DE LA RECHERCHE À L'INDUSTRIE

PRELIMINARY INVESTIGATION OF NUCLEAR DATA SAMPLING FOR THE NEW MONTE CARLO CODE TRIPOLI-5®

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DES/ISAS/DM2S/SERMA

Outline

Introduction

TRIPOLI-5, the new Monte Carlo code at CEA

Presentation of the benchmark

Neutron physics : free gas model and thermal scattering

Unresolved resonance region

Photon physics : preliminary results

Conclusion and perspectives

Introduction

- TRIPOLI-5® : new massively parellel Monte Carlo transport code developed at CEA
- Recent implementation of neutron physics
  - Free gas model
  - Thermal scattering laws (TSL)
  - Unresolved resonance range (URR) : ongoing validation
- First step of verification :
  - Code-to-code comparisons (TRIPOLI-4® and OpenMC)
  - Contribution to corrections/fix-ups
- Developement of a test environment for :
  - All isotopes from library JEFF-3.3
  - Representative energies of the neutron spectrum in a reactor
- Photon physics
  - Implementation of hoto-atomic reactions
  - Extension of the previous benchmark to photon physics

Introduction

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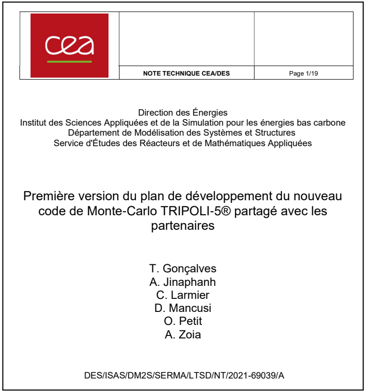
The TRIPOLI-4®5 project

- started in January 2022
- co-financed by CEA/EDF/Framatome/IRSN
- co-developed by CEA/IRSN
- builds on TRIPOLI-5®



	NOTE TECHNIQUE CEA/DES	Page 1/19

Direction des Énergies
Institut des Sciences Appliquées et de la Simulation pour les énergies bas carbone
Département de Modélisation des Systèmes et Structures
Service d'Études des Réacteurs et de Mathématiques Appliquées

Première version du plan de développement du nouveau code de Monte-Carlo TRIPOLI-5® partagé avec les partenaires

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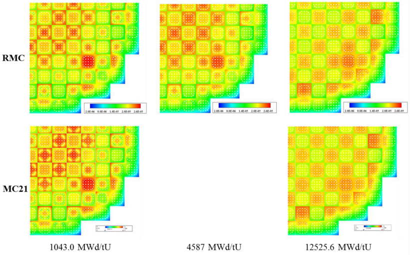
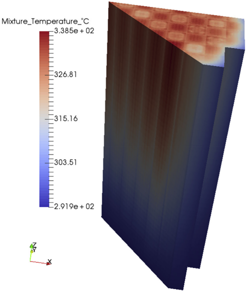
DES/ISAS/DM2S/SERMA/LTSD/NT/2021-69039/A

Challenges

- full-core simulations
- couplings
  - thermal hydraulics
  - thermo-mechanics
  - depletion
- kinetics (neutrons/precursors)
- large memory footprint
  - $\sim 10^2$ isotopes
  - $\sim 10^3$ temperatures
  - $\sim$ 1 GB per temperature
  - $\sim$ 1 TB total
- continuous burn-up of material properties
  - alternative tracking methods

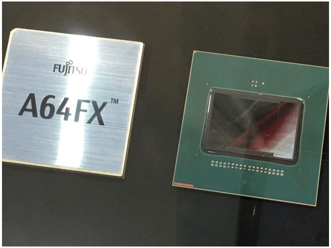




K. Wang *et al.*
Prog. Nucl. Energy 98 (2017) 301–312

D. J. Kelly *et al.*
Nucl. Eng. Technol. 49 (2017) 1326–1338

- massive parallelism
  - shared memory
  - distributed memory
  - vectorization
- computing architectures
  - heterogeneous
  - quickly evolving



Work-flow et technological choices

Work-flow

- continuous integration
- code review
- modularity

technologies

- C++14
- OpenMP + MPI
- API Python
- *CUDA*

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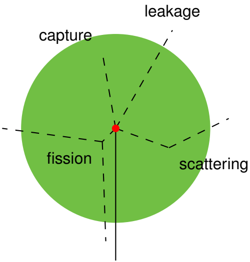
Description of the benchmark

