrid scheme allows exploitation of the strengths of both the pure continuous energy method and the pure multi-group method: a small cross section data base and accurate kinematics.

Gamma cross sections are tabulated at 176 energy points between 100 eV and 30 MeV. The same energy grid is used for all elements. Logarithmic interpolation is used to find the cross section value over the interval between tabulated points.

Note that the energy values (including the number of values) are not *hard-wired* into the MCAPM package but are determined by MCAPM by reading the data libraries. This data-driven feature allows flexibility in library characteristics without producing new code.

Projectile Multiplicities

Projectile multiplicities specify the number of projectiles of each type emerging from a reaction. Usually the multiplicity is independent of incident energy. In some cases, particularly for fission, the multiplicity is tabulated as a function of energy of the incident particle. Facilities are available for client code developers to apply a factor to projectile multiplicities in order to increase or reduce projectile production.

Projectile Characteristic Distributions

The characteristics of outgoing projectiles, except gammas undergoing scattering, are tabulated in the APM libraries in the form of equal probable distributions in either energy, angle (cosine), both energy and angle, or sometimes coupled angle-energy. The kinematics type, described below, of a particular reaction specifies which distributions are present. Typically 32 equal probable bins are used, although for some distributions, such as fission neutron spectra, more bins are used. Although this method of describing a distribution occasionally smears out some detail, it has the advantage of resolving important, high-probability portions of a distribution. It is also very computationally efficient.

Equal probable distributions are tabulated at the evaluators' choice of discrete incident energies. Linear interpolation between tabulated distributions is used to find outgoing projectile characteristics at the incident particle energy.

Gamma scattering data is described below together with kinematics types 6 and 7.

Depletion/Accretion Data

As particles traverse material, not only are their characteristics altered but they also alter the characteristics of the background medium. The target isotope is *depleted* from the background material and the resulting products are *accrued* to the background.

The philosophy governing the generation of these libraries is "maintain a closed system" meaning that any isotope created by a reaction described in the library must itself be contained in the library. For example, the (n,n'p) reaction off N14,

creates C13 which is present in the library. Problems arise with reactions such as (n,p) off Li6,

which produces He6, an isotope missing from the library. The library evaluators have attempted to solve this problem by substituting He4 for He6. This unfortunately introduces a mass error of 2 amu.

Further mass conservation errors may be introduced due to the finite number of isotopes specified by a user for a problem. Returning to the example reaction (n,n'p) off N14. If the user fails to specify C13, the client code must make some compromises. One option is to mitigate the error by substituting an isotope already present in the problem (e.g., C12 with a resulting mass error of 1 amu). MCAPM provides a facility for the client code to specify such a substitute for a missing isotope.

Kinematics Physics

All reactions have been categorized into seven kinematics types which describe the methods used to determine the characteristics of a reaction's exiting particles. Various subroutines in the bang2000 collision package perform this physics. The mapping from reaction to kinematic type is another data-driven feature of the MCAPM package.

Kinematics Type 1: Relativistic Two-Body

After sampling from a library center-of-mass frame angle distribution for the first exiting particle, kinematics type 1 determines the energy of the first particle and the energy and angle of the second particle from relativistic conservation of momentum and energy. It then transforms these characteristics back to the laboratory frame. If an outgoing particles is not a projectile, its characteristics are calculated and then discarded. All elastic scattering reactions are of this type as are other reactions such as Be7(n,p)Li7 and N14(n, α)B11 and inelastic scattering of a level.

Kinematics Type 2: Energy/Angle Uncorrelated

Kinematics type 2 simply samples separately from lab frame angle distributions and energy distributions for each projectile. Correlation errors abound: the angle for one particle is uncorrelated to its energy, the characteristic of one particle are uncorrelated to the characteristics of another emerging from the same collision. Energy and momentum are only conserved on an average, statistical sense, not for each reaction. Most reactions are of type 2 including inelastic scattering off the continuum, fission, and most (n,2n) reactions.

Kinematics Type 3: Energy/Angle Correlated

Kinematics type 3 is currently used for only one reaction: Be9(n,2n)2 α . Lab frame angle distributions are sampled for each particle. Then, a lab frame energy distribution dependent on the

sample cosine is sampled. The data set necessary to describe this reaction is quite voluminous because separate energy distributions exist for different exiting cosines.

