Nuclear data uncertainty propagation with Monte Carlo methods

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All slides can be found at: 
NRG: a leading nuclear sector service provider
Over 50 years experience in nuclear technology
Over 400 employees (10 in R&D reactor physics and simulations)
Turnover approximately Meuros 60 / per year
High Flux Reactor, Hot Cell Laboratories and Radiological labs
Who are we?

Health - Medical Isotopes world-wide
What are nuclear data?

The term "nuclear data" can have different meaning,

- dusty books, constants, mature field, code inputs,
- list, Schrödinger equation, unexciting...
- but this is not! (I’m going to prove that)
Why are nuclear data important? (Part 1)

Better nuclear data can help for:

- safety margins, fuel storage,
- life-time extension,
- cost reduction in design of new systems,
- isotope production,
- safety of people (shielding),
- waste transmutation,
- development of future systems.

Better nuclear data have a limited effect on:

- current reactor operation,
- current reactor safety,...
- accident simulation,
- proliferation,
- Chernobyl, TMI, Fukushima.
Why are nuclear data important? (Part 2)

Source: World Nuclear Association Report
Nuclear data uncertainties: general comments

- Uncertainties are not errors (and vice versa),
- they are related to risks, quality of work, money, perception, fear, safety...

Uncertainty ⇔ safety ⇔ professionalism

True uncertainties do not exist! They are the reflection of our knowledge and methods.

All the above for covariances

The importance of nuclear data uncertainties should be checked. If believed negligible, please prove it!

Our motivation:

Any justification for not providing uncertainties should become obsolete
Our mission: improve nuclear simulations

- TALYS nuclear code
- T6 software package
- Library cloning and complement
- Original nuclear data library TENDL + covariances
- Uncertainty propagation (fast) TMC
- Optimum Search and find (Petten Method)
Control of nuclear data (TALYS system) + processing (NJOY) + system simulation (MCNP/ERANOS/CASMO...)

\[ \sigma_{total}^2 = \sigma_{statistics}^2 + \sigma_{nuclear
data}^2 \]

For each random ENDF file, the benchmark calculation is performed with MCNP. At the end of the \( n \) calculations, \( n \) different \( k_{eff} \) values are obtained.

TMC for nuclear data uncertainty propagation, what else?

- No covariance matrices (no 2 Gb files) but every possible cross correlation included,
- No approximation but true probability distribution,
- Only essential info for an evaluation is stored,
- No perturbation code necessary, only “essential” codes,
- Feedback to model parameters,
- Full reactor core calculation and transient,
- Also applicable to fission yields, thermal scattering, pseudo-fission products, all isotopes (...just everything),
- Other variants: AREVA (NUDUNA), GRS (XSUSA), CIEMAT (ACAB), PSI (NUSS), CNRS Grenoble..., based on covariance files,
- Many spin-offs (TENDL covariances, sensitivity, adjustment...)
- Computer time (not human time)
- QA.
- Needs discipline to reproduce,
- Memory and computer time (not human time),
- Need mentality change.
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[ \alpha_{\text{target}} \]

\[ \alpha_{\text{compound}} \]

\[ \alpha_v \]

\[ \Gamma_v \]

\[ \Gamma_n \]

\[ \Gamma_\gamma \]

\[ (n,2n) \] \( n = 1 \)

\[ (n,\gamma) \] \( n = 1 \)

Cross section (b)

Incident Energy (MeV)

Cross section (b)

Incident Energy (eV)

Number of counts/bins

\( E_n = 500 \text{ keV} \)

\( \theta_n = 61 \text{ deg} \)

\( E_n = 5.2 \text{ MeV} \)
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[ \alpha_{\text{target}} \]

\[ \alpha_{\text{compound}} \]

\[ \alpha_v \]

\[ \Gamma_v \]

\[ \Gamma_n \]

\[ \Gamma_\gamma \]

\[ (n,2n) \quad n = 2 \]

\[ (n,\gamma) \quad n = 2 \]

\[ \theta_n = 61 \text{ deg} \]

\[ E_n = 5.2 \text{ MeV} \]

\[ E_n = 500 \text{ keV} \]

\[ (n,\text{el}) \quad n = 2 \]

\[ (n,xn) \quad n = 2 \]
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[ a_{\text{target}} \]

\[ a_{\text{compound}} \]

\[ a_v \]

\[ \Gamma_v \]

\[ \Gamma_n \]

\[ \Gamma_\gamma \]

\[ \frac{d\sigma}{d\Omega} (b/\text{sr}) \]