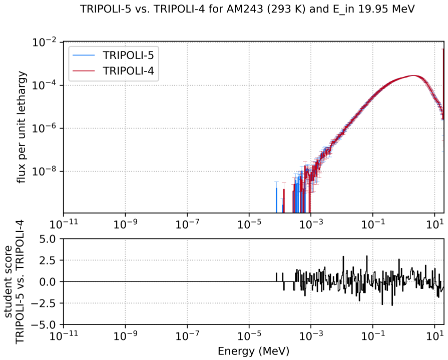
- Test configuration :
  - Sphere, radius R=30 cm
  - One single isotope
  - Isotropic, mono-energy, point source
  - Observable : flux per unit lethargy (collision estimator)
  - Number of particles : 10^6
  - Density $\gamma(E) = \frac{1}{R\hat{\sigma}_{t,i}(E)}$ with $\hat{\sigma}_{t,i}(E)$ a 4-group microscopic total cross section



- Simulation parameters :
  - 562 isotopes (free gas only) from nuclear data library JEFF-3.3
  - Source energy E_0 (MeV) : 1e-11, 2.5e-08, 1e-06, 3e-05, 0.001, 0.03, 1.0, 14.1, 19.95
  - Probability tables for unresolved resonance range : switched off
- 5058 validation configurations
- Code-to-code comparisons between 3 Monte Carlo transport codes :
  - OpenMC
  - TRIPOLI-4®
  - TRIPOLI-5®

Comparison of flux results and statistical tests

- How to compare results for the flux between two codes ?
- The Student test can be used to estimate the consistency probability of the results for a given energy bin



Comparison of flux results : Holm-Bonferroni test

- Used to solve the problem of multiple comparisons (at each energy bin)
- Calibrated with a threshold α (we choose $\alpha = 0.001$)
- We expect "false negatives" with probability α ($\sim$ 5 for 5000 configurations)

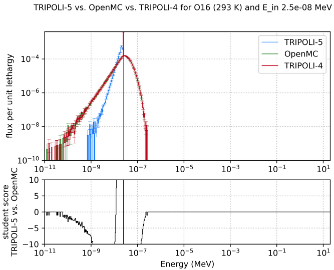


Figure 1 – Test HB : success (SVT deactivated)

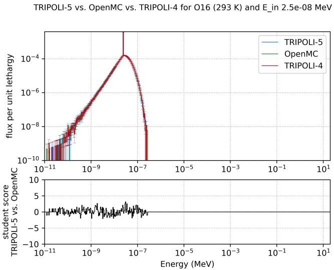


Figure 2 – Test HB : failure (SVT activated)

Example of simple fix-up : missing reactions

- Initially TRIPOLI-5® did not take into account some reactions

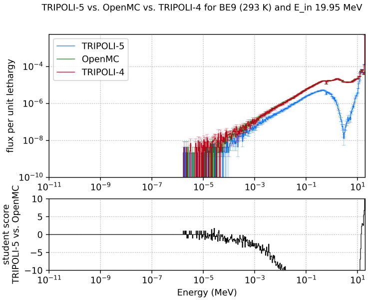


Figure 3 – Flux with only MT reaction 876

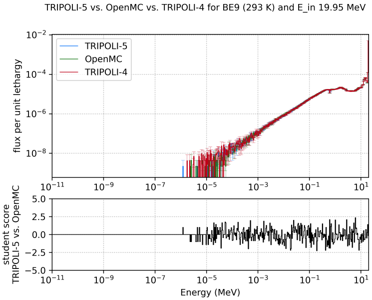
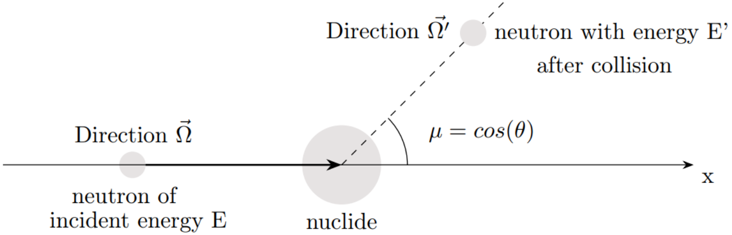


