MORET: Version 4.B
A Multigroup Monte Carlo Criticality Code

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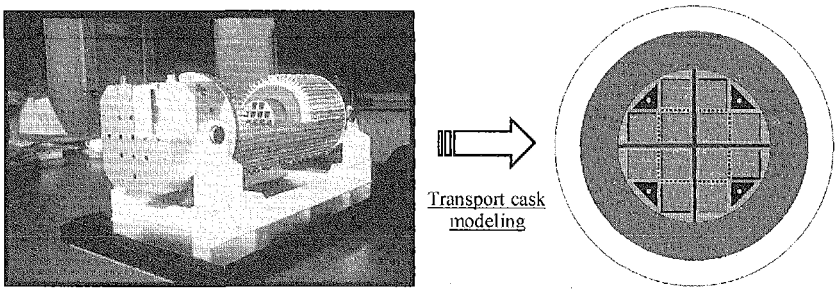
MORET 4 is a three dimensional multigroup Monte Carlo code which calculates the effective multiplication factor (keff) of any configurations more or less complex as well as reaction rates in the different volumes of the geometry and the leakage out of the system. MORET 4 is the Monte Carlo code of the APOLLO2-MORET 4 standard route of CRISTAL, the French criticality package. It is the most commonly used Monte Carlo code for French criticality calculations. During the last four years, the MORET 4 team has developed or improved the following major points: modernization of the geometry, implementation of perturbation algorithms, source distribution convergence, statistical detection of stationarity, unbiased variance estimation and creation of pre-processing and post-processing tools.

The purpose of this paper is not only to present the new features of MORET but also to detail clearly the physical models and the mathematical methods used in the code.

KEYWORDS: Monte Carlo code, simulation, perturbation, stationarity



1. Introduction

MORET is a multigroup Monte Carlo neutronics code developed by IRSN to perform criticality calculations.

It has been used for the last thirty years for most of criticality-safety studies in France and is now widely used by the French criticality safety community (IRSN, CEA and French nuclear companies).

The MORET code has been designed in order to obtain accurate calculations of effective multiplication factors for complex geometries in a reasonable calculation time. It is thus especially well suited for requirements of criticality surveys performed for fuel cycle facilities and plants and for fissile material transport packaging, which usually requires many calculations.

The efficiency of the MORET code is based mainly on the powerful association of deterministic and Monte Carlo approaches, namely:

- To treat the local heterogeneity that could be represented in simple 1D or 2D cells by deterministic methods (P_{ij} or Sn) and to apply related models for self-shielding and possibly homogenisation.
- To treat the overall heterogeneity and geometrical complexity with 3D Monte Carlo tracking without wasting computation time in treating local details since they have been taken into account in the previous step.

In the framework of the standard route of CRISTAL[1], the MORET 4 code is used in conjunction with the deterministic assembly code APOLLO2 and with the CEA93 library (172 groups structure from JEF2.2 nuclear data library).

The new 4.B version of MORET takes benefit from this successful experience and brings further enhancements to the physics and to the engineering of the code. Many developments were performed in the last few years in order to still better help users to carry out criticality safety analyses: modernization of the geometry, implementation of perturbation algorithms, source distribution convergence, statistical detection of stationarity, unbiased variance estimation and creation of pre-processing and post-processing tools.

This paper presents not only the innovations but also the whole characteristics of the physical and mathematical models implemented in the code.

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2. Physical Models and Mathematical Methods

2.1 Simulation strategies

Five strategies are available in the MORET 4 code: the conventional method, the stratified sampling[2], the super-history powering[3], the use of fission matrix[4] and the use of importance function[5,6].

The common principles of all the strategies except for the superhistory powering are:

- each cycle comprises only one generation: the starters of one generation are simulated one at the time from their 'birth' to their 'death' (absorption or leakage) and their progeny is simulated during the next cycle,
- each collision site in a fissile volume is considered as a potential fission site; the probable number of produced neutrons and the coordinates of the collision point are stored,
- the positions of the starters of the new cycle are sampled among the collision sites of the previous cycle,
- since the progeny is not considered, the number of simulated neutrons is equal to the number of starters, which is kept constant at each cycle.

