DE LA RECHERCHE À L'INDUSTRIE

BENCHMARKING OF NUCLEAR DATA FOR TRIPOLI-5

Technical Meeting on the Compilation of Nuclear Data Experiments for Radiation Characterization, AIEA | 10-14 October 2022

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DES/ISAS/DM2S/SERMA

Commissariat à l'énergie atomique et aux énergies alternatives - www.cea.fr

Outline

Introduction

- PATMOS : new massively parellel Monte Carlo transport code developed at CEA
- Recent implementation of neutron physics
  - Free gas model
  - Thermal scattering law (TSL)
- 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 (562) from library JEFF-3.3
  - Representative energies of the neutron spectrum in a reactor

Outline

The TRIPOLI-4®5 project

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

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	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

EDF

framatome

IRSN
INSTITUT DE RADIOPROTECTION
ET DE SÛRETÉ NUCLÉAIRE

The mini-app PATMOS (2015–)

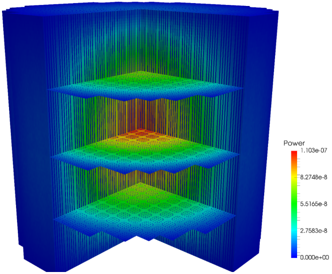
E. Brun, S. Chauveau, F. Malvagi, PATMOS : A prototype Monte Carlo transport code to test high performance architectures, in Proc. MC 2017, Jeju, Korea, April 16-20 (2017)

A testing framework for . . .

- code architecture
  - multi-level parallelism
- coupling
- new technologies
  - GPGPU
  - vectorisation

Some collaborations

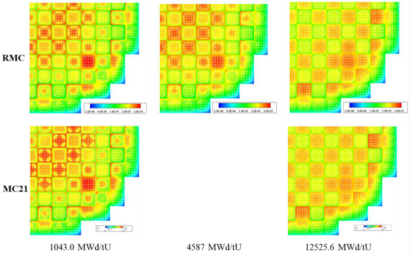
- Arm, Intel, Nvidia
- CEA/DAM, universities
- EU project DEEP-SEA

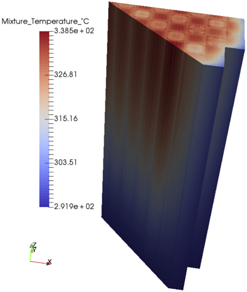


Grand Challenge on Tera1000-2 : a PWR irradidation cycle (6 $\times$ 10^6 regions) with four levels of parallelism (10^7 CPU-hours)

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



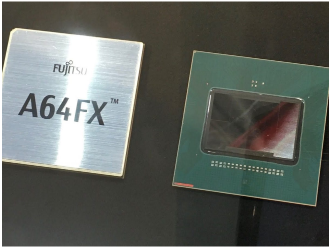


K. Wang *et al.*
Prog. Nucl. Energy 98 (2017) 301–312

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

Technological constraints

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



Work-flow et technological choices

Work-flow

- continuous integration
- code review
- modularity

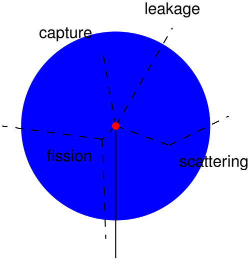
technologies

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

Outline

Description of the benchmark

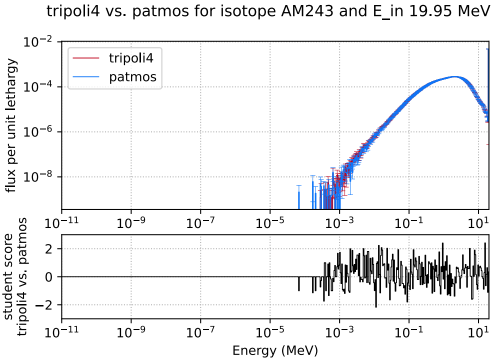
- Test configuration :
  - Sphere, radius R=30 cm
  - One single isotope
  - Isotropic, mono-energy, point source
  - Observable : flux per unit lethargy (collision estimator)
  - Number of particles : 10^6
  - Density $\gamma(E) = \frac{1}{R\hat{\sigma}_{t,i}(E)}$ with $\hat{\sigma}_{t,i}(E)$ a 4-group 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
- 5058 validation configurations
- Code-to-code comparisons between 3 Monte Carlo transport codes :
  - OpenMC
  - TRIPOLI-4®
  - PATMOS