Kinematics Type 4: Decay

Kinematics type 4 treats the initial portion of the reaction like relativistic two-body reaction. Consider, for example, $\text{Li6}(n,nd)\alpha$. Type 4 samples the center-of-mass angle of the exiting neutron from a library angle distribution. The neutron energy and the outgoing Li6 cluster's energy and angle are found in the center-of-mass frame via relativistic conservation of momentum and energy and are transformed back to the lab frame. In this model, the cluster decays immediately into its constituent parts, in this case d and α . The cluster's characteristics are discarded because type 4 samples from uncorrelated lab angle and energy distributions for the remaining projectiles. In addition to $\text{Li6}(n,nd)\alpha$, other reactions of this type include $\text{Li7}(n,n'\gamma)\text{Li7}$, $\text{Be7}(d,p\alpha)\alpha$, and $\text{C12}(n,n'2\alpha)\alpha$.

Kinematics Type 5: Cluster

In a manner similar to the decay method, kinematics type 5 calculates relativistic two-body kinematics for the first exiting particle and the remaining cluster. It retains the cluster angle and energy, assigning the angle and corresponding speed to the constituents of the cluster. Only one reaction, $d(n,2n)p$, has kinematics type 5. The first particle emerging is a neutron; the cluster is a deuteron that breaks up into a neutron and proton.

Kinematics Type 6: Coherent Scattering

The exiting angular distribution of gammas experiencing coherent scattering is modeled by the Thomson cross section modified by the square of the coherent form factor:

$$\sigma_c(E, \mu) = \frac{3T}{8} (1 + \mu^2) FF^2(m)$$

where

$$m \frac{\sin \theta/2}{\lambda_{in}}$$

$$T = 0.6652448b$$

The form factor increases the forward peaking of the angular distribution for high energy gammas. The simple Thomson distribution

$$1 + \mu^2$$

is coded into bang2000 and the form factors tabulated as a logarithmic interpolated function are read from the APM gamma data file. The exit angle is sampled by first sampling from the square of the coherent form factor via table lookup. The rejection method is used to apply the Thomson angular dependence to the sampled angle.

Kinematics Type 7: Incoherent Scattering

The Klein-Nishina cross section multiplied by the incoherent form (or scattering) factor describes the angular distribution of gammas exiting an incoherent scattering event:

$$\sigma_i(E, \mu) = \frac{3T}{8} \frac{1 - \mu^2 + \frac{\kappa^2(1 - \mu)^2}{1 + \kappa(1 - \mu)}}{[1 + \kappa(1 - \mu)]^2} SF(m)$$

where the incident energy is included in the following term

$$\kappa = \frac{E}{0.511}$$

The effect of the form factor is to decrease the extreme forward peaking of the Klein-Nishina angular distribution at high energies.

The incoherent form factor is tabulated in the APM gamma data file as a logarithmic interpolated function. The exiting characteristics of the scattered gamma are found by sampling the exiting energy and angle from the Klein-Nishina distribution using Kahn's rejection method³ for gammas with incident energies below 1.5 MeV and Koblinger's direct method⁴ for higher energy gammas. The subroutine that performs this sampling was lifted directly from MCNP.⁵ The exiting angle (and corresponding energy) is then rejected or accepted by sampling an angle from the incoherent form factor with the rejection method.

Use of MCAPM

In order for a client Monte Carlo code to take advantage of the features of MCAPM, the client code must be modified to call `gen2000` during problem generation and the appropriate routines in `bang2000` at each particle collision during the simulation. The client code calls `gen2000` once for each particle type being tracked. `gen2000` returns a pointer to the location in memory of the start of that particle's library. The contents of the library depend on the isotopes requested and the particles tracked.

Callable Routines

The client code can access individual data elements of a particle's library through a variety of supplied access routines. The data elements are requested by name in the call to the access routine. An example of accessible data is the total cross section of each isotope. This datum is necessary for the client code to calculate distance to collision.

Following a collision, the client code calls three routines to sample the target isotope, sample the reaction, and sample the number, types, and characteristics of resulting particles, respectively. The reaction sampling routine also returns information needed for the client code to properly update material compositions as a result of accretion and depletion of isotopes.

Non-Analog Physics

MCAPM provides the capability to model a slightly twisted version of reality through the use of "non-analog" physics. This may be desired in order to improve Monte Carlo statistics or to augment the effect of a particular reaction. Facilities in MCAPM exist allowing client code develop-

ers to terminate depletion and accretion isotope chains in order to limit isotope lists to a reasonable length, modify individual reaction cross sections for particular isotopes through energy group-independent multipliers, and perturb particle multiplicities through particle-dependent multipliers.

Portability

MCAPM is operational on NLTSS, UNICOS, and a variety of UNIX platforms. Coding is maintained in a single source. On all platforms, MCAPM reads binary data files produced on a Cray computer using the Cray data format. This data is translated to the platform's native format, e.g., IEEE, as the data is read. A series of routines known as PORTLIB⁶ provide this data translation capability.

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