Figure 4 – Flux with MT reactions 875 - 891

- For each code, we have developed dedicated routines in order to sample :
  - the outgoing energy distribution $f(E'|E)$
  - the outgoing cosine distribution $g(\mu|E)$

  for given parameters :
  - isotope/temperature
  - interaction (MT)
  - incoming energy E
  - number of samples (10^6)



Kolmogorov–Smirnov (KS) test

- Statistical test evaluating whether two samples stem from the same distribution or not

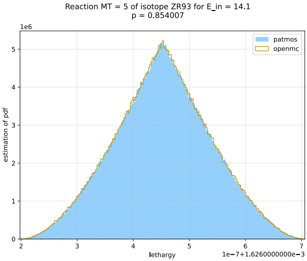


Figure 5 – KS test success : $p > 0.05$

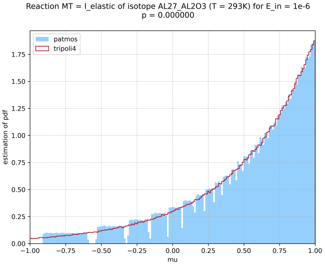


Figure 6 – KS test failure : $p < 0.05$

KS test applied to the sampling of distributions

- The test on the sampling of angle/energy distributions of outproducts enables to check the corresponding implementation

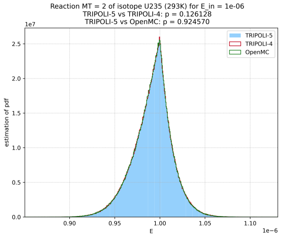


Figure 7 – Sampling of the energy distribution, ^{235}U at 293K, MT 2, $E_0 = 1$ eV

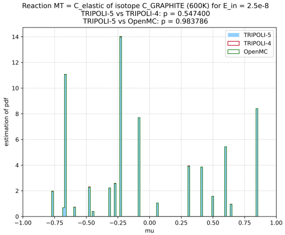


Figure 8 – Sampling of the cosine distribution, C in graphite at 293K, coherent elastic reaction, $E_0 = 0.025$ eV

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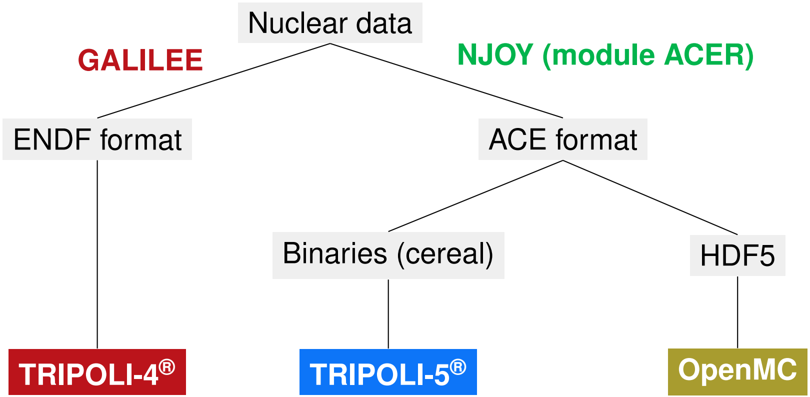
Post-treatment process of nuclear data

- For this inter-codes comparison, the data contained in different formats can differ because of the module ACER
- This makes the comparison TRIPOLI-4®/TRIPOLI-5® harder for the analysis of discrepancies



Discrepancies in (tabulated) distributions (1/2)

- The reconstruction of some distributions can be done by two methods :
  - parameters and analytic formula (format ENDF : TRIPOLI-4®)
  - pre-computed numerical values (format ACE : TRIPOLI-5®/OpenMC)
- Very frequent cases for all distributions involving tabulations with pdf/cdf tables : different size of tables between ACE and ENDF

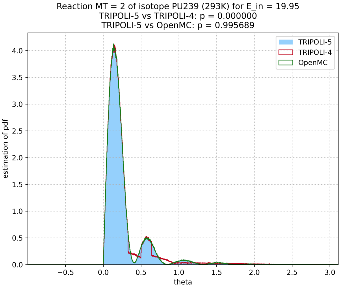


Figure 9 – Energy distribution for ^{239}Pu, MT 2, $E_0 = 19.95$ MeV

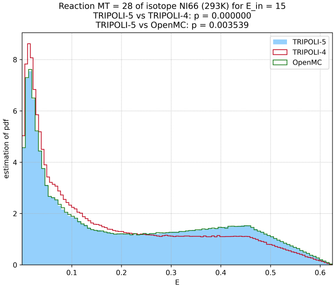


Figure 10 – Energy distribution for ^{66}Ni, MT 28, $E_0 = 15$ MeV

- The same behaviour can be observed for inelastic thermal reactions.

