



Status of the TSL activities at CEA/Cadarache in the framework of the Nausicaa collaboration

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Outlines

- × **H₂O and UO₂ measurements and Monte-Carlo analysis**
- × **Generation of TSL covariances**
- × **Future TSL activities for SG48**



H2O measurements and Monte-Carlo analysis

Inelastic neutron scattering measurements on IN5, IN4 and IN6 time-of-flight spectrometers

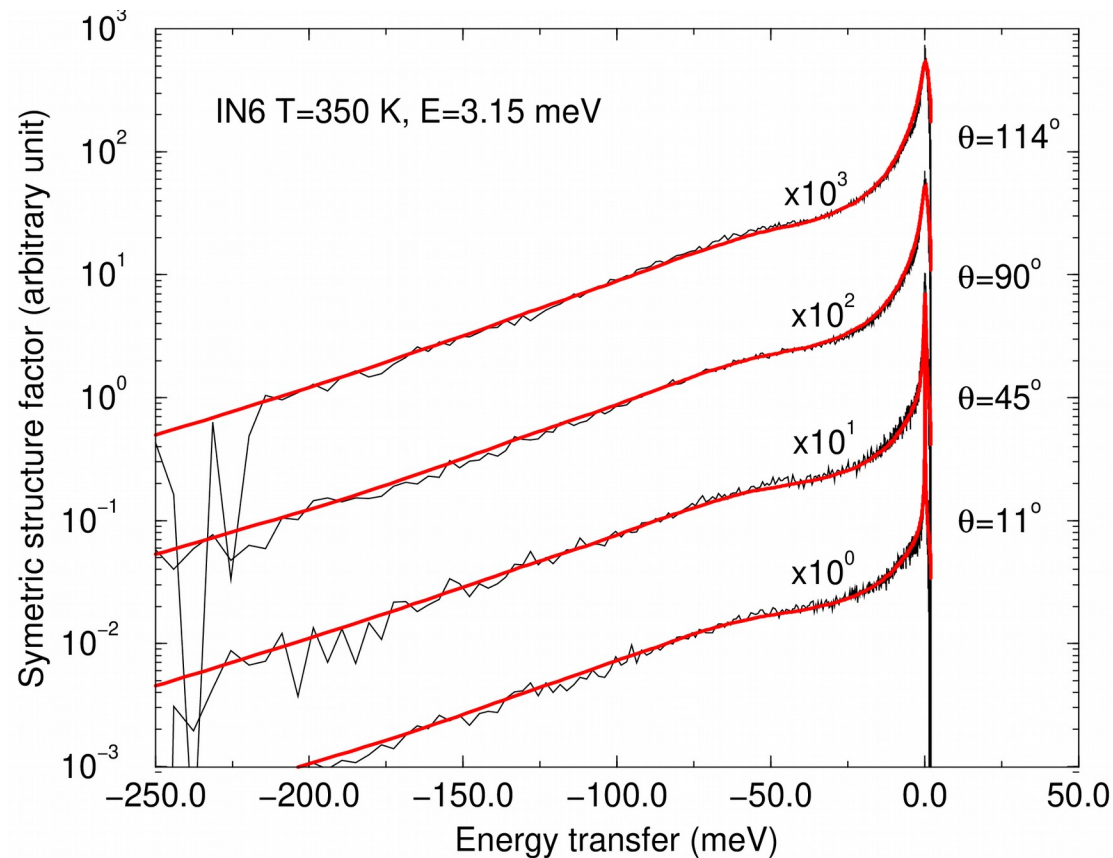
| TOF | Author | Ref. | H ₂ O sample | λ | E | Temperature | Pressure |
|-----|----------------|------|-------------------------|-----------|----------|----------------------|-----------------------------------|
| IN4 | Farhi et al. | [34] | hollow cylinder | 1.1 Å | 67.6 meV | 294, 311, 323 K | 1 bar |
| | Farhi et al. | [34] | hollow cylinder | 2.2 Å | 16.9 meV | 294 K | 1 bar |
| | Jaiswal et al. | [35] | cylinder | 2.4 Å | 14.2 meV | 300, 350, 430, 494 K | 1, 42, 94, 115, 147, 176, 185 bar |
| IN5 | Farhi et al. | [34] | hollow cylinder | 2.0 Å | 20.5 meV | 286, 293, 302 K | 1 bar |
| | Farhi et al. | [34] | hollow cylinder | 5.0 Å | 3.27 meV | 291, 302, 311 K | 1 bar |
| | Qvist et al. | [36] | capillaries | 5.0 Å | 3.27 meV | 283, 293 K | 1 bar |
| | Qvist et al. | [36] | capillaries | 8.0 Å | 1.28 meV | 283, 293 K | 1 bar |
| | Qvist et al. | [36] | capillaries | 12.0 Å | 0.57 meV | 283 K | 1 bar |
| IN6 | Jaiswal et al. | [35] | cylinder | 5.1 Å | 3.15 meV | 350, 494 K | 1, 70, 470 bar |

