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TRIMARAN : A THREE DIMENSIONAL MULTIGROUP P1 MONTE CARLO CODE FOR CRITICALLITY STUDIES

G. ERMUMCU - J. GONNORD - J.C. NIMAL

COMMISSARIAT A L'ENERGIE ATOMIQUE - Service SERMA
LABORATOIRE DE PROTECTION
SACLAY - B.P. N° 2 - 91190 GIF SUR YVETTE -
FRANCE

ABSTRACT

TRIMARAN is developped for safety analysis of nuclear components containing fissionnable materials : shipping casks, storage and cooling pools, manufacture and reprocessing plants. It solves the transport equation by Monte Carlo method in general three dimensional geometry with multigroup P1 approximation. A special representation of cross sections and numbers has been developped in order to reduce considerably the computing cost and allow this three dimensional code to compete with standard numerical program used in parametric studies.

As well as nuclear reactor safety, auxiliary components safety such as shipping cask, fuel storage pools and reprocessing plants has become of major importance and the restrictions requested by the safety regulations may effect the entire nuclear program.

Following actual safety regulations, all units containing fissile materials should'nt present any risk of nuclear chain reaction, and pre computation should guarantee that - even in all possible types of accident - such as : fire, handling error, flooding, geometric deformation following

falls or seism -the effective neutron multiplication constant (keff) is less than 1., all cross section and computation uncertainties evaluated.

The ever growing quantities of fissile materials to be stored, shipped and reprocessed demand more accurate precise calculations because large uncertainties do not allow to run such units at their optimal capacity.

Let us have a look on the following example : the effective neutron multiplication constant (keff) of a shipping cask built for 16 fuel elements is computed, assuming a total immersion in water with two methods :

A gives an uncertainty of 0.05 (3 σ)
B gives an uncertainty of 0.005 (3 σ)

Number of elements	12	14	16
method A	0.92 $\pm$ 0.05	0.93 $\pm$ 0.05	0.95 $\pm$ 0.05
method B	0.920 $\pm$ 0.005	0.932 $\pm$ 0.005	0.945 $\pm$ 0.005

knowing that the French safety regulation requires keff $\leq$ 0.95 all uncertainties included, we see from the table that using method A only the transportation of 12 elements may be allowed. The use of method B will allow the shipping of 16 elements, which represents a gain of 33 % of the shipping capacity.

However accurate methods demanding exact three dimensional treatment of the geometry and fine representation of cross section are quite expensive. Furthermore allow any type of casks or plants, the most pessimistic accident should be evaluated, involving a lot of parametric studies such as calculation of keff function of water density, poison nature, geometric deformation and eventual presence of reflectors.....

This leads to a large number of computations and a compromise must be found between cost and computational accuracy.

In order to meet this goal we have developped a simplified very fast Monte Carlo code : TRIMARAN which solves the critical Boltzmann equation in three dimensional geometry using multigroup cross sections with linear anisotropy (P1 approximation).

TRIMARAN GEOMETRY

The code uses the geometry package of the TRIPOLI system [1]. The three dimensional geometry is defined as a union of volumes filled with homogeneous composition and limited by portion of surfaces of first or second order. The geometry may be repeated by translation-rotation and symmetry and allows any type of boundary condition including albedos.

The user defines equations such as :

- general plan $ax + by + cz + d = 0$
- special plans $x + x_o = 0$
  $y + y_o = 0$
  $z + z_o = 0$
- general quadric $ax^2 + by^2 + cz^2 + dxy + eyz + fzx + gx + hy + iz + j = 0$
- sphere $(x - x_o)^2 + (y - y_o)^2 + (z - z_o)^2 - R^2 = 0$
- special cylinders $(y - y_o)^2 + (z - z_o)^2 - R^2 = 0$
  $(z - z_o)^2 + (x - x_o)^2 - R^2 = 0$
  $(x - x_o)^2 + (y - y_o)^2 - R^2 = 0$

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Then each volume will be defined by its boundary surfaces and the sign of their associated linear or quadratic forms for any point inside the volume. Any portion of boundary surface with no neighbour volume will be declared with a boundary condition such as :

- leakage
- optical reflexion
- isotropic reflexion with albedo function of energy
- symmetry
- translation
- rotation

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A special and very fast processing is used for slabs which could be inserted inside every rectangular volumes.