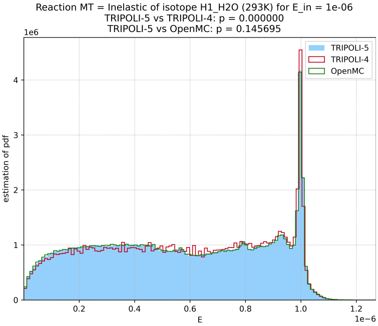


Figure 11 – Energy distribution for ^{1}H in H_2O, $E_0 = 0.1$ eV, inelastic reaction

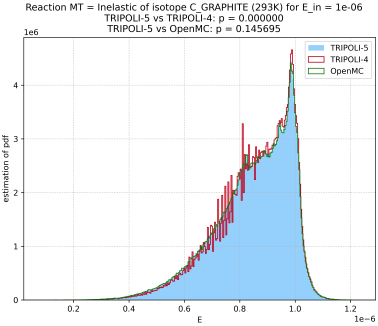


Figure 12 – Energy distribution for C in graphite, $E_0 = 0.1$ eV, inelastic reaction

Level-scattering reactions (1/3)

- Reactions identified by MT $\in$ [51-90]
- The outgoing energy of the neutron (in CM frame) is given by :

$$E_{CM} = \frac{A+1}{A}^{2} E_{in} - C$$

  - In TRIPOLI-4® : $C = E_{th}$ (reaction threshold)
  - In TRIPOLI-5® and OpenMC : $C = -Q\frac{A+1}{A}$
- In principle : $E_{th} = -Q\frac{A+1}{A}$
- However, for some isotopes : $E_{th} > -Q\frac{A+1}{A}$
- In JEFF-3.3 (T=293 K) :
  - 30 reactions
  - 18 isotopes
- A simulation option has been added to address that problem in TRIPOLI-4®.v12

Level-scattering reactions (2/3)

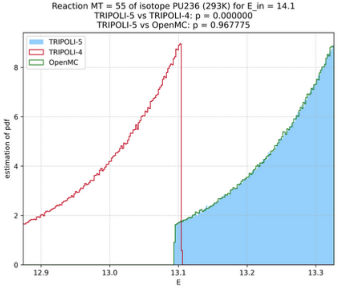


Figure 13 – Energy distribution before correction

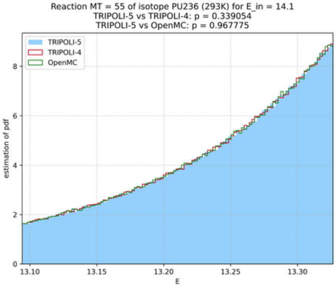


Figure 14 – Energy distribution after correction in TRIPOLI-4®.v12

Level-scattering reactions (3/3)

Isotope	MT	Energy threshold	-Q (A+1)/A	Relative error
C13	51	6.950099e+00	3.329087e+00	1.087689e+00
C13	52	6.950099e+00	3.970316e+00	7.505153e-01
C13	53	6.950099e+00	4.152748e+00	6.736144e-01
GD156	54	1.277000e+00	9.662103e-01	3.216584e-01
GD158	53	7.000000e-01	5.424426e-01	2.904591e-01
GD158	54	1.600000e+00	9.037355e-01	7.704295e-01
GD160	54	1.600000e+00	8.754871e-01	8.275541e-01
NE20	51	2.200544e+00	1.716092e+00	2.822996e-01
NI61	51	6.999999e-02	6.810912e-02	2.776236e-02
PU236	55	1.000000e+00	7.768053e-01	2.873239e-01
PU238	67	1.130530e+00	1.084677e+00	4.227341e-02
PU242	55	8.357680e-01	7.820252e-01	6.872259e-02
PU242	64	1.400000e+00	1.088517e+00	2.861535e-01
PU246	54	6.000000e-01	5.371930e-01	1.169170e-01
PU246	57	1.100000e+00	9.418450e-01	1.679204e-01