Data taken from PhD thesis of Qvist (2011), Ferran (2014), Scotta (2016), Jaiswal (2017)



H2O measurements and Monte-Carlo analysis

Symmetric form of the water dynamic structure factor **T=350**

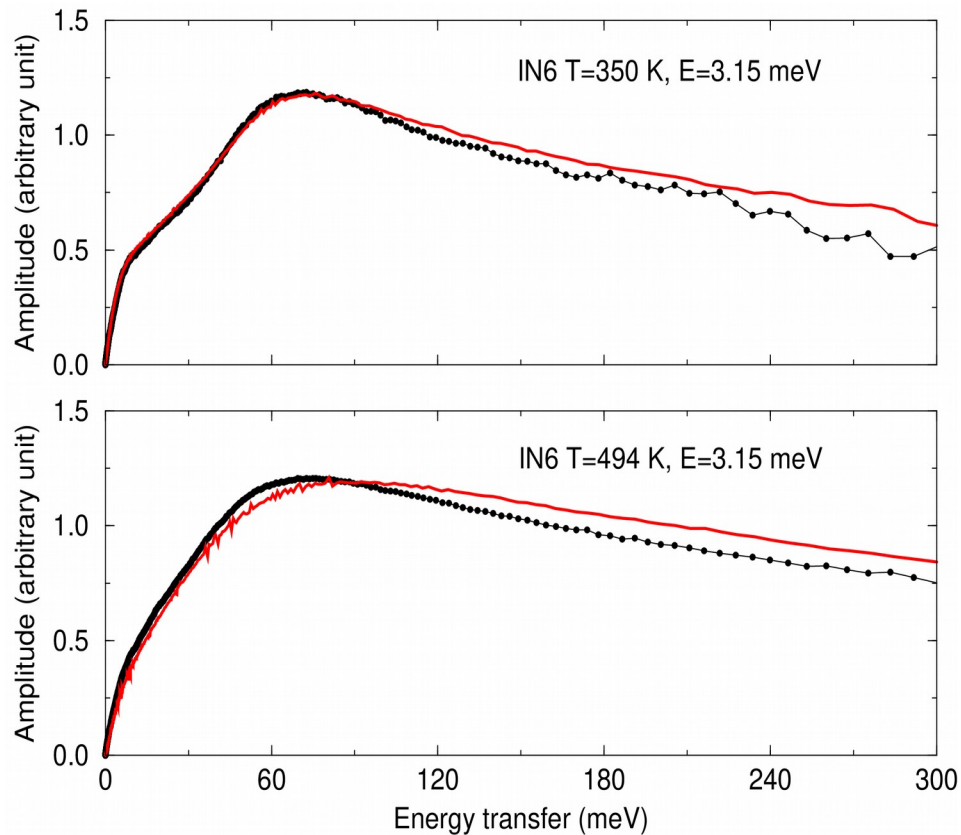


Analysis performed with the Monte-Carlo neutron transport code **TRIPOLI4** by using the **CAB model** for H in H2O (=ENDF\B-VIII)