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)

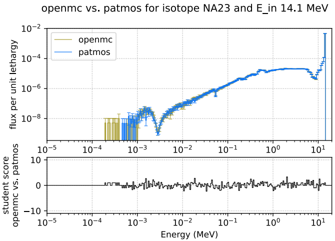


Figure 1 – Test HB : success

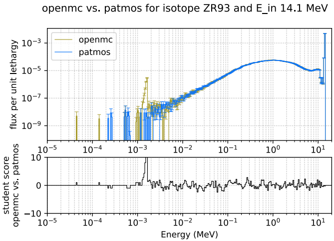


Figure 2 – Test HB : failure

Example of simple fix-up : missing reactions

- Initially PATMOS did not take into account some reactions

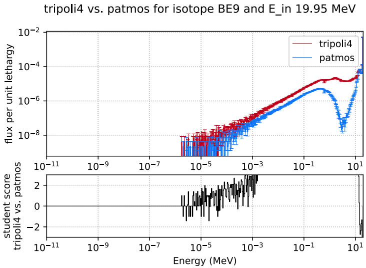


Figure 3 – Flux without MT reactions 875 - 891

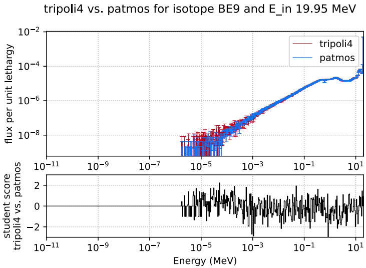
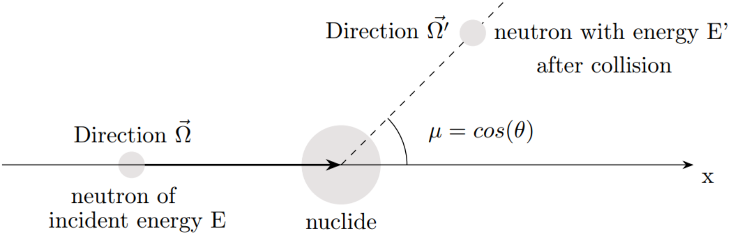


Figure 4 – Flux with MT reactions 875 - 891

An intermediate tool to verify the sampling of reactions

- 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

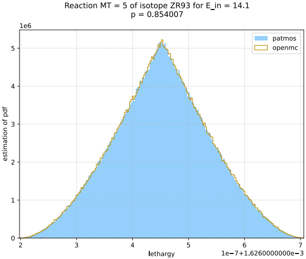


Figure 5 – KS test success : $p > 0.05$

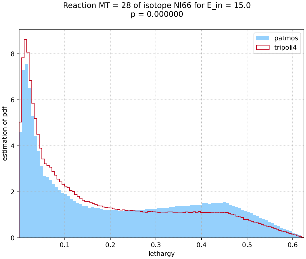


Figure 6 – KS test failure : $p < 0.05$

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

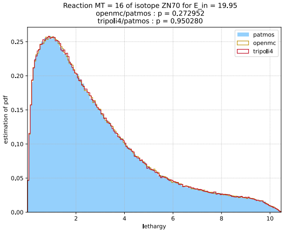


Figure 7 – Sampling of the energy distribution, ZN70 at 293K, MT 16, $E_0 = 19.95$ MeV

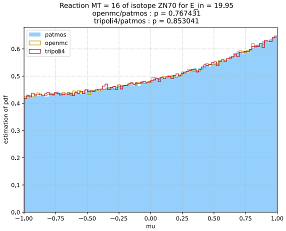
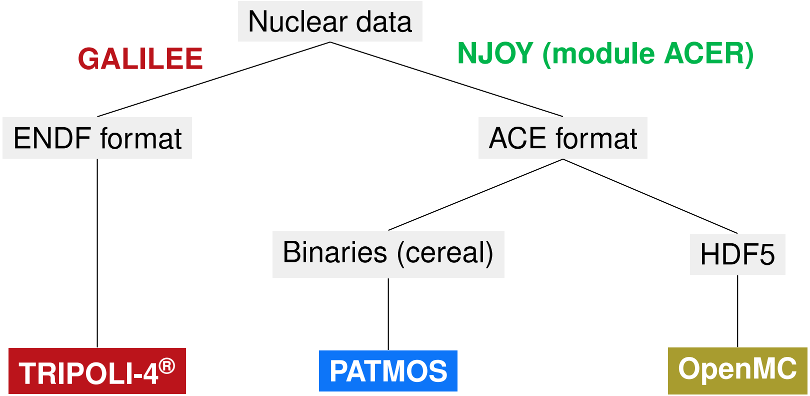