CROSS SECTION

TRIMARAN solves the Boltzmann equation without external sources :

$$(1)\quad \vec{\Omega}.\vec{\nabla}\phi(\vec{r},\vec{\Omega},E)+\Sigma_t(\vec{r},E)\phi(\vec{r},\vec{\Omega},E)=$$
$$\int_{4\pi}d^2\Omega'\int_0^\infty dE'\,\Sigma_s(\vec{r},\vec{\Omega}'\to\vec{\Omega},E'\to E)\phi(\vec{r},\vec{\Omega}',E')+\frac{\chi(\vec{r},E)}{k_{eff}}\int_{4\pi}d^2\Omega'\int_0^\infty dE'\,\nu\Sigma_f(r,E')\phi(\vec{r},\vec{\Omega}',E')$$

Using the linear anisotropy collision approximation (P1) the transfer cross section may be written :

$$(2)\quad \Sigma_s(\vec{r},\vec{\Omega}\to\vec{\Omega}',E'\to E)=\Sigma_s^0(\vec{r},E'\to E)+\vec{\Omega}.\vec{\Omega}'\,\Sigma_s^1(\vec{r},E'\to E)$$

and in the multigroup approximation (1) becomes :

$$(3)\quad \vec{\Omega}.\nabla\phi_g(\vec{r},\vec{\Omega})+\Sigma_g^t(\vec{r})\phi_g(\vec{r},\vec{\Omega})=$$
$$\sum_{g'}\left\{\left(\Sigma_{g'\to g}^{s0}(\vec{r})+\frac{\chi_g(\vec{r})}{k_{eff}}\nu\Sigma_{g'}^f(\vec{r})\right)\int_{4\pi}\phi_{g'}(\vec{r},\vec{\Omega}')d^2\Omega'+\Sigma_{g'\to g}^{s1}(\vec{r})\int_{4\pi}\vec{\Omega}.\vec{\Omega}'\,\phi_{g'}(\vec{r},\vec{\Omega}')d^2\Omega'\right\}$$

REMAINING LINES OF TYPE

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The functions $\sum_g^t(\vec{r})$, $\sum_{g\to g'}^{s0}(\vec{r})$, $\sum_{g\to g'}^{s1}(\vec{r})$, $\nu_g\sum_g^f(\vec{r})$ and $\chi_g(\vec{r})$ are constant inside a volume as defined in the geometry and are refered as the cross section library.

TRIMARAN can use any type of multigroup library with less than 256 groups. The code has its own mixing routine and may be coupled with different libraries through a simple interface.

Actually two interfaces are provided :

- one with ANISN format libraries which allows the code to use cross section processed by the AMPX system [2]
- one with a KERA library output by the cell code APPOLO[3] which computes correct self-shielded cross sections using the collision probability method.

From one of these microcopic cross section libraries, TRIMARAN computes macroscopic cross sections and probability tables :

$\sum_g^a$ absorption in group g

$\nu_g\sum_g^f$ neutron production in group g with spectrum χ_g

$$\sum_{g'\to g}^{1}(\vec{\Omega}\to\vec{\Omega}') = \sum_{g'\to g}^{s0} + \vec{\Omega}.\vec{\Omega}'\sum_{g'\to g}^{s1}$$

with g' > g for the slowing down
g' = g for in scattering
g' < g for upscattering

END TYPING

in the standard 99 groups APOLLO library, 47 are with possible upscatter.

