Preliminary results on Case R1 using various sources sampling methods

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Content

MORET as a numerical laboratory to test cross-cutting uses of the basic parameters defining different algorithms implemented in MC codes
- Overview of Sampling Techniques (ST): a new way to build his own sampling technique
- Overview of Tracking Methods (TM)
- Overview of Convergence Tests (CT)
- Overview of $K_{eff}$ Estimators (KE)

Building a numerical experimental design => list of all configurations cases launched for the benchmark case R1

Preliminary $K_{eff}$ results

Preliminary flux and fission rates results

Trends / First observations
- The question is: Is there a best mix in STxTMxCTxKE use to ensure a good react rates cv?

Future work
Samp. Tech. available in MORET: a new way to build his own sampling technique

- These methods differ only in their way of obtaining the source distribution of a new cycle => The aim is to converge from an arbitrary distribution of sources towards the true distribution of the problem => It could be interesting to mix them => paper J. Miss & O. Jacquet (MC2000)

- What is hidden behind the well known method? NATU, STRA, MKIJ, IMPO, SUPH, WIEL

- What is common between these techniques?

- An additional technique: OVERsampling

- A new one totally PARAmeterised and allowing to reproduce all the other and to highlight their real differences
Brief overview of each technique (extract of new MORET5 manual)

MORET 5 code has several (mutually exclusive) methods to perform the iteration of sources at each cycle (associated keyword in parentheses):

- The analog method (**NATURAL**), which is the default method used by the MORET code. The history of a source neutron is limited to the events specific to its generation, and ends either in absorption or a leak. This means that one step of the simulation corresponds to a single generation,

- The Stratified Sampling method (**STRAtified**), which applies certain improvements to the analog method by ensuring that each fissile set is visited at each cycle,

- The fission matrix method (**MKIJ**), which is a variant of the Stratified Sampling method, using the properties of the fission matrix to determine the distribution of the source neutrons,

- The importance method (**IMPOrtance**), which is a variant of the Stratified Sampling method, using the properties of the adjoint fission matrix to determine the distribution of the source neutrons,

- The Super History method (**SUPHistory**) which, unlike the above methods, can simulate the progeny of the source neutrons over a defined number of generations within one cycle,

- The Wielandt method (**WIELandt**), which is similar to the **SUPHistory** option, but in which the number of generations considered depends on a simulation parameter and is locally modulated by the reactivity of each fissile volume,

- The oversampling method (**OVERsampling**), which is used to adapt the number of source neutrons emitted in each fissile set in order to reduce the uncertainty on \( K_{\text{eff}} \), by oversampling the fissile sets with a high variance in production per source neutron,

- The configurable method (**PARAmeterised**): as its name suggests, this method has a set of parameters so that it can not only reproduce each of the other methods, but also combine their particular features.
<table>
<thead>
<tr>
<th>Event at which sites are created</th>
<th>KENO</th>
<th>MCNP</th>
</tr>
</thead>
<tbody>
<tr>
<td>number of sites created</td>
<td>$n = \text{INT}(W(i) + \xi)$</td>
<td>$n = \text{INT}(W(i) + \xi)$</td>
</tr>
<tr>
<td>$W(i) = \frac{\Sigma t}{\Sigma t + \Sigma a}$</td>
<td>$W(i) = \frac{\Sigma t}{\Sigma t + \Sigma a}$</td>
<td></td>
</tr>
<tr>
<td>$\xi$: random number</td>
<td>$\xi$: random number</td>
<td></td>
</tr>
<tr>
<td>sites weight</td>
<td>$W(i)/n$</td>
<td>$W(i)/n$</td>
</tr>
<tr>
<td>starters number</td>
<td>constant number $M_0$</td>
<td>constant total weight $M_0$</td>
</tr>
<tr>
<td>starters sampling algorithm</td>
<td>if more than $M_0$ sites, site bank sampled without replacement for $M_0$ starters (sites may be used more than once) if exactly $M_0$ sites, each site used once if less than $M_0$ sites, all sites used, and starters randomly sampled without replacement to get the rest of the starters</td>
<td>if more than $M_0$ sites, all the sites are used</td>
</tr>
<tr>
<td>starters weight</td>
<td>$1$</td>
<td>$1$</td>
</tr>
<tr>
<td>$W(i)/n$</td>
<td>$W(i)/n$</td>
<td></td>
</tr>
</tbody>
</table>