Figure 8 – Sampling of the cosine distribution, ZN70 at 293K, MT 16, $E_0 = 19.95$ MeV

Outline

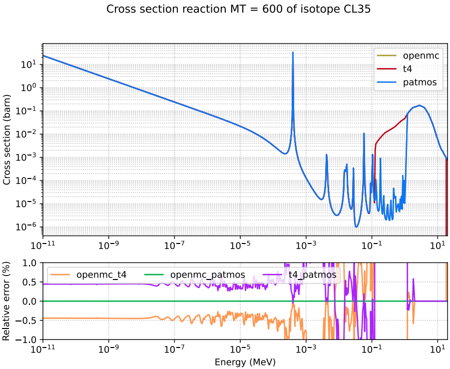
Post-treatment process of nuclear data

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



Example of discrepancies : microscopic cross section

- Full agreement on the cross section between PATMOS et OpenMC (same ACE files)
- For 22 MT reactions (over 14 isotopes), discrepancies on the cross section are observed between TRIPOLI-4®and PATMOS/OpenMC



Discrepancies in (tabulated) distributions

- 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 : PATMOS/OpenMC)
- Very frequent cases for all distributions involving tabulations with pdf/cdf tables
- Different size of tables between ACE and ENDF

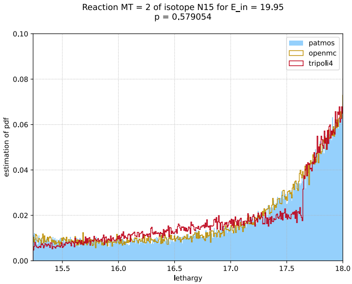


Figure 9 – Energy distribution for NI15, MT 2, $E_0 = 19.95$ MeV

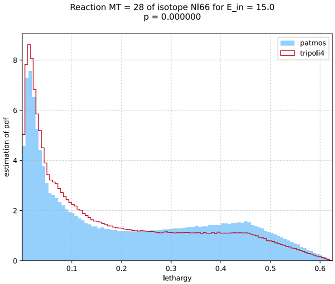


Figure 10 – Energy distribution for NI66, MT 28, $E_0 = 15$ MeV

Problem 1 : 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 PATMOS 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

Problem 1 : level-scattering reactions (2/3)

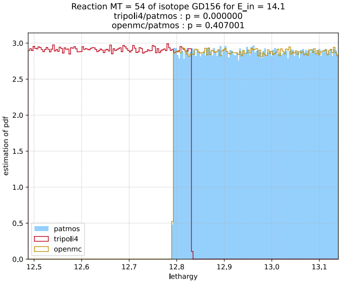


Figure 11 – Energy distribution for GD156, MT 54, $E_0 = 14.1$ MeV

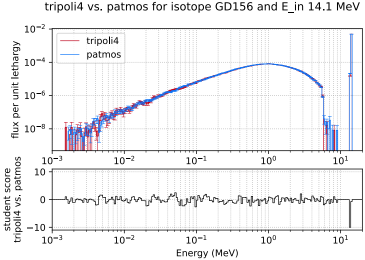


Figure 12 – Corresponding flux comparison TRIPOLI-4®/PATMOS

Problem 1 : 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 13 – List of isotopes and reactions with $E_{th} \neq -Q\frac{A+1}{A}$

Problem 2 : Case CM249 at 293K, MT 18

- Isotope CM249 at 293 K with $E_0 = 19.95$ MeV :
  - test HB KO for PATMOS/TRIPOLI-4®
  - test HB KO for PATMOS/OpenMC
  - test HB OK for TRIPOLI-4®/OpenMC