Figure 15 – List of isotopes and reactions with $E_{th} \neq -Q\frac{A+1}{A}$

"Gaps" w.r.t the energy threshold (1/2)

- Each interaction is assigned an energy threshold E_{th}
- Energy grids of the distributions of underlying outproducts start from energy E_{min}
- We expect : $E_{min} \geq E_{th}$
- However, a few isotopes at 293K contain interactions such that : $E_{min} > E_{th}$

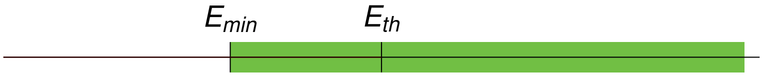


Figure 16 – Normal case

Figure 17 – Unexpected case

"Gaps" w.r.t the energy threshold (2/2)

Isotope	MT	Threshold energy	Minimal energy	Relative error
CR50	5	8.500000e-01	3.973966e+00	3.675254e+00
CR50	5	8.500000e-01	3.973966e+00	3.675254e+00
CR53	5	8.000000e-01	3.232537e+00	3.040671e+00
CR53	5	8.000000e-01	3.232537e+00	3.040671e+00
CR54	5	4.000000e+00	4.061986e+00	1.549650e-02
CR54	5	4.000000e+00	4.061986e+00	1.549650e-02
CS135	30	8.746430e+00	1.421000e+01	6.246629e-01
HF174	91	1.658000e-01	1.657890e+00	8.999337e+00
HF176	91	1.681930e-01	1.681930e+00	9.000000e+00

Figure 18 – List of isotopes/interactions (for JEFF-33.3, T=293K) for which the reaction threshold is smaller than the minimal energy of at least one grid of the underlying distribution (discrepancy with a relative error larger than 1%)

Other inconsistencies in nuclear data

- TRIPOLI-5® checks the consistency of nuclides when created
- From these consistency checks, we could observe inconsistencies in ACE files from JEFF-3.3 library at 293K [1] :
  - Some cumulative fonctions distributions (CDFs) are not sorted in the ascending way
  - Some tables associated to PDF/CDF are not sorted in the ascending way (corresponding : isotopes : AG110M, CD115M, CR50, CR53, CR54, NE20, SI32)
  - **All cumulative density functions involved in thermal inelastic reactions** have one negative value (absolute value close to 10^{-16}) : necessity to set the negative values to 0 in order to be able to generate binaries with TRIPOLI-5®
  - Non-sorted equiprobables/skewed tables (thermal reactions)
  - For thermal (continuous) inelastic reactions : the CDFs do not start at 0 !

1. ACE files generated from **NJOY 2016.42, at NEA on 2018-10-01**

Thermal reactions : the CDF does not start at 0!

- A problem **systematically** present in ACE files is cdf[0] not being equal to 0 for each energy sub-distributions of (continuous) inelastic reactions
- cdf[0] around 1^{-6}-1^{-5} for NJOY
- cdf[0] around 1^{-8} for FRENDY
- Some negative energies can be produced because of that problem within the sampling of the outgoing energy (with both OpenMC and TRIPOLI-5®) with a small probability
- We chose to complete the distribution on the left, by adding cdf[0]=0, pdf[0]=0, energy value E[0]=0 (see Eq.(1)) and a "isotropic"-like table for discrete angles
- This post-treatment is almost invisible with respect to OpenMC apart from in one case (^{20}Mg in metal) detailed further

$$\sigma(E' \rightarrow E, \mu, T) = \frac{\sigma_b}{2kT}\sqrt{\frac{E}{E'}}exp\left(-\frac{\beta}{2}\right)S(\alpha, \beta, T) \qquad (1)$$

Focus on the case MG24 in metal at 20 K (1/2)

- Energy distribution for the inelastic reaction of MG24 in metal at 20 K :
  - agreement TRIPOLI-5®/OpenMC **before** the retreatement for cdf[0]=0 : OK
  - agreement TRIPOLI-5®/OpenMC **after** the retreatement for cdf[0]=0 : KO