**Note:** $W(i)$ represents the probability of fission in each volume $V$, $M_0 = \text{INT}(P_m)$, $P_m$ is the probability to pick a site is proportional to its weight (sites may be used more than once), the weights of all starters are multiplied by the same correction factor so that the total weight of all starters is equal to $M_0$. **EGSC**
Selected remarks to show the various origins allowing to explain different simulation behaviors

- All of the methods available in the MORET code use the stratified sampling of sources, except the **PARAMeterised** method when the **STRAtification** option is not requested. The stratified sampling of sources means that instead of sampling the source neutrons of a cycle from all the source neutrons stored in the source neutron bank during the previous cycle, sampling is performed for each set of fissile volumes, maintaining the proportion of source neutrons to be emitted in each fissile set, so that the sample of source neutrons obtained is as representative as possible of the contents of the bank.

- A certain number of methods are designed to ensure that each fissile set is visited at each step: This applies to **STRAtified**, **MKIJ**, **IMPOrtance**, **OVERsampling** and **PARAMeterised** with the **STRAtification { FRNN / FREV / FEVA / OVERsampling }** option. This means:
  - that the user must place at least one source neutron in each fissile set during the description of the initial sources,
  - that the code ensures that there is always at least one source neutron in each set during the subsequent steps. This imposes the choice of the track length estimator for production in the fissile sets.
Selected remarks: differences in sources sites

The simulation methods also differ in the number of generations simulated within a cycle of the Monte Carlo calculation:

- For most of the methods (NATUral, STRAtified, MKIJ, IMPOrtance and PARAmeterised with NGEN parameter equal to 1, which is the default parameter), a cycle comprises exactly one generation, i.e. progeny (neutrons produced by fission) are not simulated in the same step as the source neutron.

- On the contrary, for certain methods (SUPHistory, WIELandt and PARAmeterised with NGEN parameter different from 1), a cycle includes several generations, meaning that the progeny (neutrons produced by fission), up to a limit generation, are simulated within the same cycle as the source neutron. To prevent an exponential increase or decrease in the number of progeny over the generations of the step, the number of neutrons produced is normalised to the last estimate of $k_{eff}$ (during the very first step, this value equals 1 by default, but it can be modified using the keyword KINI of SIMUlation).

According to the method, the sites where progeny are produced are:

- **collision sites** (PARAmeterised method with DESCendants parameter equal to 1),
- Sampled on a **track length** (elementary displacement between collisions) (PARAmeterised method with DESCendants parameter equal to 2),
- **Absorption** (SUPHistoire, WIELandt, and PARAmeterised methods with DESCendants parameter equal to 3).
XI.1.1 NATUral Method

The analog power iteration method for fission sources is the option used by default. It is however possible to specify its use via the keyword NATUral, to be placed in the SIMUlation block with the following syntax:

```plaintext
NATUral
```

Note: NATUral Method

The NATUral method is the simplest of all the power iteration methods implemented in the MORET 5 code. It reveals certain insufficiencies, which can be problematic in certain specific cases, and for which the other, more elaborate methods, attempt to compensate.
XI.1.2 STRAtified Method

The Stratified Sampling method is a variant of the analog method that can prevent the fissile sets from being deserted during the simulation.

The following modifications, concerning the method of re-sampling neutron sources in the subsequent cycle, have been introduced with respect to the **NATUrAl** method:

- **The user must place source neutrons in each of the fissile sets.**
- The *track length* estimator is used to estimate the neutron production in each fissile set.
- The number of source neutrons to be emitted in each fissile set is never zero. When the real number $X_{NS}$ of source neutrons to be emitted in the set should be less than 1, a source neutron is generated with a weight equal to $X_{NS}$.

The key word **STRAtified** must be placed in the **SIMUlation** block. Its syntax is as follows:

```
STRAtified
```
XI.1.3 MKIJ Method

The Fission Matrix method is a variant of the STRAtified method (see Section XI.1.2, p. 262) aiming to accelerate the convergence of the sources towards the physical distribution.

The keyword MKIJ must be placed in the SIMUlation block. Its syntax is as follows:

\[
\text{MKIJ freq}
\]

where

- freq is the frequency (number of cycles) of use of the eigenvector of the Kij matrix. Order of magnitude: \( freq \approx 10 \).

\[\text{Note: Restriction:}\]

Like the STRAtified method, the MKIJ method requires at least one neutron to be positioned by the user in each fissile set.
XI.1.4 **IMPOrtance Method**

The Importance method is a variant of the Stratified Sampling method (see Section XI.1.2, p. 262) aiming to accelerate the convergence of the sources towards the physical distribution.