The probability tables are stored in memory in a special format presenting two important advantages :

- it reduces considerably the memory occupied by the cross section
- the format is specially adapted to the neutron simulation by the Monte Carlo method.

SIMULATION

A batch of neutrons is simulated using the Monte Carlo method. Scoring is made for absorption, neutron production and leakage and an estimation of :

$$keff = \frac{\text{neutron production}}{\text{absorption+leakage}}$$ is computed.

In the same time, the next batch of neutrons is generated with the fission spectrum of the composition where they are created.

This process is repeated until the variance on the mean value of keff reached the user precision or the iteration limit.

To initiate the process a guess batch of neutrons is generated in fissile materials using a flat flux approximation.

Starting from a neutron characterised by :

its position $\vec{r}$ its direction $\vec{\Omega}$

its group g and its weight π

a track length is sampled. Then absorption and production rate are computed and scored along the track using two different but highly correlated ways :

- track length estimator :

- collision estimator

At the end of the track the neutron either leaves the system or has a collision. In the latter case the weight is multiplied by the probability of no absorption and a new group g' and direction $\vec{\Omega}'$ are sampled from $\Sigma_s^0(g\ g')$ and $\Sigma_s^1(g, g')$. If the material is fissile, neutrons for the next generation are sampled from $\nu_g \Sigma_g^f$ and χ_g

The neutron history is simulated until the particle leaves the system or its weight becomes less than .

The program offers two options :

- russian roulette
- weight transfer, which seems to give a better variance.

At the end of the batch the different values of the keff estimation are used to accelerate the convergence.

The code outputs :

- absorption and production rates with their variance for each volume
- leakage through boundary surfaces
- mean value and variance of keff computed by three different ways :
- number of neutrons generated at each batch
- $keff = \frac{production}{absorption+leakage}$ from collision estimator
- $keff = \frac{production}{absorption+leakage}$ from track length estimator

SPECIAL TECHNICAL FEATURES OF TRIMARAN

The computing cost is a function of 3 parameters :

- number of input/output operations
- size of memory occupied during the exection
- central processing unit time (CPU)

The code has been specially programmed to obtain a significant reduction of the contribution to the cost of each parameter.

The input/output operations are reduced to the minimum necessary to run a computation : reading the user input, the microscopic cross sections and printing the results. All the data used during the execution is stored at the beginning in the central memory. This programming usually leads to a large utilization of the computer memory : for example, using our standard 99 groups library the cross sections matrices ($\sum_{1}^{0}$ - $\sum_{4}^{1}$) will occupy for only one composition 99x99x2 words. For a typical shipping cask problem where about 10 compositions are described 800 K would be necessary only to store the cross sections !

TRIMARAN uses a special binary coding which reduces the size occupied by the cross sections by a factor between 10 to 15. Using that method most of our problems can be run within a region less than 300 K.

Furthermore this coding leads us to give up nearly completely floating point operations for fixed binary operations 4 to 5 times faster on IBM machines.

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This type of binary coding is specially adapted to Monte Carlo method for two reasons :

- the limited variation of numbers used during the simulation : probabilities belongs to (0,1)..

- the inherent uncertainties brung by the Monte Carlo method allows to simulate floating point operations by binary operations as long as we control the numerical uncertainties in order that their cumulated values stay negligible in respect to the variance of the result.

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In a Monte Carlo run the variance on the result decreases like the square root of the number of histories, and if it is quite easy to obtain rapidly a poor variance (10/15 %) it becomes hopeless to reach better variance than .5 to.4% in a reasonable computing time. This limit allows to use numerical methods giving uncertainties between 10^{-5} - 10^{-4} instead of the 10^{-7} - 10^{-6} of standard floating points operations, but 5 to 10 times faster. This is well shown on figure 1 where the variance is plotted as a function of time for 3 different Monte Carlo simulations of the same benchmark.