\( E_n = 500 \text{ keV} \)

\( \theta_n = 61 \text{ deg} \)

\( E_n = 5.2 \text{ MeV} \)

\( n = 3 \)
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[ \alpha_{\text{target}} \]

\[ \alpha_{\text{compound}} \]

\[ \alpha_{\nu} \]

\[ \Gamma_{\nu} \]

\[ \Gamma_{n} \]

\[ \Gamma_{\gamma} \]

\[ a_{\text{target}} \]

\[ a_{\text{compound}} \]

\[ a_{\nu} \]

\[ \Gamma_{\nu} \]

\[ \Gamma_{n} \]

\[ \Gamma_{\gamma} \]

\[ (n,2n) \quad n = 4 \]

\[ (n,\gamma) \quad n = 4 \]

\[ \text{Cross section (b)} \]

\[ \text{Cross section (b)} \]

\[ \text{Energy (MeV)} \]

\[ \text{Number of counts/bins} \]

\[ \text{Cross section (b)} \]

\[ \text{Cross section (b)} \]

\[ \text{Cross section (b)} \]

\[ \text{Cross section (b)} \]

\[ \text{Incident Energy (MeV)} \]

\[ \text{Incident Energy (MeV)} \]

\[ \text{Incident Energy (MeV)} \]

\[ \text{Incident Energy (MeV)} \]

\[ \text{Cross section (b)} \]

\[ \text{Cross section (b)} \]

\[ \text{Cross section (b)} \]

\[ \text{Cross section (b)} \]

\[ \theta_n = 61 \text{ deg} \]

\[ E_n = 5.2 \text{ MeV} \]

\[ E_n = 500 \text{ keV} \]
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[ \alpha_{\text{target}} \]
\[ \alpha_{\text{compound}} \]
\[ \alpha_v \]
\[ \Gamma_n \]
\[ \Gamma_\gamma \]

\( \Gamma_n \) a compound a target \( \Gamma_\gamma \)

\begin{align*}
\text{Cross section (b)}
\end{align*}

\begin{align*}
\text{Cross section (b)}
\end{align*}

\( d^2\sigma/d\theta/dE \text{ (b/MeV/sr)} \)

\begin{align*}
\text{Number of counts/bins}
\end{align*}

\begin{align*}
\text{Number of counts/bins}
\end{align*}

\( k_{\text{eff}} \) value

\begin{align*}
\text{Number of counts/bins}
\end{align*}

\( \theta_n = 61 \text{ deg} \)

\begin{align*}
\text{Number of counts/bins}
\end{align*}

\( E_n \) = 500 keV

\begin{align*}
\text{Number of counts/bins}
\end{align*}

\( E_n \) = 5.2 MeV

\begin{align*}
\text{Number of counts/bins}
\end{align*}

\( n = 5 \)

\( n = 5 \)

\( n = 5 \)

\( n = 5 \)
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[ \Gamma_n \]

\[ \Gamma_\gamma \]

\[ a_{\text{target}} \]

\[ a_{\text{compound}} \]

\[ a_v \]

\[ \theta_n = 61 \text{ deg} \]

\[ E_n = 500 \text{ keV} \]

\[ E_n = 5.2 \text{ MeV} \]

\[ \sigma / d\theta (b/\text{s}) \]

\[ d\sigma / d\Omega (b/sr) \]

\[ d^2\sigma / dE d\Omega (b/eV/sr) \]

\[ k_{\text{eff}} \text{ value} \]

\[ n = 6 \]

\[ n = 6 \]

\[ n = 6 \]

\[ n = 6 \]

\[ n = 6 \]
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[ a_{\text{target}} \]

\[ a_{\text{compound}} \]

\[ a_v \]

\[ \Gamma_n \]

\[ \Gamma_{\gamma} \]
Hands on “1000 \times (Talys + ENDF + NJOY + MCNP) calculations”

\[ \alpha_{\text{target}} \]

\[ \alpha_{\text{compound}} \]

\[ \alpha_v \]

\[ \Gamma_n \]

\[ \Gamma_\gamma \]