In the case of the superhistory powering:

- each cycle comprises L generations: the starters of the first generation of the cycle and their progeny are followed one at the time from their 'birth' to their 'death' (absorption or leakage),
- each absorption site in a fissile volume during the last generation of the cycle is considered as a potential fission site; the probable number of produced neutrons and the coordinates of the absorption point are stored,
- the positions of the starters of the new cycle are sampled among the absorption sites of the last generation of the previous cycle,
- the number of starters is kept constant but the number of simulated neutrons is variable at each cycle since the progeny is considered.

These strategies differ from the point of view of the estimation of the source distribution between the cycles (see section 2.4).

Some of these strategies have been compared on a modified version of the configuration studied by Kadotani et al. (a 5 × 5 × 1 array of metal spheres in vacuum) in which the initial source is chosen to be far from the converged source distribution.[7]

They are currently tested in the framework of the Expert Group in Source Convergence Analysis, which was set up by the NEA.[8]

2.2 Sources description

The MORET 4 code provides three automatic options to describe the first generation source neutrons:

- punctual distribution (which requires specifying the coordinates of source neutrons, an operation that may be tedious),
- uniform distribution of a specified number of source neutrons in specified fissile volumes,
- automatic sampling of starting points in all fissile volumes, by generating the same number of neutrons in each volume and by uniformly distributing them in each volume.

2.3 Neutron tracking

The life of a neutron is a succession of separated events in space: birth, elementary motion, collision, crossing of surfaces, leakage or absorption.

The energy group of the starting neutrons is drawn randomly from the fission spectrum of the medium supplied by the APOLLO2 code. The motion direction of the starting neutrons is drawn randomly from a uniform angular distribution.

If the distance to the closest surface in the direction of the neutron is smaller than the probable distance to the next collision drawn randomly, the neutron leaves the volume otherwise a collision takes place.

If the neutron leaves the volume and enters a new one, a new probable distance is drawn randomly, accounting for the different material environment. The direction of motion is kept the same.

If the neutron reaches one of the outer boundaries of the system, depending on the type of boundary conditions, it can be reflected or leak out. If the neutron leaks out of the system, the neutron 'dies' and the tracking is stopped.

If a collision takes place, the choice between absorption and scattering is randomly determined.

In the case of scattering, the (n,xn) reactions are accounted for by introducing a weight to the neutron which is increased at each collision by the factor:

$$\frac{\Sigma_{s,(n,n')} + 2\Sigma_{s,(n,2n)} + 3\Sigma_{s,(n,3n)} + \cdots}{\Sigma_{s,(n,n')} + \Sigma_{s,(n,2n)} + \Sigma_{s,(n,3n)} + \cdots}$$

with $\Sigma_{s,(n,xn)}$ being the cross section for the (n,xn) reactions.

A new energy group is selected from the cumulative transfer probability distribution. This group-to-group transfer determines an angular scattering distribution, usually expressed as a Legendre expansion of the cross section transfer array supplied by the APOLLO2 code. According to the order of expansion available, the MORET 4 code uses one of the three following methods preserving the moments of the Legendre expansion of the angular scattering distribution[9]:

- the Coveyou semi-linear method (P1),
- the Lux semi-continuous method (P3),
- or the discrete angle method (P5 and higher).

In the case of absorption, the neutron 'dies' and the tracking is stopped.

2.4 Source distribution estimation

At each cycle, the number of neutrons is not rigorously renormalized to the initial number of

starting neutrons, M_0, but the total weight of the starters is renormalized to M_0.

At the end of a cycle, the proportions of neutrons P_V to be emitted in each fissile volume V are determined in the following way:

$$P_V = \frac{\text{fission productions in V}}{\text{total fission productions}} M_0$$

The fission productions are estimated either with the collision estimator (conventional strategy), or with the track-length estimator (stratified sampling, use of fission matrix and importance function), or with the absorption estimator (superhistory powering). The track-length estimator guarantees a non-null estimate of the fission productions in each fissile volume if at least one neutron is emitted in each fissile volume.