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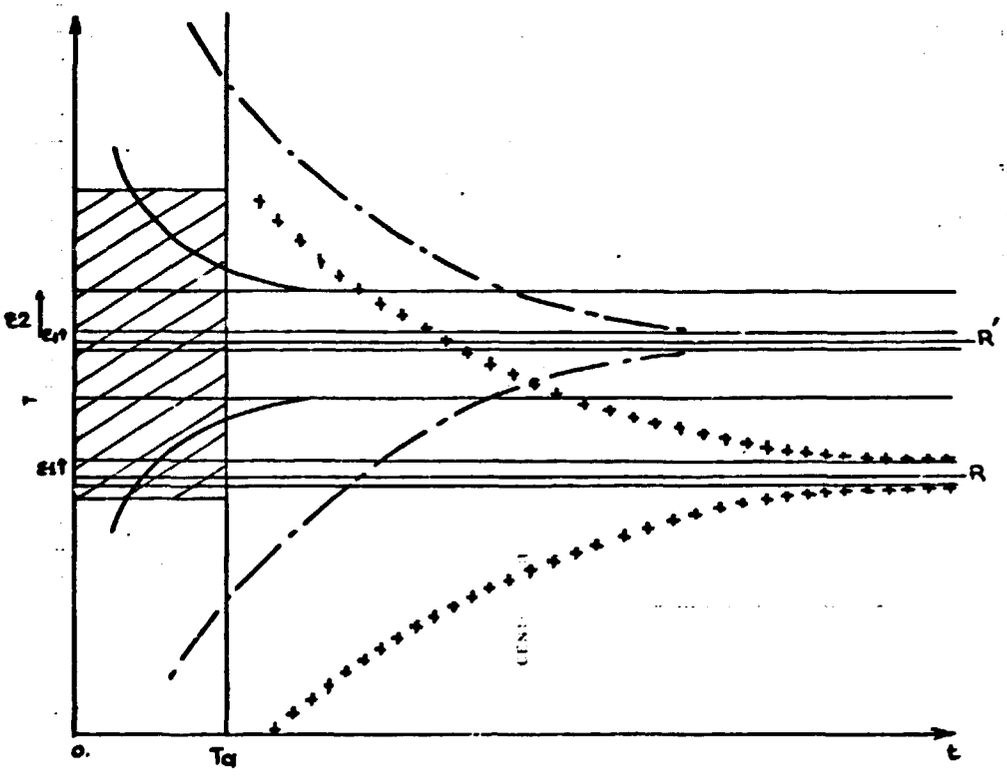
FIGURE 1



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R_{ex} exact result R' approximate result

ε_1 numerical uncertainty from floating point operations

ε_2 numerical uncertainty from binary method

Ta acceptable computing time for engineering calculations

++ exact Monte Carlo

•|— multigroup P1 with floating point

—— TRIMARAN

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The exact Monte Carlo computation converges very slowly to the exact result limited only by the accuracy on floating point operations $\mathcal{E}1$. But the computing time limits its use to physical studies or special applications.

Simplified Monte Carlo keeping the advantages of three dimensional geometry but using approximated description of cross sections and anisotropy converges to an approximate result R' much faster but still not enough to compete with the analytical or numerical codes used in nuclear engineering.

TRIMARAN, using binary coding, falls in the range of these engineering codes, the counter part being a larger theoretical uncertainty. But anyway this theoretical uncertainty cannot be reached in the range of accuracy and computing time where the code is used. This proves the advantages of the method.

CONCLUSION

By reducing the cost of a three dimensional Monte Carlo run, as shown by preliminary results, by a factor 8 to 10 we dispose of a code able to satisfy three dimensional demands of some calculations and still in the range of price of analytical or numerical codes used in nuclear engineering.

TRIMARAN is going to be implemented in the shielding code system PROMETHEE [4] which will supply it with the input output facilities of a modular system. We think then to extend the field of this method to deep penetration problems.