TALYS \hspace{1cm} MCNP

\[ \frac{d\sigma}{d\theta} (b/sr) \]

\[ \frac{d^2\sigma}{dE/d\theta} (b/\text{eV}/\text{sr}) \]

\[ n = 8 \]

\[ E_n = 500 \text{ keV} \]

\[ \theta_n = 61 \text{ deg} \]

\[ E_n = 5.2 \text{ MeV} \]
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[ \alpha_{\text{target}} \]
\[ \alpha_{\text{compound}} \]
\[ \Gamma_v \]
\[ \Gamma_n \]
\[ \Gamma_\gamma \]

\[ (n,2n) \quad n = 9 \]
\[ (n,\gamma) \quad n = 9 \]

\[ \text{Cross section (b)} \]

\[ \text{Incident Energy (MeV)} \]

\[ d\sigma/d\theta (b/\text{sr}) \]

\[ \frac{d^2\sigma}{dE/d\theta} (b/\text{eV/ sr}) \]

\[ \text{Number of counts/bins} \]

\[ \text{Incident Energy (MeV)} \]

\[ \text{Cross section (b)} \]

\[ \text{Energy (MeV)} \]

\[ E_n = 500 \text{ keV} \]

\[ E_n = 5.2 \text{ MeV} \]

\[ \theta_n = 61 \text{ deg} \]
Hands on “1000 \times (Talys + ENDF + NJOY + MCNP) calculations”

\[ \alpha_{\text{target}} \]

\[ \alpha_{\text{compound}} \]

\[ \alpha_v \]

\[ \Gamma_n \]

\[ \Gamma_\gamma \]

\[ (n,2n) \quad n = 10 \]

\[ (n,\gamma) \quad n = 10 \]

\[ \sigma/d\theta (b/\text{sr}) \]

\[ d\sigma/d\theta (b/\text{sr}) \]

\[ d^2\sigma/d\theta dE (b/\text{eV/\text{sr}}) \]

\[ \text{Number of counts/bins} \]

\[ k_{\text{eff}} \text{ value} \]
Hands on "1000 \times (\text{Talys} + \text{ENDF} + \text{NJOY} + \text{MCNP}) \text{ calculations}"

\[ \alpha_{\text{target}} \]
\[ \alpha_{\text{compound}} \]
\[ \alpha_v \]
\[ \Gamma_v \]
\[ \Gamma_n \]
\[ \Gamma_\gamma \]

\[ (n,2n) \quad n = 15 \]
\[ (n,\gamma) \quad n = 15 \]

\[ \begin{array}{c|c|c|c|c|c|c}
\hline
\text{Cross section (b)} & 2.0 & 1.5 & 1.0 & 0.5 & 0.0 & 0.5 \\
\text{Incident Energy (MeV)} & 10 & 15 & 20 & 25 & 30 & 35 \\
\end{array} \]

\[ \begin{array}{c|c|c|c|c|c|c}
\hline
\text{Cross section (b)} & 10^{-1} & 10^{-2} & 10^{-3} & 10^{-4} & 10^{-5} & 10^{-6} \\
\text{Incident Energy (eV)} & 200 & 400 & 600 & 800 & 1000 & 2000 \\
\end{array} \]

\[ \begin{array}{c|c|c|c|c|c|c}
\hline
\text{Number of counts/bins} & 0 & 2 & 4 & 6 & 8 & 10 \\
\text{k\textsubscript{eff} value} & 0.99 & 1.00 & 1.01 & 1.02 & 1.03 & 1.04 \\
\end{array} \]