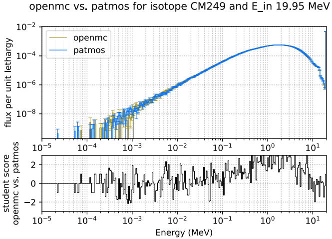


Figure 14 – Flux before correction

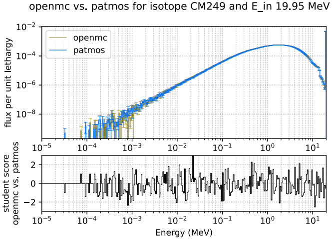


Figure 15 – Flux after correction

- In a case where there is no delayed neutrons explicitely provided by ACE, PATMOS used ν_{prompt} instead of ν_{total}

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

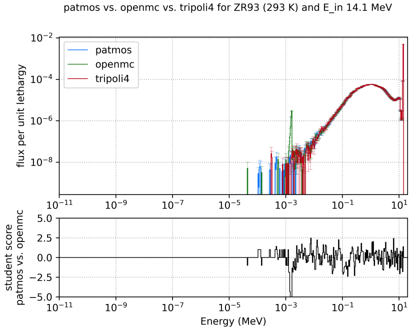


Figure 16 – Flux before correction

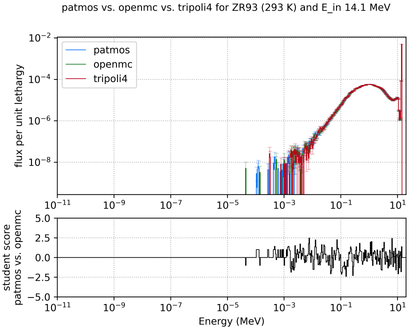


Figure 17 – Flux after correction

Problem 3 : 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.

```
diff --git a/src/physics.cpp b/src/physics.cpp
index 472fd1cd0..7d1d9a138 100644
--- a/src/physics.cpp
+++ b/src/physics.cpp
@@ -1127,6 +1127,10 @@ void inelastic_scatter(const Nuclide& nuc,
const Reaction& rx, Particle& p)

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

Figure 18 – Fix-up in OpenMC

"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, for 6 isotopes at 293K (CR50, CR53, CR54, CS135, HF174 and HF176), there are interactions such that : $E_{min} > E_{th}$

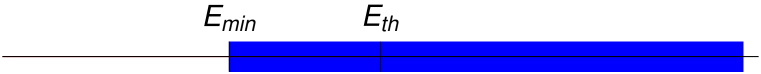


Figure 19 – Normal case

Figure 20 – Unexpected case

Isotope	MT	Threshold energy	Minimal energy	Relative discrepancy
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 21 – 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

- PATMOS checks the consistency of nuclides when created
- From these consistency checks, we could observe small problems in ACE files from JEFF-3.3 library at 293K :
  - Some cumulative fonctions distributions (cdf) are not sorted in the ascending way
  - Some tables associated to pdf/cdf are not sorted in the ascending way
  - Isotopes : AG110M, CD115M, CR50, CR53, CR54, NE20, SI32
  - ACE files generated from **njoy 2016.42, at NEA on 2018-10-01**

