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New features of the Monte Carlo Neutron Transport Code MORET 6

Wilfried Monange^{1*}

¹IRSN 31 avenue de la Division Leclerc, 92260 Fontenay-aux-Roses, France

The MORET code is a simulation tool that simulates the transport of neutrons using the Monte Carlo method. It allows users to create complex three-dimensional geometrical configurations in a user-friendly way. New features have been introduced to extend the application field of MORET beyond the usual criticality calculations. The most important change is the addition of an analog fixed source mode. Other useful improvements have been added concerning the geometry, the fission matrix, multigroup sensitivity coefficients and outputs. This paper provides an overview of these new features.

1 Introduction

Inherited from the French MACAO program of the 1960s, the MORET code simulates the transport of neutrons using the Monte Carlo method. One of the main objectives of IRSN is to provide a user-friendly code that has undergone an extensive validation. The code allows users to model complex three-dimensional geometrical configurations, use various evaluations and nuclear data processing to describe the materials, select the best adapted simulation method for neutron transport and define tallies. The configuration is described through an ASCII file containing several blocks that correspond to material compositions, geometry modeling, simulation parameters and desired outputs. These blocks are defined with a flexible format making the final input data easily readable by any users.

Initially designed to perform criticality calculations to support criticality safety assessments, releases 4 and 5 of the MORET code are a fundamental part of the “standard route” of the French criticality calculation package CRISTAL V1 [1] and V2 [2] since it oversees the multigroup criticality calculation path thanks to a coupling with APOLLO2 cell code [3]. IRSN also developed a continuous route for MORET 5 to perform reference criticality calculation for the safety assessment. The continuous and multi-group routes of MORET are developed and validated by IRSN.

This paper presents the new functionalities and the main changes brought to release 6 of the MORET code compared to release 5. For a description of the existing functionalities in MORET 5, readers may refer to [4]. The first section introduces the main evolutions of the code, notably the addition of an analog fixed source calculation mode. The next section addresses the geometry aspect of MORET 6, which now handle tracking within random media. Another improvement is the MORET 6’s capacity to utilize alternative geometry engines besides the default one provided with MORET. The third section details new features only available in the criticality mode. First, in addition to the continuous-energy sensitivity

* Corresponding author: wilfried.monange@irsn.fr

coefficient calculation already available in MORET 5, MORET 6 now handle the multigroup-energy sensitivity coefficient calculation. The second modification involves a complete rewrite of the fission matrix calculation to improve its use with large systems (power reactor for example). Finally, minor modifications have been added to the output of MORET 6 in both criticality and analog fixed source modes to enhance modeling design and users verification.

2 Analog fixed source calculation

Until release 5, all developments of MORET focused on criticality calculations. However, in recent years, IRSN has shown an increasing interest in analog fixed source calculation. Among the fields concerned are the so-called nuclear neutron noise methods (also known as zero power neutron noise). These methods are now extensively used in various fields, including the validation of nuclear data through subcritical experiments, the characterization of fissile materials (in waste drums for example), etc. Another area of interest is the detailed study of the neutron population in reactors, where temporal and spatial correlation phenomena (commonly referred as "clustering") have recently been demonstrated [5]. The most straightforward way to accurately study the evolution of neutron population over time is to perform analog fixed source calculations. This type of calculation aims at simulating the life of neutrons in the most realistic manner, from their birth to their death, without employing variance reduction techniques, and necessitates careful management of the time dimension. The following sections present the main modifications of the code.

2.1 Neutron source

At the root of any fission chain is a source event that generate neutrons. Currently, MORET 6 provides source events of two types: spontaneous fission and external neutron source. In the first case, MORET 6 uses the characteristics of the material where spontaneous fission occurs to configure the fission process (which is described later). In the second case, the user defines the energy spectrum to be used. Regardless of the source type, users can also specify a set of spatial and time distributions. For specific needs, users can define initial neutrons sources in a file. This file can also be generated by MORET 6 at the end of a calculation.