The keyword **IMPOrtance** must be placed in the **SIMUlation** block. Its syntax is as follows:

```
IMPOrtance  freq
```

where

- `freq` is the frequency (number of steps) of updating of the eigenvector of the Kij adjoint matrix. Order of magnitude: `freq ≈ 10`.

**Note: Restriction:**

*Like the Stratified Sampling method, the Importance method requires at least one neutron to be positioned by the user in each fissile set.*
XI.1.5 OVERsampling Method

The oversampling method (OVERsampling) is a variant of the stratified sampling method (see Section XI.1.2, p. 262), which is used to adapt the number of source neutrons emitted in each fissile set in order to reduce the uncertainty on $k_{\text{eff}}$, by oversampling the fissile sets with a high variance in production per source neutron.

Without biasing the proportion of source neutrons to be emitted in each fissile set, but by modifying the weight of source neutrons, the method generates more source neutrons in the fissile sets where neutron production is high according to the simulated history. Splitting is used when the weight of neutrons in each set can be significantly different.

The keyword OVERsampling must be placed in the SIMUlation block. Its syntax is as follows:

```
OVERsampling
```

**Note: Restriction:**

Like the Stratified Sampling method, the Oversampling method requires at least one neutron to be positioned by the user in each fissile set.
XI.1.6 SUPHistory Method

The super-history method (SUPHistory) is a simulation method used to track a source neutron and its progeny over a limited number of generations within a cycle, in order to avoid recalculating source distribution at each generation.

The keyword SUPHistory must be placed in the SIMUlation block. Its syntax is as follows:

```
SUPHistory L
```

where

- L is the limit number of generations that will be simulated per 'super-history'. Order of magnitude: L ≈ 10.

The SUPHistory method is distinct from the NATUral, MKIJ, STRAtified and IMPOrtance methods on the following points:

- Refer to the MORET5 manual
I.1.1 **WIELandt Method**

The Wielandt Method (**WIELandt**) is a simulation method that improves the quality and stability of source convergence in slowly converging systems.

The Wielandt method is used to handle a modified problem where the inverse eigenvalues are offset by the same constant without any change to the eigenfunctions (distribution of sources associated with the eigenvalues).

The syntax of the **WIELandt** keyword is as follows:

```
WIELandt  delta_aimed
```

where:
- `delta_aimed` refer to MORET5 manual

---

The **CVSP** option is used to modify the period of convergence of the parameter $\Delta = k_e - k_{eff}$ towards the desired value.

The syntax to be used is as follows:

```
CVSP  period_cv
```
A totally generic approach to build its sampling technique

The syntax of the PARAmeterised

PARAmeterised

[ FISSion esti_F ]
[ DESCendant esti_D ]
[ NGENeration n_generation ]

STRAtification

[ FRNN ]
[ PRODuction esti_P ]
[ FREV freq_FREV ]
[ FEVA freq_FEVA ]
[ OVERsampling ]

WIELandt delta_aimed
[ CVSP period_cv ]

- **FISSion** is used to specify the estimator to be used to determine the fission sites (esti_F = 1 for collision, 2 for track length and 3 for absorption). By default, esti_F = 1.
- **DESCendant** is used to specify the estimator to be used to determine the sites where progeny are produced following fission (esti_D = 1 for collision, 2 for track length and 3 for absorption). By default, esti_D = 1. This option is usable only if n_generation ≠ 1.
- **NGENeration** is used to specify the maximum number of generations per cycle. n_generation = 0 signifies an unlimited number of generations. By default, n_generation = 1.
- **STRAtification** is used to activate the source stratification option (deactivated by default). The distribution of sources in each fissile element respects the fraction of source neutrons calculated according to the various options available inside STRAtification. This option uses the fissile sets defined by DFIS (Section XI.4, p. 275) or, by default, considers each fissile volume as a distinct set.
  - **FRNN** (Nonzero Fraction) ensures at least one source neutron in each fissile set at each cycle (disabled by default).
  - **PRODuction** is used to specify the estimator to be used to estimate the production in each fissile set for the calculation of the fraction of sources to be emitted in each set (esti_F = 1 for collision, 2 for track length and 3 for absorption). By default, esti_P = esti_F.
  - **FREV** is used to specify the frequency of use of the eigenvector of the fission matrix to determine the fractions of sources in fissile sets (disabled by default); freq_FREV is the number of cycles between two uses of the fission matrix eigenvector.
  - **FEVA** is used to specify the frequency of updating of the eigenvector of the adjoint fission matrix used to estimate the production in each fissile set based on the importance values (disabled by default); freq_FEVA is the number of cycles between two updates of the adjoint fission matrix eigenvector.
  - **OVERsampling** is used to activate the oversampling of source neutrons: The fraction of sources in a fissile set increases with increasing variance of the production per history in this set (disabled by default). Without biasing the proportion of source neutrons to be emitted in each fissile set, but by modifying the weight of source neutrons, this method generates more source neutrons in the fissile sets where neutron production is high according to the simulated history. Splitting is used when the weight of neutrons in each set can be significantly different.
- **WIELandt** is used to deploy the Wielandt method (described in Section XI.1.7, p. 267).