Summary of the results (free gas)

Summary of the code-to-code comparison for the flux (5058 configurations) :

- PATMOS/TRIPOLI-4® : 91.7% of success rate (HB test)
- PATMOS/OpenMC : 99.9% of success rate (HB test), 7 failures including :
  - 6 'false negatives' (we obtain a passing HB test after modification of the seed in one code), consistent with the probability of rejection for HB test (α=0.1)
  - 1 resolved case : ZR93 at 293K, E_0 = 14.1 MeV

Outline

Inelastic 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 1e-16-1e-5 for NJOY
- cdf[0] around 1e-8 for FRENDY
- Some negative energies can be produced because of that problem within the sampler (with both OpenMC and PATMOS) 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 (MG in metal) detailed further...

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

Other inconsistencies

- **All cumulative density functions involved in 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 PATMOS (because of our consistency checks)
- Non-sorted equiprobables/skewed tables, etc.
- We can sort them but does that make sense for skewed distributions ?

- Perfect agreement OpenMC/PATMOS for all distributions (apart from one single case : energy distribution of the inelastic reaction of MG24 in metal at 20K)

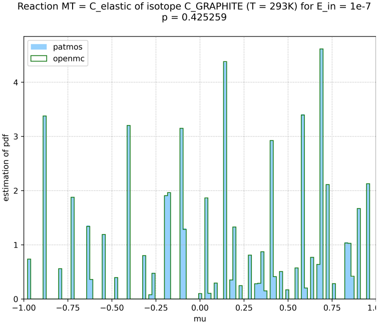


Figure 22 – Cosine distribution for C in graphite, $E_0 = 0.1$ eV, coherent elastic reaction

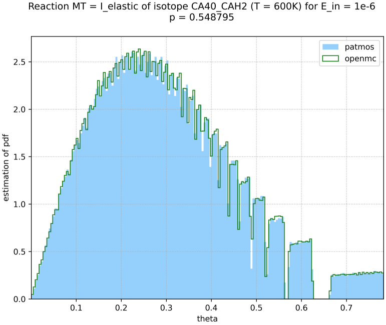


Figure 23 – Angle distribution for CA40 in CAH2, $E_0 = 0.1$ eV, inelastic reaction

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

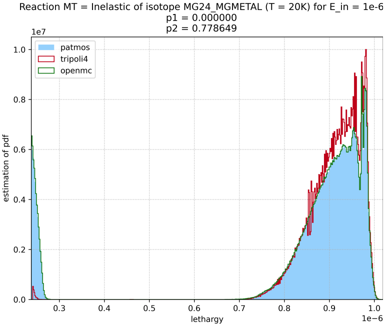


Figure 24 – Before retreament in PATMOS

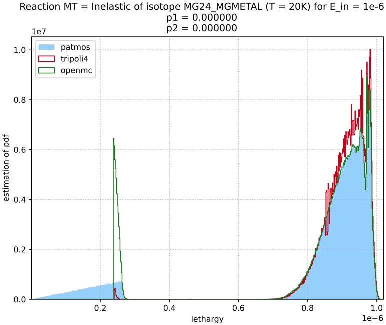