2.2 Simulation modes

To address various user requirements and the very different behavior of the neutron population between negative and positive reactivity, MORET 6 handles two simulation modes named "sequential" and "chronological".

In the sequential simulation mode, histories (i.e. all the neutrons emitted by the source event and their progeny induced by fissions) are simulated one after another. To properly work, the sequential mode assumes that all histories end, i.e. that the system's reactivity is negative. However, for positive reactivity system, at least one of the fission chains may be infinite and subsequent histories will not be simulated. To address this issue, users may opt for the chronological simulation mode.

The purpose of the chronological simulation mode is to respect the "real" chronology to some extent. The time interval of source events is divided into time bins of equal length. MORET 6 simulates time bins one after the other, i.e. only those portions of histories that

belong to the current time bin are simulated. An unfinished history at the end of a time bin is paused and continued when MORET 6 simulates the next time bin. Within a time-bin, the algorithm is like the sequential algorithm. Conditions based on physical criteria (maximum rate of induced fission for example) or computer-oriented criteria (such as memory use) are available to prematurely halt the simulation.

2.3 Fission process

Since the fission process must be simulated as realistically as possible in the analog fixed source mode, the management of these processes differs from that used in the criticality mode of MORET and relies on the LLNL Fission Library [6]. This library allows for the simulation of neutrons from both spontaneous and induced fission. Neutron characteristics are derived from statistical sampling of distributions based on a combination of measured data and analytical models. This library also includes the Fission Reaction Event Yield Algorithm (FREYA) that allows the creation of fully correlated fission neutron for the most common isotopes.

For both spontaneous and induced fissions, IRSN added two options to the available parameters of the LLNL Fission Library multiplicity distribution:

- the use of the Terrel approximation;
- the use of random rounding of the average number of neutrons produced by fission, as employed in criticality calculation.

Only for the induced fission, an additional option has been incorporated to allow the sampling of the energy, velocity and direction cosines using the same energy distributions from the ACE cross-sections libraries as those used for a criticality calculation.

The management of delayed neutron remains the responsibility of MORET as the LLNL Fission Library does not handle them. The following simplified model of delayed neutron is used:

- At most one delayed neutron can be emitted by fission event;
- No correlation between delayed neutron emission probability and the number of prompt neutrons;
- The emission direction is assumed to be isotropic.

2.4 Outputs

The main output of MORET 6 analog fixed source mode is the NTRAC file, which contains complete characterization of all events (such as time, position, energy, family relationship, etc.) in either a text file (CSV type) or binary file. To be recorded, events must satisfy an event filter, i.e. specific conditions that an event must satisfy. Eventually, users can also specify a history filter; in that case, only events that satisfy both the event filter and belong to histories meeting the history filter are recorded. Both filters are defined using the following elements:

- The locations of the event(s),
- The isotopes involved,
- The reactions type (spontaneous fission, induced fission, diffusion, etc.).

In addition to the NTRAC files, several output files record in real time the characteristics of the simulation (such as fission chain length, reactivity estimation, fission multiplicity, etc.). Dedicated output files for the sequential mode (providing information by history) and chronological mode (providing information by time step) are also available.

2.5 Validation

For the analog fixed source mode, the list of observables to be considered is not as well-defined as for the criticality mode (where the main observable is the k_{eff}) since the basic objective of an analog fixed source code is to perform a realistic simulation of the neutron population behavior. However, different observables can be computed with analog fixed source simulation and depends both on user objectives and configuration reactivity. For the validation of MORET 6's analog fixed source mode, the following three reactivity ranges have been distinguished: subcritical, critical and delayed supercritical configurations since they focus on different observables. Prompt supercritical configurations have not been retained as they deemed unnecessary.