The various options in STRAtification can be combined.
It is obviously possible to obtain all of the simulation methods using the PARAmeterised option.

- For the Analog method:

- For the Stratified Sampling method:
- For the Fission Matrix method:
  
  \[ MKIJ \ n \]
  
or
  
  \[
  \begin{array}{l}
  \text{PARA} \\
  \quad [ \text{FISS 1} ] \\
  \quad [ \text{NGEN 1} ] \\
  \quad \text{STRA} \\
  \quad \quad [ \text{PROD 2} ] \\
  \end{array}
  \]
  
  Nature of the fission sites (unnecessary): 1 (= collision) by default
  
  Number of generations (unnecessary): 1 by default
  
  Production estimator (unnecessary): if not specified, 2 (= track length)
  
  when there must always be sources in each fissile set
  
  \[ \text{FREV} \ n \]

- For the Importance method:
  
  \[ \text{IMPO} \ n \]
  
or
  
  \[
  \begin{array}{l}
  \text{PARA} \\
  \quad [ \text{FISS 1} ] \\
  \quad [ \text{NGEN 1} ] \\
  \quad \text{STRA} \\
  \quad \quad [ \text{PROD 2} ] \\
  \end{array}
  \]
  
  Nature of the fission sites (unnecessary): 1 (= collision) by default
  
  Number of generations (unnecessary): 1 by default
  
  Production estimator (unnecessary): if not specified, 2 (= track length)
  
  when there must always be sources in each fissile set
  
  \[ \text{FEVA} \ n \]
- For the Oversampling method:
  
  **OVER**
  
  or
  
  **PARA**
  [ FISS 1 ]
  [ NGEN 1 ]
  STRA
  [ PROD 2 ]
  **OVER**

  Nature of the fission sites (unnecessary): 1 (= collision) by default
  Number of generations (unnecessary): 1 by default
  Production estimator (unnecessary): if not specified, 2 (= track length)
  when there must always be sources in each fissile set

- For the Super-History method:
  
  **SUPH n**
  
  or
  
  **PARA**
  FISS 3
  [ DESC 3 ]
  NGEN n
  STRA
  [ PROD 3 ]

  Nature of sites where progeny neutrons are produced (unnecessary): if not specified, it is the same estimator as for potential fission sites
  Production estimator (unnecessary): if not specified, it is the same estimator as for potential fission sites
For the Wielandt method:

\[ \text{WIEL \ delta\_aimed} \]

or

\[ \text{PARA [ FISS 1 ] DESC 3 NGEN 0 STRA [ PROD 1 ] WIEL \ delta\_aimed} \]

Nature of the fission sites (unnecessary): 1 (= collision) by default

Production estimator (unnecessary): if not specified, it is the same estimator as for potential fission sites
Overview of Tracking Methods (TM): **Conventional / Woodcock**

Overview of Convergence Tests (CT): Normality test based on the **Lilliefors** or **KHI2** to add Shannon entropy

Overview of Keff Estimators (KE)

**Source-type k\textsubscript{eff} estimators**

The \( k\text{eff} \) for the current cycle is equal to the number of neutrons produced in the system during the cycle, normalised to a source neutron.

The mean \( k\text{eff} \) is the arithmetic mean of the \( k\text{eff} \) values per cycle.

The code calculates three source-type \( k\text{eff} \) estimators:

- Collision-source,
- Track length-source,
- Absorption-source,

based on the collision, track length, and absorption estimates respectively of the production rates in all of the fissile volumes.
Balance-type $k_{\text{eff}}$ estimators

The step $k_{\text{eff}}$ is equal to the number of neutrons produced in the system during the cycle (normalised to one source neutron) divided by the neutron balance for the cycle (normalised to one source neutron).