Figure 25 – After retreament in PATMOS

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

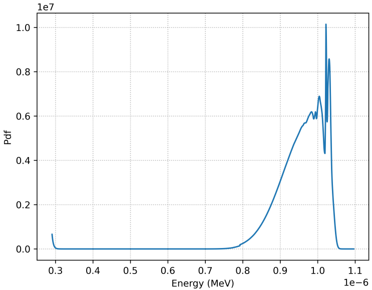


Figure 26 – PDF before retreament in PATMOS

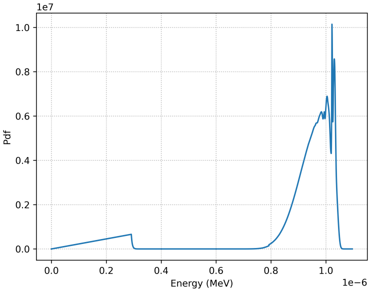


Figure 27 – PDF after retreament in PATMOS

Sampling of thermal reactions : PATMOS/TRIPOLI-4®

- Unperfect agreement TRIPOLI-4®/PATMOS for some distributions
- Several explanations :
  - inelastic reactions : different size of values/pdf/cdf for energy distributions in continuous mode
  - incoherent elastic reactions : different sampling (see next slides)

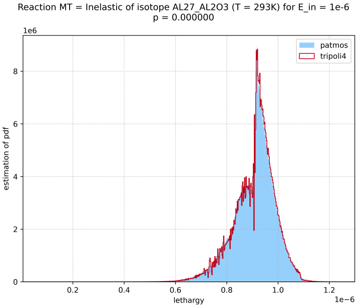


Figure 28 – AL27 in AL2O3 at 293K, E_0 =1eV, inelastic reaction

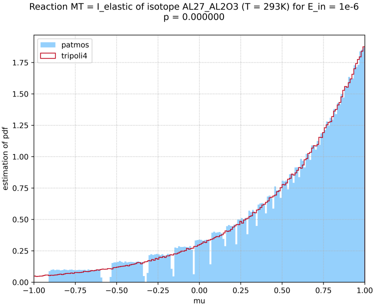


Figure 29 – AL27 in AL2O3 at 293K, E_0 =1eV, incoherent elastic reaction

Incoherent elastic reaction and Debye-Waller factor

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

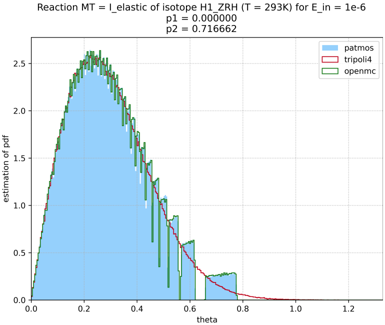


Figure 30 – PATMOS uses ACE data

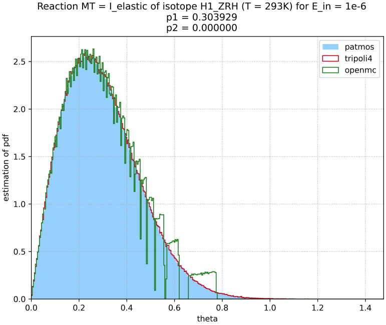


Figure 31 – PATMOS uses Debye-Waller factor from ENDF files

- No impact of the sampling of the incoherent elastic reaction on the flux for H1 in ZRH at 293K : the discrepancy stems probably from another distribution (probably in inelastic reaction)

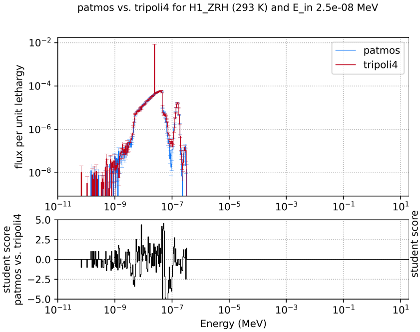


Figure 32 – PATMOS uses ACE data

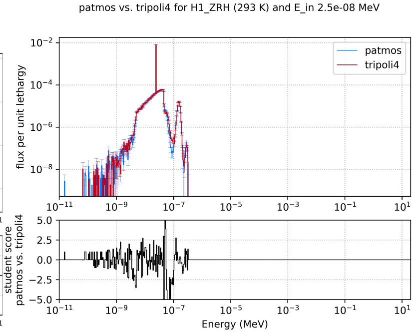


Figure 33 – PATMOS uses Debye-Waller factor from ENDF files

Errors in some thermal ACE files : wrong NATOM (1/4)

- Total cross sections do not match between TRIPOLI-4®and PATMOS/OpenMC for some isotopes (namely H1 in ZRH at 293K)
- There is a problem with the NATOM parameter in thermal ACE files produced by AEN (available on the website)