The sub-critical domain has been validated using three neutron noise benchmarks of the Los Alamos National Laboratory and one of the Lawrence Livermore National Laboratory. The LANL benchmarks consist of a plutonium sphere surrounded with variable thickness of reflectors. The reflector materials were nickel for the BeRP Nickel benchmark [7], tungsten for the BeRP Tungsten benchmark [8] and a mix between copper and polyethylene for the SCR α P benchmark [9] as illustrated in **Figure 1**. The k_{eff} range from about 0.77 to about 0.94. The LLNL benchmark, called ISSA [10], is composed of a variable number of uranium assemblies inside a water pool, as illustrated in **Figure 1**. For this benchmark, the highest k_{eff} was equal to about 0.95 (9 assemblies).

Neutron detectors with coincidence capabilities were used to measure noise observables such as the single counting rate R_1 (i.e. number of detections per second) and the double counting rate R_2 (i.e. rate at which two neutrons coming from the same fission chain are detected). For all configuration MORET 6 gives consistent and satisfactory results with the measured data. For illustration, **Figure 2** shows a comparison of R_1 and R_2 measured with the IRSN MORET 6 results and the LANL MCNP 6 results for all SCR α P benchmark configurations. The nuclear data library used was ENDF/B7.1. To simulate this benchmark, a detailed modeling has been used and the sequential mode has been used for the MORET 6 simulation. These results have been extracted from [9].



Figure 1. Left picture: SCR α P benchmark during assembly, the plutonium sphere is in the center and surrounded with polyethylene (white layers) and copper (gold layers) shells. Right picture: ISSA benchmark with all available assemblies.

Regarding reactivity levels close to criticality, an experiment has been carried out in 2019 with the Reactor Critical Facility of the Rensselaer Polytechnic Institute, focusing on the neutron population fluctuations and on time and spatial neutron correlations. Intensive calculations with MORET 6 using both chronological and sequential modes have been performed. Multiple observables, as well as raw neutron population behavior, have been calculated and compared with experimental measurement, demonstrating a perfect

agreement. The experiment, the MORET 6 results and a theoretical analysis of the results are presented in reference [5].

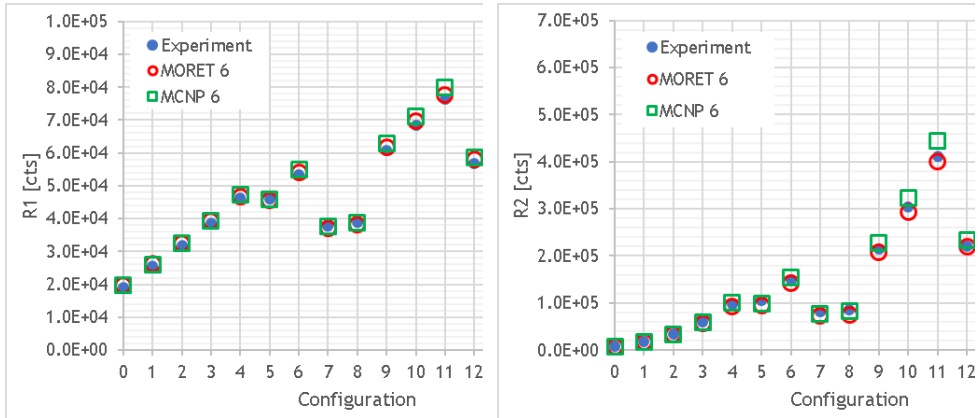


Figure 2. Comparison of R_1 (left) and R_2 (right) between measured data (filled point), MORET 6 calculations (circle) performed by IRSN and MCNP 6 calculation (square) performed by LANL for each configuration of the SCR α P benchmark.

Regarding configurations with a positive reactivity, calculations have been performed to simulate the GODIVA experiment [11]. The reactivity equals $\rho / \beta_{\text{eff}} = 0.7$. Comparisons were made on the pulsation and on the average time to reach a fission rate equal to $2.7 \cdot 10^{11}$ fissions/seconds. A total of 6000 calculations have been performed with MORET 6 using ENDF/B7.1 library. Table 1, presenting the comparisons, shows slight disagreements between the experimental results and MORET 6 results. These disagreements must be softened by some experimental uncertainties. The intrinsic neutron source has been assumed to be equal to 46.22 spontaneous fissions per second only, whereas other values exist in the literature.