\[ \begin{array}{c|c|c|c|c|c|c}
\hline
\text{d\sigma/d\theta (b/sr)} & 1.0 & 1.2 & 1.4 & 1.6 & 1.8 & 2.0 \\
\text{Angle (deg)} & 0 & 20 & 40 & 60 & 80 & 100 \\
\end{array} \]

\[ \begin{array}{c|c|c|c|c|c|c}
\hline
\text{d\sigma/dE (b/MeV)} & 10^{-7} & 10^{-8} & 10^{-9} & 10^{-10} & 10^{-11} & 10^{-12} \\
\text{Energy (MeV)} & 2.0 & 2.5 & 3.0 & 3.5 & 4.0 & 4.5 \\
\end{array} \]

\[ (n,\text{el}) \quad n = 15 \]
\[ (n,\text{xn}) \quad n = 15 \]

\[ \theta_n = 61 \text{ deg} \]
\[ E_n = 5.2 \text{ MeV} \]
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[ a_{\text{target}} \]

\[ a_{\text{compound}} \]

\[ a_v \]

\[ \Gamma_v \]

\[ \Gamma_n \]

\[ \Gamma_\gamma \]

\[ k_{\text{eff}} = 1.01451 \pm 703 \text{ pcm} \]

TALYS  \hspace{1cm}  MCNP

\[ n = 20 \]

Number of counts/bins

0 2 4 6 8 10

0.99 1.00 1.01 1.02 1.03 1.04

k_{\text{eff}} \text{ value}
Hands on “1000 \times (Talys + ENDF + NJOY + MCNP) calculations”

\[ a_{\text{target}} \]

\[ a_{\text{compound}} \]

\[ a_v \]

\[ \Gamma_v \]

\[ \Gamma_n \]

\[ \Gamma_{\gamma} \]

\[ k_{\text{eff}} = 1.01403 \pm 0.696 \text{ pcm} \]

Number of counts/bins

<table>
<thead>
<tr>
<th>Number of counts/bins</th>
<th>10</th>
<th>8</th>
<th>6</th>
<th>4</th>
<th>2</th>
<th>0</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.99</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.00</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.01</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.02</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.03</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.04</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

\[ n = 25 \]
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[ k_{\text{eff}} = 1.01395 \pm 678 \text{ pcm} \]

\[ n = 30 \]

Number of counts/bins

0.99 1.00 1.01 1.02 1.03 1.04

k_{\text{eff}} value

Number of counts/bins

0 2 4 6 8 10
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[
\begin{align*}
\Gamma_n &= 40 \\
\kappa_{eff} &= 1.01337 \pm 712 \text{ pcm}
\end{align*}
\]
Hands on “1000 \times (\text{Talys} + \text{ENDF} + \text{NJOY} + \text{MCNP}) \text{ calculations}”

\[ a_{\text{target}} \]

\[ a_{\text{compound}} \]

\[ a_v \]

\[ \Gamma_v \]

\[ \Gamma_n \]

\[ \Gamma_\gamma \]

\[ k_{\text{eff}} = 1.01429 \pm 0.676 \text{ pcm} \]

Number of counts/bins

\[ n = 60 \]

TALYS \hspace{1cm} MCNP

\[ k_{\text{eff}} \text{ value} \]
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[
\begin{align*}
\alpha_{\text{target}} & \\
\alpha_{\text{compound}} & \\
\alpha_v & \\
\Gamma_v & \quad \text{TALYS} \quad \text{MCNP} \\
\Gamma_n & \\
\Gamma_\gamma & \\
\end{align*}
\]

Number of counts/bins

\[
\begin{array}{cccccccc}
1.04 & 1.03 & 1.02 & 1.01 & 1.00 & 0.99 & 1.00 & 1.01 & 1.02 & 1.03 & 1.04 \\
\end{array}
\]

\[
k_{\text{eff}} = 1.01358 \pm 693 \text{ pcm}
\]

\[
n = 100
\]
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[ a_{\text{target}} \]

\[ a_{\text{compound}} \]

\[ a_{\nu} \]

\[ \Gamma_{\nu} \]

\[ \Gamma_{n} \]

\[ \Gamma_{\gamma} \]

\[ k_{\text{eff}} = 1.01306 \pm 766 \text{ pcm} \]