- Works only for H1 in H2O or similar stoechiometry

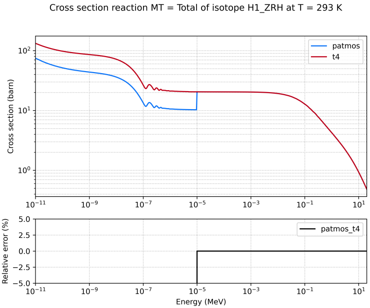


Figure 34 – Thermal ACE file from AEN

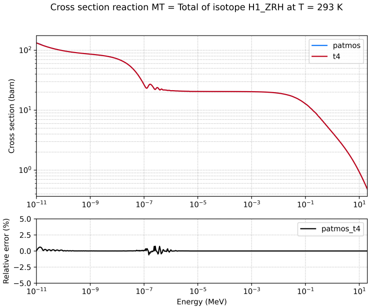


Figure 35 – PATMOS uses re-processed thermal ACE

- Focus on the inelastic reaction : factor of 2 between associated cross section read by PATMOS/OpenmC and by TRIPOLI-4®

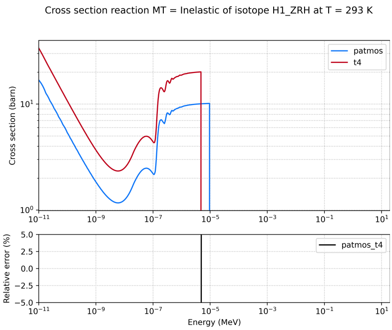


Figure 36 – Thermal ACE file from AEN

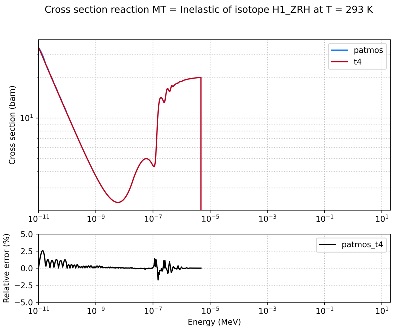


Figure 37 – PATMOS uses re-processed thermal ACE

- Focus on the incoherent elastic reaction : factor of 2 between associated cross section read by PATMOS/OpenmC and by TRIPOLI-4®

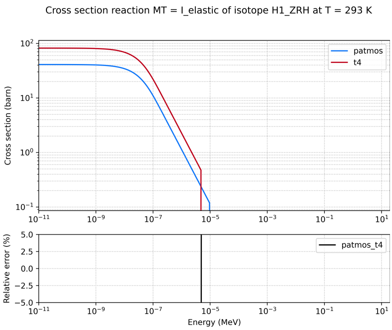


Figure 38 – Thermal ACE file from AEN

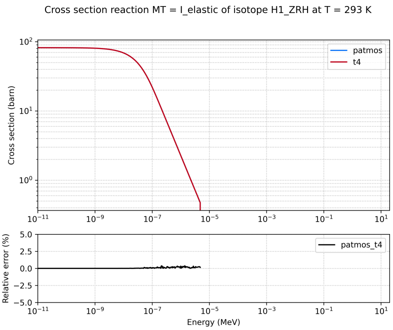


Figure 39 – PATMOS uses re-processed thermal ACE

- Impact on the flux : huge discrepancy between TRIPOLI-4®and PATMOS/OpenMC

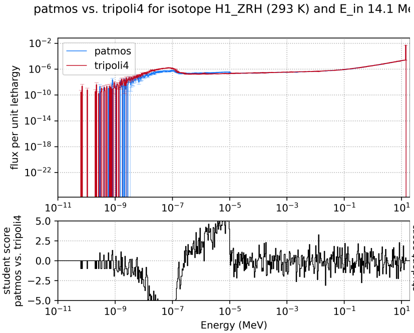


Figure 40 – Thermal ACE file from AEN

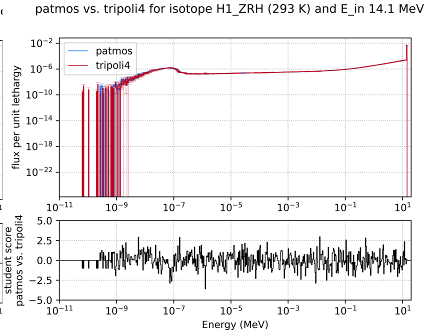


Figure 41 – PATMOS uses re-processed thermal ACE

Discrepancies due to (TSL) threshod

- Some discrepancies stem from the TSL threshold that differ from a code to another one

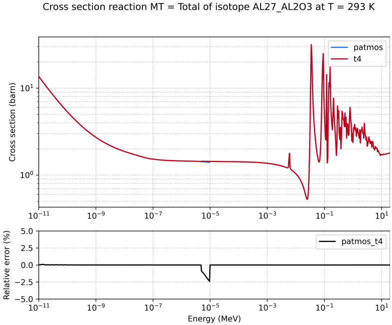


Figure 42 – ACE data with a threshold at 9.86 eV

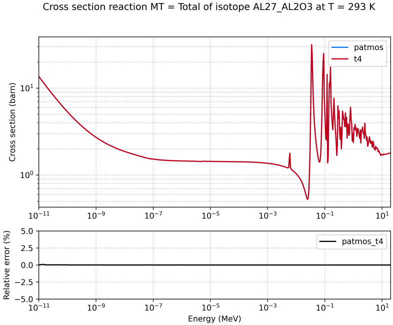


Figure 43 – ACE data with a threshold at 4.95 eV

Degradation due to ACE module

- For some itosopes, the size of the energy grid is significantly reduced (factor around 2-3) from ENDF files to corresponding ACE files
- This can lead to relative errors around 2.5% on interpolated cross sections for H1 in H2O at 293K at low energy.

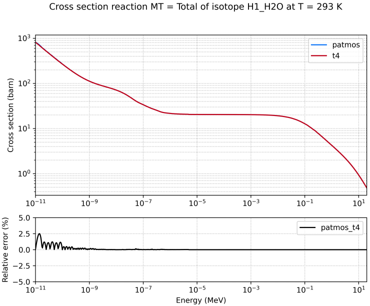


Figure 44 – Interpolated total cross section for H1 in H2O