Table 1. Comparison between measured and calculated result of a GODIVA experiment.

Observable	Measured	MORET 6
Inverse of the period	0.57 s^{-1}	$0.52 \text{ s}^{-1} (\sigma = 0.02)$
Time to achieve $2.7 \cdot 10^{11}$ fission/seconds	$31.8 \text{ s} (\sigma = 4.58 \text{ s})$	$37.5 \text{ s} (\sigma = 7.3)$

The addition of the fixed-source analog mode has the collateral effect of extending MORET's validation process beyond the usual k_{eff} comparisons by enabling to verify the correct treatment of effective cross-sections by performing comparisons with the OpenMC [12] (release 0.14.0) code. This involves comparing the spectrum of collision rates obtained from both OpenMC and MORET6 using a neutron source and a very simple geometry: A mono-energetic neutron source is placed at the center of a sphere containing a single isotope. The concentration of this isotope is adjusted to achieve a collision rate close to one collision per neutron source. Several energies ranging from a few keV to 10MeV have been tested. All isotopes in each library (including thermal nuclear data) are tested separately. The libraries tested are JEFF33, ENDF/B7 and ENDF/B8. The nuclear data used for both codes (ACE file for MORET6 and MD5 files for OpenMC) are consistent across nuclear libraries. The results obtained show only small differences for isotopes that are rarely used.

3 Improvement of geometry engine

3.1 Random media

The capability to transport the neutrons within random media is useful to calculate observables (k_{eff} , β , α , neutron noise values, etc.) for configurations with pieces of fissile material randomly distributed. The most common applications include fuel degradation during and after a severe accident, waste tank assessment, fuel dissolution, fuel fabrication process (e.g. during the mixing of UO_2 powder and additives), etc.

A random medium consists of many volumes, each with its own dimensions. The use of a regular lattices – such as the one available within MORET - is then impossible and modeling each volume individually poses a challenging task for users and could significantly slow down the neutron tracking. Thus, the geometry engine of MORET 6 code has been extended to specifically supports neutron tracking in random media. Since this modification only impacts the geometry engine, this feature is available for both critical and analog fixed source mode. According to [13], there are various ways to represent random media. However, due to its ease of implementation and good performance, the Poisson-box tessellation method has been chosen for the random media representation in MORET 6.

To use this feature, users simply define volumes of the geometry to be filled by one or more random media. A volume defined as a random medium is divided into several cells. Each cell is associated with a single chemical medium. The randomness of the media comes both from the distribution of the planes and the assignment of the chemical media to all cells. The splitting of cells is done with planes perpendicular to the three axes, which produces a non-regular non-conform rectangular lattice. The distance between two successive planes is governed by a Poisson process. User can adjust:

- The volume proportions of each of the chemical media in the random medium;
- The tolerance of these proportions;
- The density of the Poisson process, indicating the average number of cells per unit length.

Figure 3 shows the principle of the construction of the geometry. The algorithm starts by generating the positions of the planes according to a Poisson process. This determines the dimensions, volumes proportion and positions of each cell in the Poisson lattice. Then, a preliminary check assesses if the geometry will inevitably lead to a violation of the by the user-requested proportions. If this check fails, a new geometry is generated (maximum 1000 times). An algorithm is then used to associate a chemical medium to each cell. If the proportions are not within the tolerances, the process is repeated up to 1000 times.

Within a random medium, neutron tracking is optimized in the same way to a standard lattice with a regular pitch. When the neutron enters the random medium, the entry cell is determined by dichotomy. When the neutron exits a cell, knowledge of the exit face of this cell allows direct determination of the neighboring cell it enters. The management of random media is an integrated part of the geometry (not an overlay). Thus, a volume containing a random medium can undergo most of the geometric operations available in MORET, such as intersection, overwriting, rotation, etc. **Figure 4** shows a model created using MORET 6, illustrating a hypothetical fuel melt of a reactor.