Number of counts/bins

\[ n = 200 \]

\[ k_{\text{eff}} \text{ value} \]
Hands on “1000 \times (\text{Talys} + \text{ENDF} + \text{NJOY} + \text{MCNP}) \text{ calculations}”

\[ a_{\text{target}} \]
\[ a_{\text{compound}} \]
\[ a_v \]
\[ \Gamma_v \]
\[ \Gamma_n \]
\[ \Gamma_\gamma \]

\[ n = 300 \]

\[ k_{\text{eff}} = 1.01304 \pm 743 \text{ pcm} \]

Number of counts/bins

\[ \begin{align*}
0.99 & \quad 1.00 & \quad 1.01 & \quad 1.02 & \quad 1.03 & \quad 1.04 \\
0 & \quad 2 & \quad 4 & \quad 6 & \quad 8 & \quad 10
\end{align*} \]
Hands on “1000 \times (\text{Talys} + \text{ENDF} + \text{NJOY} + \text{MCNP}) calculations”

\[
\begin{align*}
\Gamma_n &= 400 \\
k_{\text{eff}} &= 1.01355 \pm 769 \text{ pcm}
\end{align*}
\]
Hands on “1000 × (Talys + ENDF + NJOY + MCNP) calculations”

\[
\alpha_{\text{target}} \quad \alpha_{\text{compound}} \\
\alpha_v \quad \Gamma_v \\
\Gamma_n \quad \Gamma_\gamma
\]

TALYS \quad MCNP

\[
k_{\text{eff}} = 1.01372 \pm 745 \text{ pcm}
\]

Number of counts/bins

\[
n = 600
\]

\[
0.99 \quad 1.00 \quad 1.01 \quad 1.02 \quad 1.03 \quad 1.04
\]

k_{\text{eff}} \text{ value}
Hands on “1000 \times (\text{Talys} + \text{ENDF} + \text{NJOY} + \text{MCNP}) \text{ calculations}”

\[ a_{\text{target}} \]

\[ a_{\text{compound}} \]

\[ a_v \]

\[ \Gamma_v \]

\[ \Gamma_n \]

\[ \Gamma_\gamma \]

\[ k_{\text{eff}} = 1.01363 \pm 744 \text{ pcm} \]

Number of counts/bins

\[ n = 800 \]

TALYS \hspace{1cm} MCNP
Hands on “1000 \times (Talys + ENDF + NJOY + MCNP) calculations”

\[ \Gamma_n \]

\[ \Gamma_\gamma \]

\[ n = 800 \]

\[ k_{eff} = 1.01363 \pm 744 \text{ pcm} \]

Statistical uncertainty \(\simeq 68 \text{ pcm}\)

\[ \Rightarrow \text{uncertainty due to nuclear data} \simeq 740 \text{ pcm} \]
Considered data in TMC (or fast TMC)

Several hundreds of random ENDF files for transport + depletion

- 3 Major actinides: \(^{235}\text{U},^{238}\text{U},^{239}\text{Pu}\),
- Light elements: lighter than oxygen,
- Thermal scattering data: H in H\(_2\)O, D in D\(_2\)O, C in Carbon,
- All Fission yields (e.g. \(^{234,235,236,238}\text{U},^{239,240,241}\text{Pu},^{237}\text{Np},^{241,243}\text{Am},^{243,244}\text{Cm}\)),
- All Minor actinides (e.g. \(^{234,236,237}\text{U},^{237}\text{Np},^{238,240,241,242}\text{Pu},\text{Am},\text{Cm}\)),
- All fission products (e.g. from Ge to Er), and decay data,

(fast) TMC can be applied to any input data, propagating uncertainties to any outputs
Considered data in TMC (or fast TMC)