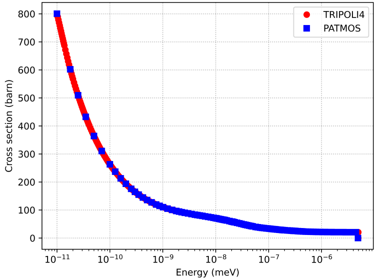


Figure 45 – Inelastic cross sections (points of the energy grid only)

Comparisons PATMOS/OpenMC

- We performed the comparison over about 217 configurations (configuration = isotope, temperature, energy of the source)
- HB test success rate : 100%

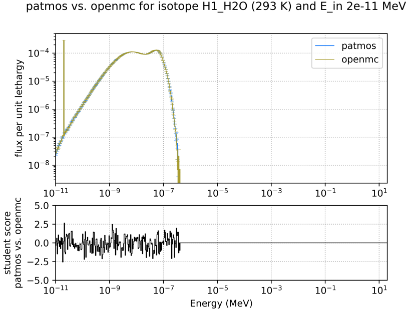


Figure 46 – H1 in H2O at 293K, E_0 = 2e-11 MeV

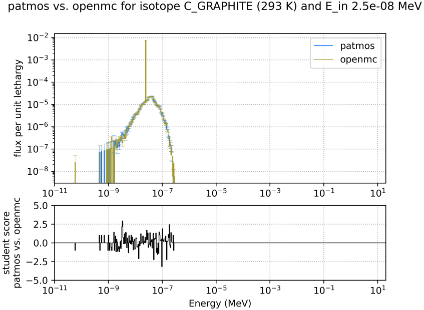


Figure 47 – C in graphite at 293K, E_0 = 2.5e-08 MeV

Comparisons PATMOS/TRIPOLI-4®

- We performed the comparison over about 217 configurations (configuration = isotope, temperature, energy of the source)
- HB test success rate : $\sim$ 70%

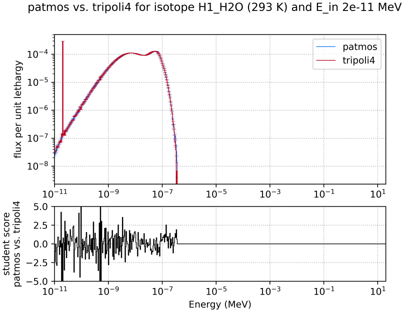


Figure 48 – Interpolated total cross section for H1 in H2O

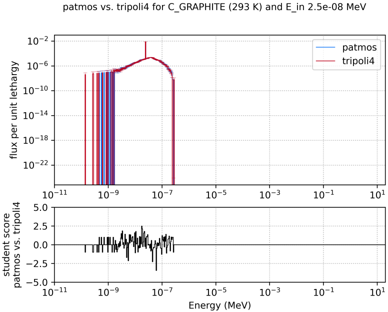


Figure 49 – Inelastic cross sections (points of the energy grid only)

Conclusion

- Implementation of a routine to verify neutron physics implemented in PATMOS
  - Comparison of the flux spectrum with TRIPOLI-4® / OpenMC
  - Free gas model (without URR) : more than 5000 validation configurations from library JEFF-3.3
  - Thermal scattering : around 200 validation configurations from library JEFF-3.3
- Final success rate of the code-to-code comparison :
  - Free gas :
    - PATMOS / TRIPOLI-4® : 91.7%
    - PATMOS / OpenMC : 99.9% (6 'false negative' cases + 1 resolved case)
  - S(α,β) :
    - PATMOS / TRIPOLI-4® : $\sim$ 70%
    - PATMOS / OpenMC : 100%
- PATMOS is in excellent agreement with OpenMC, 2 discrepancies only :
  - ZR93 at 293K, due to MT 5 and yield 0
  - MG24 in metal at 20K, due to a problem in nuclear data for the inelastic reaction (discrepancy is spotted only from the sampling of cosine distributions)