H2O measurements and Monte-Carlo analysis

Experimental density of states at 350 and 494 K



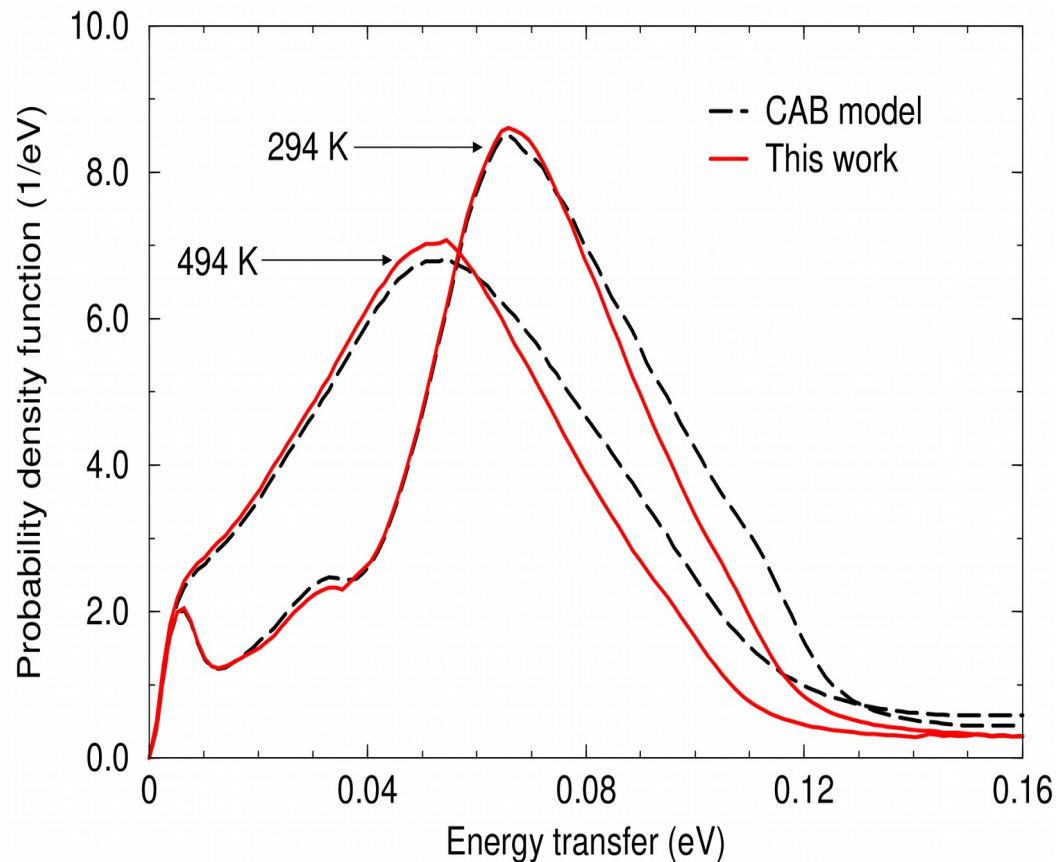
Water Librational mode:

- Reasonable agreement between the data and the TRIPOLI4 simulations (CAB model)
- Slight improvement is needed (frequency shift is overestimated at elevated temperature)