In the case of the use of fission matrix, the calculation of P_V differs from the usual way every N cycles (N is fixed by the user). In this case, the proportions of neutrons P_V to be emitted in each fissile volume V are given by the components of the eigenvector associated to the highest eigenvalue of the fission matrix which is calculated all N cycles.

The fission matrix is a square matrix of size the number of fissile volumes defined as follows: $k_{ij} = P_{ij}/S_j$, P_{ij} being the cumulative (over all the cycles) fission production in fissile volume i due to neutrons emitted in volume j, S_j being the cumulative (over all the cycles) weight of sources emitted in volume j. P_{ij} is estimated with the three combined estimators (collision, track-length, absorption).

In the case of the use of the importance function, the fission productions are estimated with the track-length estimator but not in the usual way. The contribution of a neutron born in the volume j and moving in volume i is multiplied by the ratio of the importance of volume i over the importance of volume j. The estimation of the importance function is renewed all N cycles (N is fixed by the user). It is the eigenvector of the highest eigenvalue of the adjoint of the fission matrix.

The number of starting neutrons for the next cycle in a fissile volume V is: $M_V = \text{NINT}(P_V)$.

In the case of stratified sampling, if M_V is null (i.e. $P_V < 0.5$), M_V is set to 1, in order to have at least one neutron in each fissile volume.

If M_V differs from 0, all starters in volume V have the weight P_V / M_V.

The M_V starters in fissile volume V are sampled from the potential fission sites (either collision sites or absorption sites in the case of superhistory powering) in volume V stored during the previous cycle. The probability to pick a potential fission sites is proportional to its weight.

The weights of all starters are possibly multiplied by the same correction factor in order to keep the total weight of all starters equal to M_0.

2.5 Keff estimators

An aspect that deserves a lot of attention is the estimator of keff.[10] Using the three usual estimators of the reaction rates (collision, track-length and absorption) and two cycle keff definitions:

- "source" keff = fission productions / sources,
- "balance" keff = fission productions / neutron balance (absorption + leakage – excess),

MORET 4 has 6 individual keff estimators, computed as the average of cycle keff estimates at each cycle.

In the case of superhistory powering, a supplementary keff estimator based on the absorption estimator is used (average of fission productions at each cycle / average of sources).

All the keff estimators have the same expected value but not the same standard deviation. This implies that, depending on configurations, a keff estimator can require more or less cycles than the others to reach a fixed uncertainty. In other words, no estimator is universally better than others.

The linear combination of estimators allows creating a higher performance estimator whose variance is equal to the minimum of individual variances, in the worst conditions.

Thus, the MORET 4 code evaluates:

- on each step, two combinations of three keff estimators (the combined "source" estimators and the combined "balance" estimators); the simulation stops when the minimum number of cycles is achieved and as soon as the standard deviation of one of the available keff estimators is lower than the precision level wished by the user,
- on the ultimate step, a more general combination of 5 keff estimators (the 3 "source" estimators and 2 "balance" estimators: collision and track-length) and of 2 control variables (neutron balance estimated with the collision estimator and the track-length estimator).

3. New Features of MORET

3.1 Modernization of the geometry

Since the first releases of MORET, the geometry has been described in a combinatory manner, via simple-shape convex elementary volumes (sphere, cylinder with any direction axis, parallelepiped box, cone with axis parallel to a reference axis, semi-solid limited by a plane, prism with hexagonal section) and geometric operators derived from the theory of sets (inclusion, intersection, union, penetration, truncation). The whole system is placed in an external volume whose surfaces may totally or partly reflect the neutrons.

Up to the previous version, only one rectangular array could be described in the geometry. The description of hexagonal arrays is now available. As explained below, several arrays and arrays in arrays are now allowed thanks to the new modular geometry.