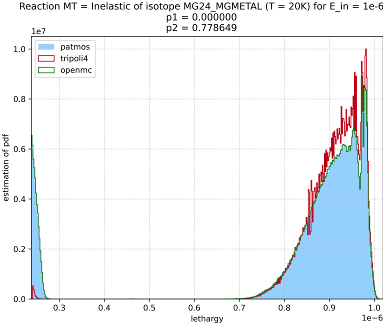


Figure 19 – Before retreament in TRIPOLI-5®

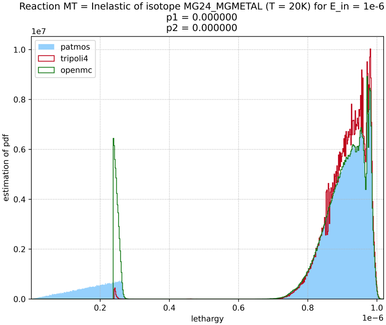


Figure 20 – After retreament in TRIPOLI-5®

Focus on the case MG24 in metal at 20 K (2/2)

- Looking at the "guilty" probability density function, we observe that the behaviour of this quantity looks pathological (decreasing slope at low energy)
- With such non-physical data, our work-around for the case cdf[0]=0 leads to significantly different results w.r.t OpenMC

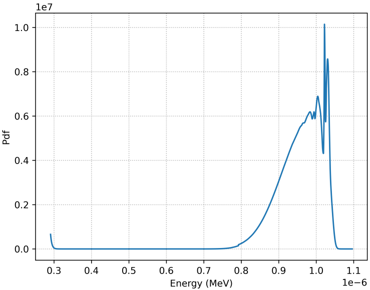


Figure 21 – PDF before retreament in TRIPOLI-5®

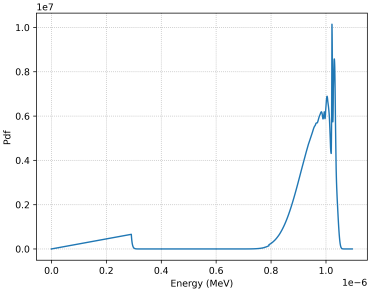


Figure 22 – PDF after retreament in TRIPOLI-5®

Incoherent elastic reaction and Debye-Waller factor

- Two ways to sample the cosine :
  - TRIPOLI-4® uses the analytic formula $\mu = 1 + \frac{log(\xi+(1-\xi)e^{-4EW'})}{2EW'}$
  - TRIPOLI-5® uses tables (OpenMC can do both methods)

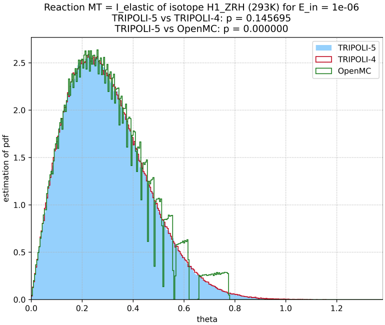


Figure 23 – TRIPOLI-5® uses ACE data

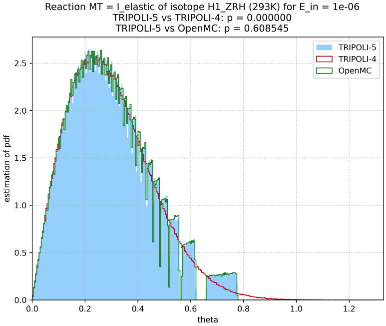


Figure 24 – TRIPOLI-5® uses Debye-Waller factor from ENDF files

Case ZR93 at 293K, MT 5 (1/2)

- Isotope ZR93 at 293K with $E_0 = 14.1$ MeV :
  - test HB OK for TRIPOLI-5®/TRIPOLI-4®
  - test HB KO for TRIPOLI-5®/OpenMC
  - test HB KO for TRIPOLI-4®/OpenMC

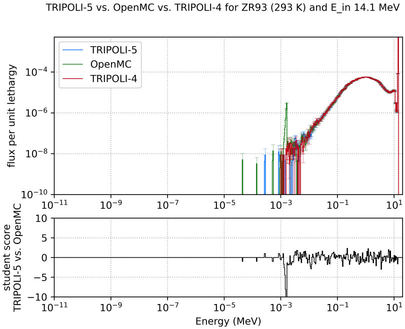


Figure 25 – Flux before correction

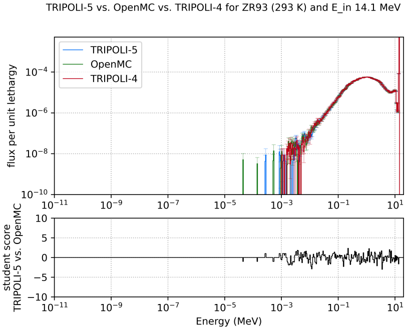


Figure 26 – Flux after correction

Case ZR93 at 293K, MT 5 (2/2)