H₂O measurements and Monte-Carlo analysis

**Iterative Bayesian least-squares fitting procedure
implemented in the nuclear data code CONRAD**

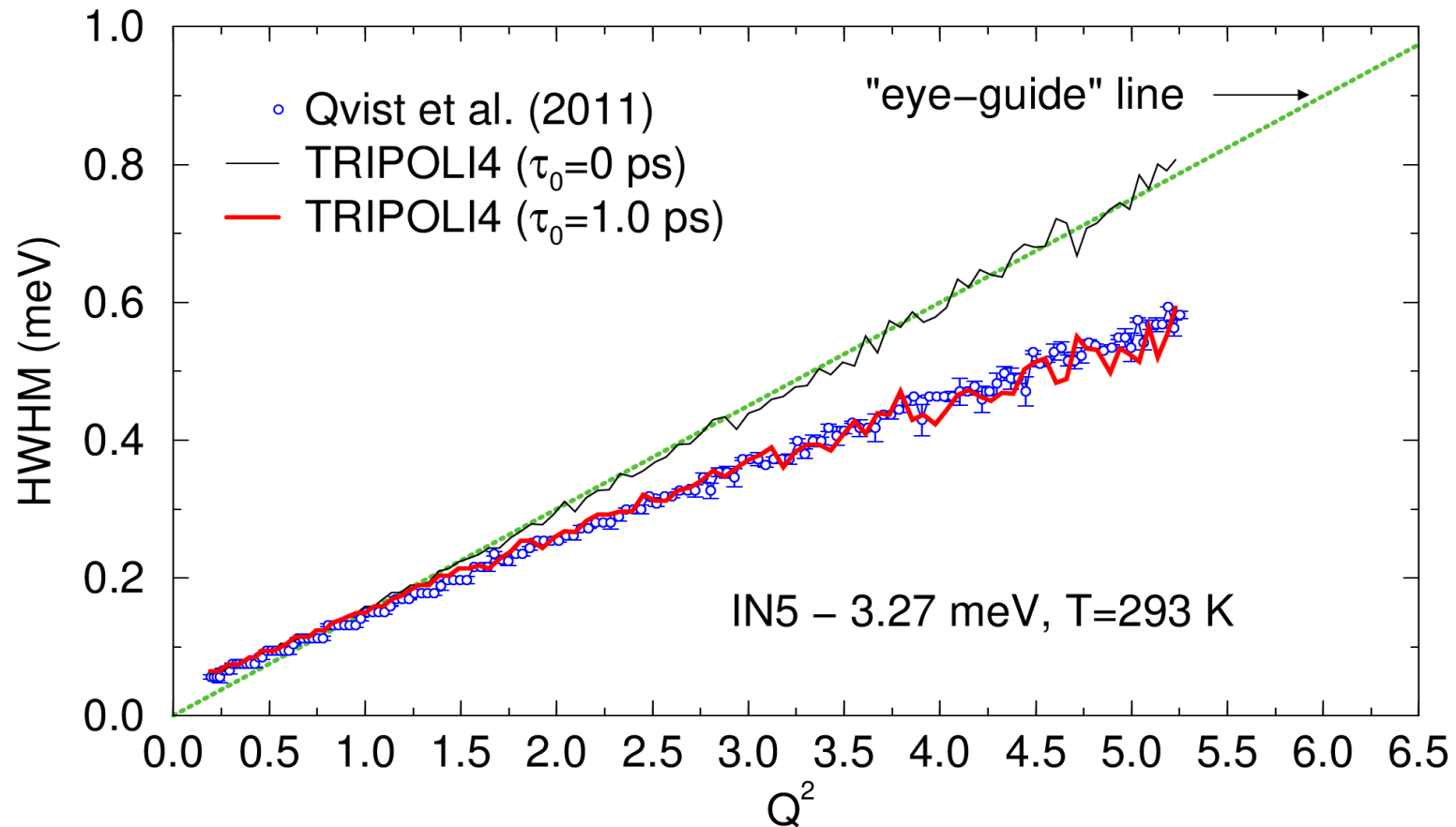


ILL data provide a narrower
water librational band than
predicted by MD simulations