The modular geometry, implemented in MORET 4.B, allows to model more complex geometries. It is based on the use of basic building blocks (parts of the whole geometry), called

"modules", that can be embedded one in another (via holes) to form sub-systems usable from one study to another without modifications. The geometry of each sub-system is always described in a combinatory manner via simple-shape volumes.

Here are summarized the features of modules:

- There is one main module (numbered 0) for the whole geometry (see examples Figure 1).
- The way of modelling the geometry within each module is unchanged compared to the previous versions.
- Modules have their own local coordinates and can be used from one calculation to another without any modification. This is particularly interesting for users who can choose modules or add their own modules in a common database.
- Modules can be embedded one in another without any restriction via holes (keyword TROU: hole in French).
- Modules allow modelling several arrays, and arrays in arrays (one array per module) whereas only one array could be described with the previous versions of the code.

As illustrated in Figure 1, suppose sub-modules 1, 2 and 3 have been already modelled for the study 1 and stored in a database, the writing of the geometry part of the input file for the study 2 would consist in pasting the description of sub-modules 1, 2, 3 and in writing the following description of the main module:

```
MODUle 0
  TYPE 1 BOITe 15. 10. 10.
  TYPE 2 BOITe 2. 2. 2.
  TYPE 3 SPHEre 3.
  VOLUme 1 0 1 1  0.  0. 0.
  * Hole 1: in vol. 1, of type 2, filled with module 2,
  * at coordinates (-8.,5.,0.)
  TROU   1 1 2 2  -8.  5.  0.
  * Hole 2: in vol. 1, of type 2, filled with module 2,
  * at coordinates (7.,0.,0.)
  TROU   2 1 2 2  7.  0.  0.
  * Hole 3: in vol. 1, of type 3, filled with module 3,
  * at coordinates (-5.,-5.,0.)
  TROU   3 1 3 3 -5.  -5.  0.
FINModule
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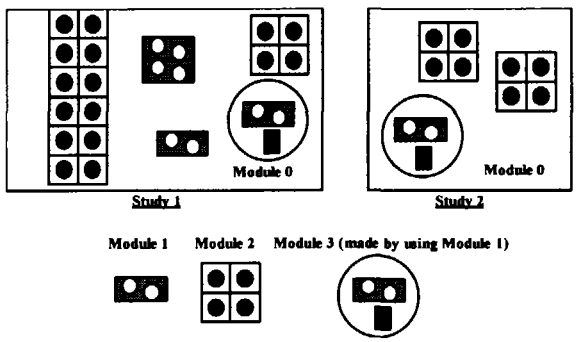

Fig. 1 Example of modular geometries

3.2 Implementation of perturbation algorithms

The correlated sampling method was implemented in the MORET 4 code. This new feature allows estimating during the same simulation the keff and the variation of the keff due to "low" perturbations of chemical compositions, while not noticeably increasing the calculation time. The validity extent of this method is currently being studied.

A numerical and physical validation of MORET 4 perturbation calculations against 'Physical' type fission products experiments is exposed in a paper of Anno et al. in this conference.[11]

3.3 Statistical detection of convergence

The settling of the source distribution convergence can require a very variable number of cycles during which the estimation of keff can be erroneous.

The suppression of non-converged cycles is necessary to obtain an accurate determination of the keff confidence interval but the checking of the source convergence is a longstanding difficulty of Monte Carlo calculations.

Up to the last release of MORET, the user could check the convergence of the calculation only by the following different indicators:

- chi-square tests performed by the code to check the normality of the distribution of the cycle keff (for each keff estimator),
- the recalculation of the final keff and its standard deviation after the suppressing of a variable number of initial cycles,
- the plot of the distribution of the cycle keff in order to be visually compared to the theoretical normal distribution (Figure 2),
- the plot of the cumulative keff versus the number of active cycles in order to visualize the presence of an initial transient (Figure 3).

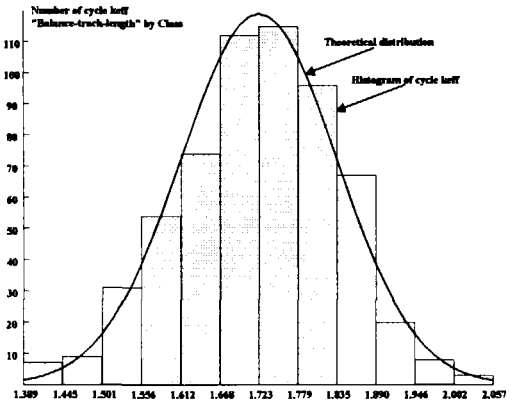