Several hundreds of random ENDF files for transport + depletion

- 3 Major actinides: $^{235}\text{U}$, $^{238}\text{U}$, $^{239}\text{Pu}$,
- Light elements: lighter than oxygen,
- Thermal scattering data: H in H$_2$O, D in D$_2$O, C in Carbon,
- All Fission yields (e.g. $^{234,235,236,238}\text{U}$, $^{239,240,241}\text{Pu}$, $^{237}\text{Np}$, $^{241,243}\text{Am}$, $^{243,244}\text{Cm}$),
- All Minor actinides (e.g. $^{234,236,237}\text{U}$, $^{237}\text{Np}$, $^{238,240,241,242}\text{Pu}$, Am, Cm),
- All fission products (e.g. from Ge to Er), and decay data,

(fast) TMC can be applied to any input data, propagating uncertainties to any outputs

TMC was already applied to

- criticality-safety, shielding, pincell/assembly burn-up, full core, activation,
- PWR, BWR, Gen-IV systems,
- UO$_2$, MOX fuels,
- MCNP, SERPENT, FISPACT, DRAGON, PANTHER, RELAP-5
Application: thermal scattering for H in H₂O or S(α,β) tables (with MCNP)

Random parameters of the S(α,β) for inelastic scattering

- **lmt1-1**
  - $k_{\text{eff}} = 0.99813 \pm 80 \text{ pcm}$

- **hst42-1**
  - $k_{\text{eff}} = 0.99646 \pm 210 \text{ pcm}$

- **pst1-1**
  - $k_{\text{eff}} = 1.00286 \pm 350 \text{ pcm}$

- **pst12-10**
  - $k_{\text{eff}} = 1.00561 \pm 400 \text{ pcm}$
Systematical study on UO$_2$/MOX assembly uncertainties

- Different UO$_2$/MOX assemblies (PWR, BWR, VVER, AGR, CANDU, fast systems),
- Burn-up calculated with SERPENT,
- All major nuclear data taken into account.
- $\Rightarrow$ systematical study on $k_{\text{eff}}$, inventory, heat...
Comparison of $\Delta k_{\infty}$ for assemblies and full core (SERPENT)

$\Delta k_{\infty}$ uncertainty for different assemblies

- PWR UO$_2$ (no Gd)
- PWR UO$_2$ (w Gd)
- PWR MOX (1 assembly)
- PWR MOX (4 assemblies)
- EPR MOX
- BWR MOX (w Gd)
- BWR UO$_2$ (w Gd)
- BWR MOX (w Gd)
- VVER UO$_2$
- VVER MOX
- CANDU
- AGR

Burn-up (GWd/tHM)
TMC applied to PWR assembly burn-up calculations with DRAGON

- Due to fission yields
- Due to resonance $\sigma_\gamma$
- Due to $\nu$
- Due to transport data
- Due to MF3
- Due to fission yields

238U

Burn up (GWd/tHM)

Uncertainty on $k_{eff}$ (%)
TMC applied to PWR assembly burn-up calculations with DRAGON

![Graphs showing burn-up calculations for different isotopes and uncertainties on k_{eff}.](image-url)

- **239Pu**
  - Due to transport data
  - Due to fission yields
  - Due to resonance $\sigma_f$
  - Due to MF3

- **240Pu**
  - Due to transport data
  - Due to fission yields
  - Due to resonance $\sigma_{\gamma}$

- **241Pu**
  - Due to transport data
  - Due to fission yields
  - Due to resonance $\sigma_f$
  - Due to MF3

- **FP**
  - Due to transport data
  - Due to fast $\sigma_{\gamma}$
  - Due to MF2
TMC applied for burn-up calculations: decay heat

Burn-up (GWd/tHM)

Decay heat (arb. unit)

Burn-up & cooling time (years)

UO2

MOX

50
40
30
20
10
0

0
10
20
30
40
50

10
20
30
40
50

5.10^0
5.10^1
5.10^2
5.10^3
1.10^5

0.1
1
2
3
4
5

43210.1
TMC applied for burn-up calculations: decay heat uncertainties

![Graph showing burn-up (GWd/tHM) vs. Relat. Heat Uncert. (arb. unit) for UO2 and MOX fuel.](image)