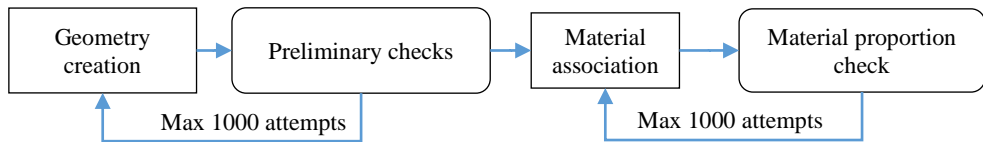


Figure 3. Principle of algorithm for creating the random medium.

Since the constructed geometry remains fixed during the calculation, users have de flexibility to perform many simulations of unique realization of the random geometry to assess the distribution of calculate observables (k_{eff} , etc.).

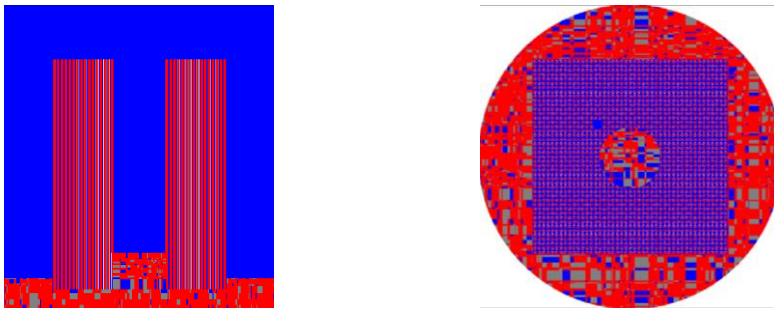


Figure 4. Modelling with MORET 6 of a fuel melt of a reactor.

For the validation of the randomized geometry, MORET 6 produces the equivalent geometry as if each cell of the random media had been modelled with boxes in a dedicated output file. IRSN also participated – with MORET6 - in a NEA work aiming at comparing various random geometry models [14].

3.2 Coupling to other geometries

MORET 6 is now enabled to be coupled with other geometric engines. Having the possibility to switch from one geometric engine to another provides multiple advantages:

- avoiding the conversion step from another code input to a MORET 6 input;
- offering to users the possibility to describe the geometry with the best geometric engine (combinatory-based, surface-based, etc.).

To achieve this feature, the geometry engine is now an independent module. The API (application programming interfaces) has been designed so that MORET 6 does not need to know the specificities of a geometry engine.

A side effect of the generalization of the geometry engine, is that the volume selection mechanism of MORET 5, which is too specific to its own geometry, has to be replaced in MORET 6 with a more generic one based on regular expressions.

To validate the implementation of this API, MORET 6 has been coupled with the geometry engine of the ROOT framework [15]. An significant issue of ROOT is the lack of reflection operator. To address this, MORET 6 allows to define - in case of a ROOT geometry

- the creation of faces defined as the interface between two volumes. The created faces are then used for reflection as for a MORET 6 geometry.

4 Criticality calculation

4.1 Multigroup sensitivity coefficients

Since release 5.C.1, the MORET code supports the calculation of continuous energy sensitivity coefficients [16] for the following quantities: total, elastic scattering, total inelastic scattering, fission, total capture and radiative capture cross sections, average number of neutron produced by fission, scattering cosine distribution and fission spectrum. These coefficients and their corresponding standard deviations are provided per material, per isotope, per reaction based on a user-defined energy binning. The new release of MORET extends this feature to multigroup cross sections with the same technical choices as for the continuous energy calculations [17, 18, 19, 20]:

- Use of the differential operator;
- Sensitivity coefficient of first order;
- Use of the estimation of the adjoint source (estimation of the fission source derivatives);
- Sensitivity of material composition only.