H2O measurements and Monte-Carlo analysis

QENS data analysis

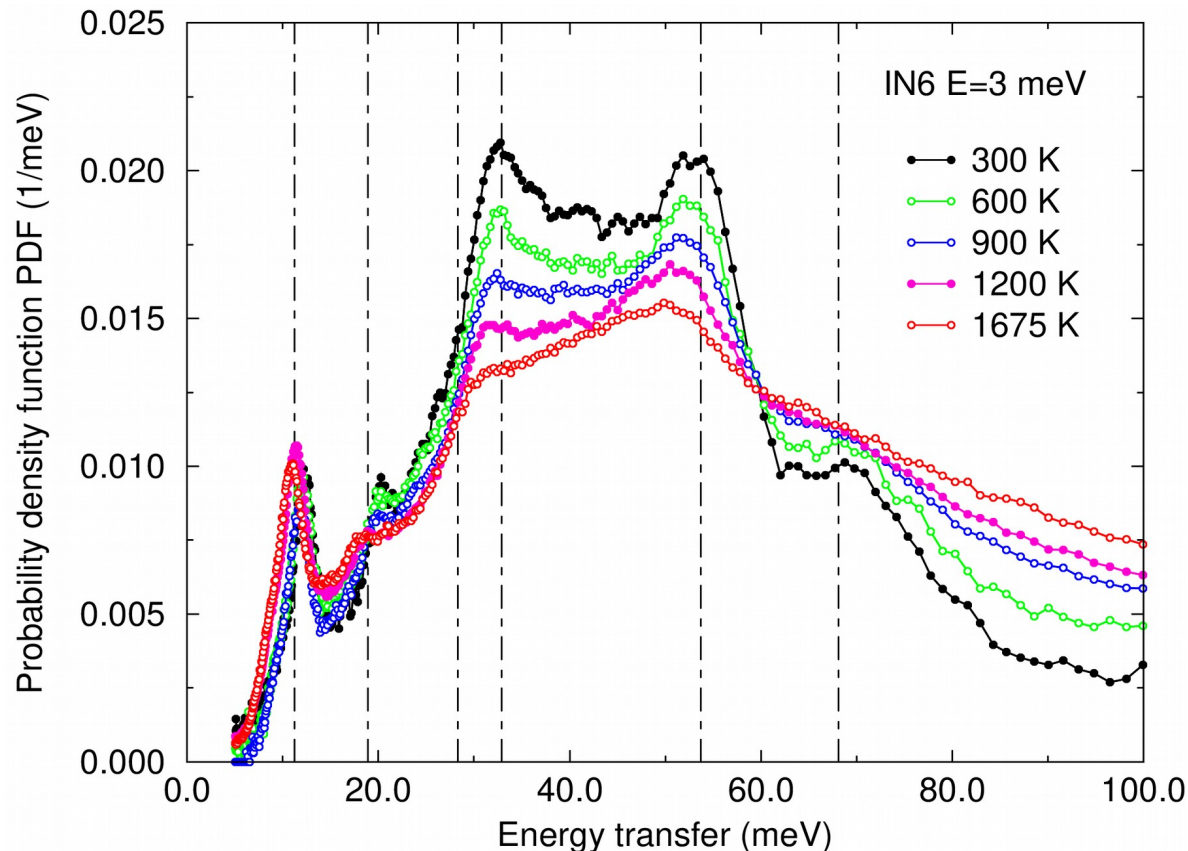


Translational diffusion part : Egelstaff-Schofield diffusion model with a Singwi-Sjolander residence time correction



UO₂ measurements and Monte-Carlo analysis

Inelastic neutron scattering measurements on IN6 time-of-flight spectrometer (T=294 to 1675 K)