- For this isotope, the yield associated to MT 5 (n, other) can be equal to 0 for some incoming energies.
- It is necessary to treat the reaction as a capture instead of as a scattering.

```
   // evaluate yield
   double yield = (*rx.products_[0].yield_)(E_in);
-  if (std::floor(yield) == yield) {
+  if (std::floor(yield) == yield && yield > 0) {
     // If yield is integral, create exactly that many secondary particles
     for (int i = 0; i < static_cast<int>(std::round(yield)) - 1; ++i) {
       p.create_secondary(p.wgt(), p.u(), p.E(), ParticleType::neutron);
```

Figure 27 – Fix-up in OpenMC

- Fixup integrated in OpenMC in November 2022

Neutron physics : summary of the results

Table 1 – Summary of the results based on the Holm-Bonferroni (HB) test for the code-to-code comparison of neutron flux.

Free gas only		
	TRIPOLI-5® versus TRIPOLI-4®.v12	TRIPOLI-5® versus OpenMC
Number of configurations	4953	4939
Number of HB test failures	418 [a]	19 [b]
HB test success rate	91.56%	99.62%
Final HB test success rate	-	99.85%

Free gas and TSL		
	TRIPOLI-5® versus TRIPOLI-4®.v12	TRIPOLI-5® versus OpenMC
Number of configurations	279	279
Number of HB test failures	102	2
HB test success rate	63.44%	99.28%

a. with correction of the level scattering thresholds, without : 446, i.e. success rate 91.00%

b. with correction of ^{93}Zr

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Presentation of the benchmark

Neutron physics : free gas model and thermal scattering

Unresolved resonance region

Photon physics : preliminary results

Conclusion and perspectives

Unresolved resonance region : preliminary results

- We have recently extended the comparison with activation of the treatment of cross sections in the unresolved resonance region
- TRIPOLI-5® : implemention with probability tables provided by ACE files
- Preliminary results : excellent agreement with OpenMC

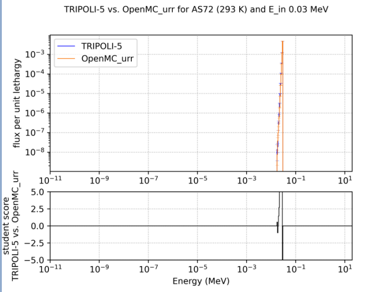

Figure 28 – TRIPOLI-5® : URR off, OpenMC : URR on

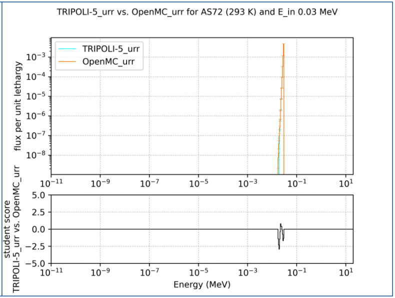

Figure 29 – TRIPOLI-5® : URR on, OpenMC : URR on

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Photon physics in TRIPOLI-5®

- Recently, electromagnetic interactions performed by photons with atoms have been implemented into TRIPOLI-5®
- Photo-atomic reactions :
  - Rayleigh photon scattering
  - Compton inelastic scattering
  - pair production
  - photo-electric capture
- Electron transport modeled with Thick-Target-Bremsstrahlung (TTB)
  - TTB can be switched off
- TRIPOLI-5® uses :
  - ENDF-formatted EPICS data
  - data from G4EMLOW library for Compton profile and TTB
  - data from ESTAR library for collision stopping powers
- TRIPOLI-5® supports EPICS 2014 and EPICS 2017 libraries
- Extension of the benchmark :
  - Data library : EPICS 2014 (for compatibility with OpenMC)
  - Adaptation of energy sources and of the energy tally grid
  - Adding the photon/electron transport code PENELOPE to the comparison

Photon physics : results with TTB witched off

- TRIPOLI-4® : does not support Relativistic Impulse Approximation (RIA)
- TRIPOLI-5®/TRIPOLI-4® : different treatment of atomic relaxation : TRIPOLI-5® uses a larger number of sub-shells to simulate fluorescence
- TRIPOLI-5®/PENELOP :good agreement but differences due to fluorescence
- TRIPOLI-5®/OpenMC : significant discrepancy, which originates from an approximation in the RIA sampling algorithm used by OpenMC