- **Burn-up (GWd/tHM)**: 0, 10, 20, 30, 40, 50
- **Relat. Heat Uncert. (arb. unit)**: 0.1, 1, 2, 3, 4
- **Burn-up & cooling time (years)**: 0.1, 1, 2, 3, 4, 5, 10^0, 2, 10^2, 5, 10^3, 1, 10^5
- **Lines**: Red line for UO2, Blue line for MOX
Effect of H in H$_2$O for a full core PWR (courtesy of O. Cabellos, UPM, Spain)

Method: TMC applied to COBAYA (3D multigroup core calculations) + SIMULA (coupled neutronic-thermohydraulics 3D core calculations)
Effect of H in H\(_2\)O for a full core PWR (courtesy of O. Cabellos, UPM, Spain)

![Graph showing the effect of H in H\(_2\)O for a PWR full core](image)

- **Boron concentration**
- **Moderator Temp. coeff.**
- **Power coeff.**

<table>
<thead>
<tr>
<th>Uncertainties (%)</th>
<th>Burn-up (GWd/TMU)</th>
</tr>
</thead>
<tbody>
<tr>
<td>8</td>
<td>0.1</td>
</tr>
<tr>
<td>4</td>
<td>0.2</td>
</tr>
<tr>
<td>2</td>
<td>0.5</td>
</tr>
<tr>
<td>1</td>
<td>1.0</td>
</tr>
<tr>
<td>1</td>
<td>2.0</td>
</tr>
<tr>
<td>1</td>
<td>4.0</td>
</tr>
<tr>
<td>1</td>
<td>8.0</td>
</tr>
</tbody>
</table>

Legend:
- Red line: Boron concentration
- Blue dashed line: Moderator Temp. coeff.
- Dotted line: Power coeff.
In TMC:

*If we can do a calculation once, we can also do it a 1000 times, each time with a varying data library.*
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Well, then uncertainty propagation with TMC takes $1000\times$ longer than a single calculation...

(Each $\sigma_{\text{statistics}}$ needs to be small)

There is a solution with Monte Carlo codes:
(in fact 2 solutions)

- fast GRS method,
- and fast TMC.

"Efficient use of Monte Carlo: uncertainty propagation",
2012: fast GRS method

First presented in PHYSOR-2012 by W. Zwermann et al.. It takes advantage of conditional expectations:

If two output variables $k^{(1)}$ and $k^{(2)}$ are identically distributed and conditionally independent given the vector of nuclear data input then

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In practice:

1. perform $i = 1..500$ MCNP short calculations with random nuclear data and a fixed seed $s_1 \Rightarrow k_{\text{eff}}^{(1)}(i)$
2. repeat for $j = 1..500$, same random nuclear data but fixed seed $s_2 \Rightarrow k_{\text{eff}}^{(2)}(j)$

There is no necessity to have small $\sigma_{\text{statistics}}$!!

each run can be (very) short
2 × 500 "short" runs ∼ 2 × "long" run in time
If a single calculation takes \( m \) histories (\( \sigma_{\text{stat}} \) small enough), then repeat it \( n \) times with \( m/n \) histories, random nuclear data and random seeds.

\[
\sigma_{\text{total}}^2 = \sigma_{\text{statistics}}^2 + \sigma_{\text{nuclear data}}^2 \text{ still holds.}
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still holds.

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<th>Run</th>
<th>ENDF/B-VII.1</th>
<th>Seed</th>
<th>Histories</th>
<th>Time</th>
<th>Result</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>ENDF/B-VII.1</td>
<td>$s_0$</td>
<td>$m$</td>
<td>$T$ sec.</td>
<td>$k \pm \sigma_{\text{stat}}$</td>
</tr>
<tr>
<td>1</td>
<td>Nuclear data</td>
<td>$s_1$</td>
<td>$m/n$</td>
<td>$T/n$ sec.</td>
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<tr>
<td>run 1</td>
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<td>seed s_1</td>
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<tr>
<td>run 2</td>
<td>nuclear data 2</td>
<td>seed s_2</td>
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<th>run ( i )</th>
<th>data ( j )</th>
<th>seed ( s_i )</th>
<th>histories</th>
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<th>( k \pm \sigma_{\text{stat}} )</th>
</tr>
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<tr>
<td>run 0</td>
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$$\left\{ \begin{align*}
\sigma_{\text{total}}^2 &= \frac{1}{n-1} \sum_{i=1}^{n} (k_i - \bar{k})^2 \\
\sigma_{\text{statistics}}^2 &= \frac{1}{n} \sum_{i=1}^{n} \sigma_i^2
\end{align*} \right.$$
The fast methods