Fig. 2 Part of the postscript output file: Comparison of the distribution of the cycle keff with the theoretical normal distribution

Statistical tests based on the Brownian bridge theory have been implemented in MORET 4.B and its post-processing tool (OPOSSUM) to automatically suppress the initial transient of the cycle keff series.[12,13]

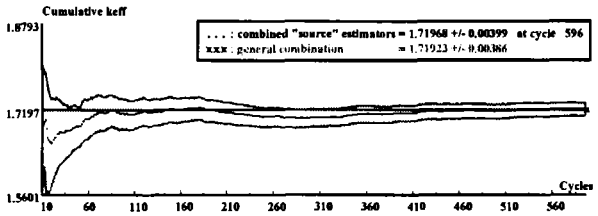

Fig. 3 Part of the postscript output file: Cumulative keff versus the number of active cycles

3.4 Unbiased standard deviation estimation

Various methods have been proposed to better take into account the correlations between generations in the calculation of the standard deviation of any Monte Carlo results (batching method, method of Ueki et al., use of time series methodology...).[14]

At present, none of them gives really satisfactory results. Developments are still in progress in this area.

Nevertheless, the method proposed by Ueki et al. has been chosen because, without a great effort of adaptation, it gives a more realistic estimation of the standard deviation than the conventional method assuming no correlation.

The principle of the method of Ueki et al. and the adaptations of the method are explained hereafter.

Let consider a cycle keff series of length N.

Ueki et al. established the theoretical expression of the bias of the conventional estimation of the variance of the mean of the cycle keff series, denoted as $\hat{\sigma}^2$:

$$B\left(\hat{\sigma}^2\right)=-\frac{2}{N(N-1)}\sum_{i=1}^{N-1}(N-i)c(i),$$

c(i) being the true autocovariance coefficients of the cycle keff series.

Ueki et al. also established the theoretical expression of the bias of the conventional estimation of the autocovariance coefficients of the cycle keff series, denoted as $\hat{c}(i)$, for the small values of i:

$$B\left(\hat{c}(i)\right)=-\sigma^2$$

σ^2 being the true variance of the mean of the cycle keff series.

Ueki et al. consider only the first p (p = 10) autocovariance coefficients, assuming that the autocovariance function c(i) quickly decreases to 0 when the lag i increases.

The method of Ueki et al. consists in iterating the estimation of the variance of the mean σ_u^2:

$$\sigma_u^2=\hat{\sigma}^2+\frac{2}{N(N-1)}\sum_{i=1}^{p}(N-i)c(i)$$

with $c(i)=\hat{c}(i)$ for the first iteration and $c(i)=\hat{c}(i)+\sigma_u^2$ for the next iterations.

So the successive estimates of the variance of the mean with the method of Ueki et al. define a linear recurring sequence of order 1: $\sigma_{u,k+1}^2=a\cdot\sigma_{u,k}^2+b$

with $\sigma_{u,0}^2=0$, $a=\left[2p\left(N-\frac{p+1}{2}\right)\right]\Big/\left[N(N-1)\right]\approx\frac{2p}{N}$ and

$$b=\hat{\sigma}^2+\frac{2}{N(N-1)}\sum_{i=1}^{p}(N-i)\hat{c}(i)$$

When the number of cycle N is about a few hundreds, a is very small and the number of iterations needed is very low: 1 or 2.

An improvement of the method of Ueki et al. consists in estimating directly the limit l of the sequence ($l=a\cdot l+b$):

$$\sigma_u^2=\left[\hat{\sigma}^2+\frac{2}{N(N-1)}\sum_{i=1}^{p}(N-i)\hat{c}(i)\right]\Big/\left[1-\frac{2p\left(N-\frac{p+1}{2}\right)}{N(N-1)}\right]$$

One of the major difficulties of the method of Ueki et al. is the fact that σ_u^2 can be negative! Indeed, due to the uncertainties on the estimates $\hat{c}(i)$ of the first p autocovariance coefficients, the corrective term $\frac{2}{N(N-1)}\sum_{i=1}^{p}(N-i)\hat{c}(i)$ can be negative and greater in absolute value than $\hat{\sigma}^2$.

An adaptation has been made to the method of Ueki et al. consisting in initialising the number p of autocovariance coefficients taken into account to 10 and in decreasing p while σ_u^2 is negative.

3.5 Creation of pre-processing and post-processing tools

The new tools for the MORET code are written in JAVA and are available on all environments (Windows, Linux, Unix).