Given that a neutron (and the excess neutrons it generates) ends up either absorbed or escaped, the neutron balance is defined as the sum of the absorption and leakage rates, minus the excess rate, where all of these quantities are normalized to one source neutron. The neutron balance is said to be a control variable because it has a known expected value: its value is 1.

The mean $k_{\text{eff}}$ is the arithmetic mean of the $k_{\text{eff}}$ values per cycle.

The code calculates three balance-type $k_{\text{eff}}$ estimators:

- Collision-balance,
- Track length-balance,
- Absorption-balance,

from the collision, track length, and absorption estimates respectively of the production, absorption, and excess rates in all volumes and based on the leakage estimate.

An exception to the above must be stated with regard to the absorption-balance estimator: the absorption estimate of the excess rate is not legitimate (because the excess reactions are scattering reactions, not absorption), and is therefore replaced by the collision estimate of the excess rate.
**$k_{\text{eff}}$ estimators obtained by linear combination of estimators**

These different $k_{\text{eff}}$ estimators have the same means, but not the same standard deviation. Given that one estimator is not always better than the others (their performance depends on the configuration), new estimators are built from the previous ones, so that their variance is always less than the smallest of the individual variances. These new estimators are obtained by linear combination of different $k_{\text{eff}}$ estimators (and possibly some control variables: Variables with a known expected value), without affecting the mathematical expectation of the result.

From the tenth cycle, the MORET code systematically calculates the following:

- a linear combination of the three source-type estimators,
- a linear combination of the three balance-type estimators,
- a 'general' combination obtained from the three source-type estimators, from two balance-type estimators (collision and track length) and two control variables (the neutron balance estimated per collision and per path).
List of all configurations cases launched for the benchmark case R1

- Sampling Techniques (ST): NATU / STRA / IMPO 10 / MKIJ 10 / OVER / SUPH 5
  All usual techniques + OVER

- Overview of Tracking Methods (TM): Conventional (no Woodcock)

- Overview of Convergence Tests (CT): Lilliefors / KHI2

- Overview of Keff Estimators (KE): all

- Npart(=M) x Ncycles = 10^6

- Npart inactive = 10^7

- Npart = 100, 200, 500
  1000, 2000, 5000
  10000, 20000, 50000
Visual check of convergence tests: non conclusive
Visual check of $k_{eff}$ convergence curves: non conclusive
\[ \text{KEFF(btrack)} = \text{fct(sampling techniques)} \]

Inactive part = \(10^7\)
Active part = \(N\text{Part} \times N\text{Cycles} = 5 \times 10^6\)
\(\sigma < 0.00025\)

\[ M = 1 / \text{Npart} \]
\[ \text{KEFF} = fct(\text{keff estimator} \ ; \ \text{sampling techniques}) \]

Inactive part = \(10^7\)
Active part = \(N\text{Part} \times N\text{Cycles} = 5 \times 10^6\)

\(\sigma < 0.00025\)

\[ M = \frac{1}{N\text{part}} \]
Keff = fct(keff estimator ; STRA)

KEFF(bcoll) = fct(sampling techniques)

Inactive part = \(10^7\)
Active part = \(N_{Part} \times N_{Cycles} = 5.10^5\)
\(F < 0,00025\)

\(M = 1 / N_{part}\)
Flux in $220/221 = \text{fct(}\text{fixed rod, sampling techniques)}$
Flux in 220 / 221 = fct(fixed rod, sampling techniques)

Flux in Assembly(2,2,0) Core(2,2,1)
err ~1.5%
Fission rates in assembly 2 2 1 = (rods positionning, sampling techniques)

Fissions rates convergence (NATU) in one assembly, in different cells center of the core ($\sigma < 3\%$)
Flux in $2\,2\,0\,/\,4\,4\,1 = fct(\text{fixed rod, sampling techniques})$

Flux in Assembly(2,2,0) Core(4,4,1)  
err $\sim 1.5\% \,(0.00002)$
Flux in $220/671 = \text{fct(fixed rod, sampling techniques)}$

Flux in Assembly(2,2,0) Core(6,7,1)
err $\sim$3% (0.00001)
Observations / Additional work

- No time to perform a real deep analysis
- Need: several 100M part => qq B
- Work in progress
- Any advice / suggestion is welcome
- To be completed => planned for the EGAMCT report 1