In the framework of multigroup energy, a sensitivity coefficient is the result of the sum of explicit and implicit components [21]. Explicit terms refer to parameters appearing explicitly in the multigroup neutron-balance equation, whereas implicit terms refer to perturbations in the resonance self-shielded cross sections. Currently, for sensitivity coefficients calculation, MORET relies on APOLLO2 self-shielded cross sections and thus does not consider the implicit part.

The verification of this new feature is carried out through a comparison between the sensitivities obtained with the continuous cross section treatment of MORET 6.

4.2 Fission matrix

Previously, the calculation of the fission matrix was rarely used with earlier releases of MORET. However, in response to the demand for more sophisticated configuration studies, particularly in nuclear power reactors, the fission matrix calculation has undergone a complete redesign. In MORET 5 the discretization of the fission matrix was limited to the fissile volumes, which makes the data set description and the results interpretation quite complicated for users. Now, in MORET 6, it is possible to use a cartesian mesh such as it is available in most Monte-Carlo codes.

Another improvement concerns improved estimation of the uncertainties of eigenvalues and eigenvectors. Indeed, the technique used in MORET 5 consisted simply in generating 1000 fission matrices and computing for each of them the eigenvalues and eigenvectors and then deducing the uncertainty. This process has limitations since it wrongly assumes that each term of the matrix follows an independent normal distribution (while terms within a same column are correlated). MORET 6 now uses an algorithm [22] based on the fact that at first order a variation of the eigenvalue and the eigenvector is related to their derivative with respect to each term of the fission matrix. This way of working requires computing the variance-covariance matrix of the terms of the fission matrix. All these matrices are stored in memory with a "compressed sparse column" representation in order to limit the memory usage of MORET 6. Finally, users can also choose to perform the filling of the fission matrix

using one of the three estimators available (track-length, collision or absorption) as one estimator may outperform the others depending on the configuration.

5 Output

5.1 Geometry plotting function

MORET 5's plotting system was only vector-based: the code calculates the intersection between the volumes and the visualization plane and then creates 2D shapes that are written to a PostScript file. However, this way of proceeding is not compatible with all geometric engines. Thus, it is now possible to request "raster" type plotting (i.e. built from pixels). The principle is based on the scanning of rays included in the section plane. By using the neutron tracking system (contrarily to former vector-based graphics) the resulting graph is a faithful representation of the geometry "really" considered by the code during neutron tracking. The plots can be drawn with a horizontal or vertical scan of the rays and in one of the two ways (left/right, up/down), resulting therefore in four ways to draw a graphical section, all of which must be consistent. This principle is used in the MORET 6 verification process to ensure that the tracking engine accurately "sees" the same geometry in both directions.

5.2 Volume calculation

MORET 6 also integrates the calculation of volumes. The principle is based, as for the "raster" graphic sections, on the scanning of rays within a space defined by the user. As for the "raster" type plotting, calculations are performed for both directions and both ways and consistency of the four values are checked in the verification process of MORET 6 to ensure that the tracking engine "sees" the same geometry in both directions and in both ways.

This volume calculation capability has been coupled with the score manager so that users can request MORET to produce score volume normalized by cubic centimetres.

6 Conclusions

The new release of MORET introduces new capabilities that underwent continuous testing during development. Initially designed for criticality calculation, these new features enhance the MORET code criticality capabilities with multigroup sensitivity coefficient calculation, new fission matrix calculation algorithm, and the possibility to simulate randomized geometry. The major evolution of MORET code is the possibility to perform analog fixed source simulations. MORET 6 results on neutron noise benchmarks show a good agreement with experimental values. Consequently, IRSN will continue experimental validation of MORET 6 and will use the analog fixed source simulations for safety-relevant applications. Finally, multiple features have been added in order to improve the use of MORET code: enhancements for creating and checking input data, option to utilize other geometric engine and additional output capabilities. A MORET 6 code license can be requested from IRSN (email to M. W. Monange).

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