- as fast as S/U methods (1-2 × longer than 1 single calculation),
- tested on criticality & shielding benchmarks, burn-up ($k_{eff}$ and inventory),
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- Example: the Martin-Hoogenboom benchmark

MCNP6 model: 241 fuel assemblies, with 264 fuel pins each
Fast TMC & GRS methods on a full core

- $357 \times 357 \times 100$ regions ($1.26 \times 1.26 \times 3.66 \text{ cm}^3$): 6.4 million cells for generated power (f7)
- 1 calculation takes $2 \times 10^{11}$ histories ($\sigma_{\text{statistics}} = 0.25 \%$ at the center, 500 weeks on 1 cpu)
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- Uncertainty on local pin power due to $^{235}\text{U}$, $^{238}\text{U}$, $^{239}\text{Pu}$ and H in H₂O thermal scattering in each cell?

![Graph of F7 local generated power density](image)
Fast TMC & GRS methods on a full core

- TMC: 500 random runs of $2 \times 10^{11}$ histories (500 weeks for each),
- TMC is not applicable,
- Uncertainties with the fast TMC and fast GRS methods,
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1. Source convergence

- For both methods, a first calculation is run with fixed nuclear data to obtain a reasonably converged fission source.
- All subsequent short simulations start with this fission source:
  - each with 10 inactive cycles and 90 active cycles of $4 \times 10^6$ histories, and random nuclear data,
  - source convergence tested with the MCNP6 built-in indicator (fission source entropy).
- 362 short runs out of 508 were then accepted for fast TMC.
- 2 × 122 short runs out of 2 × 328 were then accepted for fast GRS.
(2) Statistical uncertainty estimation

- In MCNP eigenvalue calculation, $\sigma_{\text{stat}}$ is usually underestimated.
- An independent estimation of $\sigma_{\text{stat}}$ is therefore necessary for fast TMC,
- From the 508 short runs, the first 389 were repeated with fixed nuclear data,
- 274 were then accepted due to source convergence.
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- An independent estimation of $\sigma_{stat}$ is therefore necessary for fast TMC,
- From the 508 short runs, the first 389 were repeated with fixed nuclear data,
- 274 were then accepted due to source convergence.
- 9% difference for $k_{eff}$
- for generated power ($f7$):
  ratio is $1.019 \pm 0.040$.

Therefore, for local power, the MCNP estimation of $\sigma_{stat}$ is good enough.
Fast TMC & GRS methods on a full core: $k_{\text{eff}}$ uncertainty

![Graph showing $k_{\text{eff}}$ uncertainty vs number of runs for Fast TMC and Fast GRS methods.]

- Fast TMC: 740 pcm
- Fast GRS: 760 pcm
Fast TMC & GRS methods on a full core: generated local power

![Graph showing uncertainty in generated power (f7) with Fast GRS method and Fast TMC methods compared.](image)

- **Y-axis (cm):** y (cm)
- **X-axis (cm):** x (cm)
- **Uncertainty [%]:** 0%, 2%, 4%, 6%
- **Uncertainty on generated power (f7):** Fast GRS method, Fast TMC

Nuclear data Uncertainties (%)

- n.a.
- guide
- tube
- 1
- 2
- 3
- 4
- 5
- 6
- 7
- 8

Uncertainty on generated power (f7)

- Fast GRS method
- Fast TMC
The previous uncertainties can be fitted using $f(x) = a_0 + a_2 x^2$
Conclusions

Anyone can do it with the random nuclear data files from www.talys.eu/tendl-2012 (actinides, thermal scattering...)

D. Rochman – 33 / 33
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fast TMC and GRS methods:
If we can do a calculation once, we can also get nuclear data uncertainties in twice the time (or less).