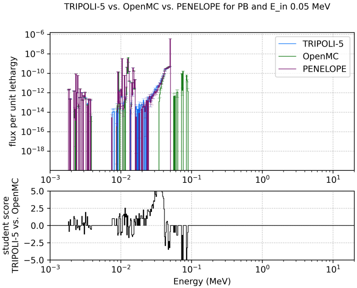

Figure 30 – Element Pb, $E_0 = 0.05$ MeV, inhibited TTB

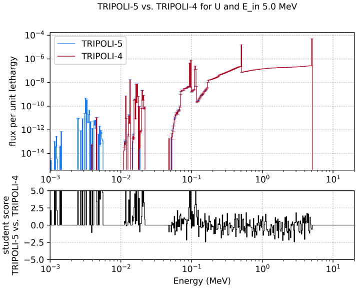

Figure 31 – Element U, $E_0 = 5$ MeV, inhibited TTB and RIA

Photon physics : results with TTB (1/2)

- Left : reasonable agreement among all the codes, but with significant differences that again originate from the treatment of Compton scattering
- Right : small, but statistically significant discrepancy between TRIPOLI-5® and PENELOPE/OpenMC due to the difference in stopping power data, since TRIPOLI-5® uses values from NIST ESTAR database, while OpenMC and PENELOPE calculate collision stopping powers internally

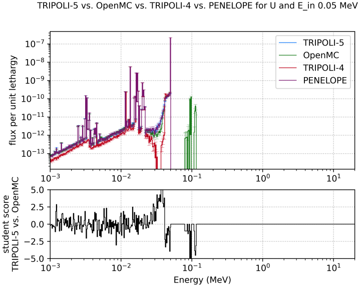

Figure 32 – Element U, $E_0 = 0.05$ MeV, TTB activated

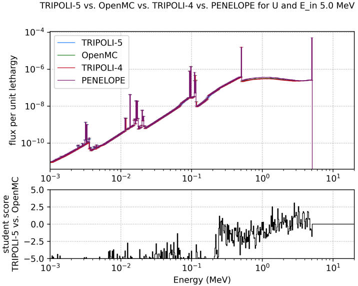

Figure 33 – Element U, $E_0 = 5$ MeV, TTB activated

- The discrepancies due to stopping power data become less significant for lower atomic number materials (and for lower energies)

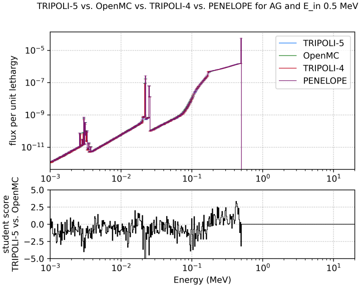

Figure 34 – Element Ag, $E_0 = 0.5$ MeV, TTB activated

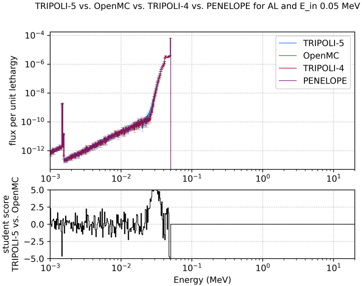

Figure 35 – Element Al, $E_0 = 0.05$ MeV, TTB activated

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Conclusion and perspectives

- Implementation of a routine to verify neutron physics (free gas and TSL) implemented in TRIPOLI-5®
  - Comparison of the neutron spectrum with TRIPOLI-4® / OpenMC over 500 isotopes from JEFF-3.3
  - TRIPOLI-5® is in excellent agreement with OpenMC for neutron physics
  - The investigation of discrepancies with respect to TRIPOLI-4® is more complicated because of non-equivalent nuclear data
- Some inconsistencies have been detected in nuclear data for neutron physics as well as problems in the sampling of codes.
- Excellent agreement for unresolved resonance range modeled with PURR probability tables between TRIPOLI-5® and OpenMC
- Perspective : compare the results obtained with PURR and CALENDF probability tables
- Photon physics : good agreement with other codes but the statistical HB-test is not adapted due to important differences of modeling among all codes. Future work : resort to a convenient benchmark.