3.5.1 Pre-processing Tool EJM

EJM[13] is a text editor offering users the possibility to display the construction of their geometry at the same time as they write it. Its principal panel is divided into two parts: the left part is used to write the modelling of the geometry and the right one to visualize it with various cuts (in the three directions) at various levels in real time.

3.5.2 Post-processing Tool OPOSSUM

OPOSSUM[13] is a post-processing tool allowing users to visualize the results of their MORET 4 calculations through graphs and curves and to compare several calculations results. This new tool will include three main features to help users to analyze the calculations results:

- a tool displaying the curves from the output data (cross sections, reaction rates, fluxes...),
- a graphical tool giving 2D representations of various tallied parameters (source distribution, reaction rates) in the MORET geometry model,
- a statistic tool used to determine the well-done stationarity of the Monte Carlo calculation.

3.5.3 Post-processing tool to assist code bias estimation

The three main functionalities of this tool[15] are:

- definition of the characterization's working database (user selected experiments),
- graphical visualization of a practical case among the experiments of the working database,
- bias estimation with statistical uncertainty evaluation.

4. MORET project

At present, the MORET team regroups at least 5 persons for the development of the code and associated tools, verification, experimental validation, installation and user support.

4.1 Software characteristics

MORET 4 is a modular code written in Fortran 90. The routines are grouped in specific modules (physics, mathematics or purely IT domains). The memory is dynamically managed.

A software engineering tool, called PAPYRUS, allows configuration management.

4.2 Verification and Installation

An extensive verification is done at each new development's step to validate the new functionalities as well as the old ones. A verification database of more than 200 test cases is automatically launched on each platform referred above (see section 4.1) and then analysed. New test cases are added to this database at each new development.

The same database of tests is used to demonstrate that the software is properly installed and functioning correctly.

MORET 4 runs on various platforms: IBM (AIX), SUN (Solaris), DEC (OSF1), HP (HP-UX), SGI (IRIX), PC (Windows and Linux).

4.3 Experimental Validation

Within the scope of the French CRISTAL package, the MORET 4 code undergoes an important experimental validation program[16] with systematic analysis of critical experiment results from various origins (experimental programs performed in Valduc facility, in the USA, in Japan...). The greater part of these experiments is assessed by the ICSBEP working group (International Criticality Safety Benchmark Evaluation Project).

4.4 Users Support

A huge effort has been achieved to assist MORET 4 users:

- combined classroom and hands-one training,
- public and private access website with online documentation (www.irsn.fr/cristal),
- users hot line, forum and users club,
- bugs report, maintenance.

5. Conclusion

This paper has introduced the main improvements implemented in the Monte Carlo code MORET 4.B. The "kits" approach for the geometry making is an original way to improve the efficiency of users to build and verify their criticality safety models.

Future developments of MORET will particularly concern:

- the diversification of the origin of cross sections,
- the development of source convergence criteria,
- the improvement of simulation algorithms to guarantee the source convergence,
- the development of pre-processing and post-processing tools.

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