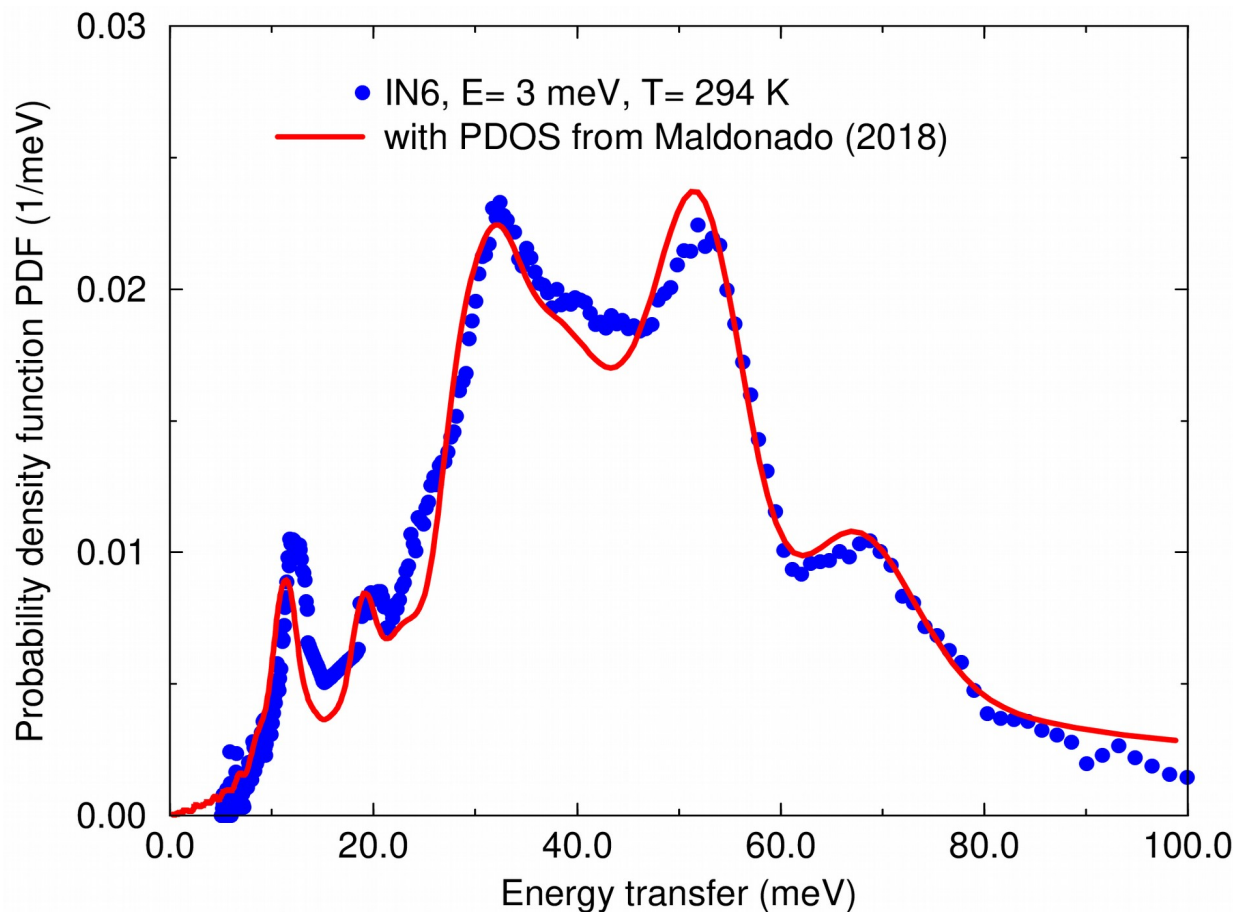


Data taken from PhD thesis of Scotta (2016) and Xu (ongoing)



UO₂ measurements and Monte-Carlo analysis

Experimental density of states at 294 K



Analysis of the data with the neutron transport code TRIPOLI4 by using the abinitio density of states of Maldonado (Uppsala University)



Generation of TSL covariances

Different strategies were investigated:

- × Covariance matrix between MD parameters
- × Covariance matrix between LEAPR parameters
- × Covariance matrix between $S(\alpha, \beta)$

Propagation of TSL uncertainties to integral parameters via **direct perturbation method**, **Iterative Fission Probability** and **TMC**



Generation of TSL covariances

Table 6. Example of uncertainties on the reactivity (UOX configuration at room temperature) in pcm due to the nuclear data. The contribution of ^1H in H_2O comes from the present work. The other contributions were calculated with the covariance data base COMAC [32] developed at the CEA of Cadarache.

| Isotopes | (n,f) | Capture | (n,n) | (n,n') | (n,xn) | ν_{tot} | χ_{fast} | χ_{th} | Total |
|--------------------------------------|-------|---------|-------|--------|--------|-------------|---------------|-------------|-------|
| ^1H in H_2O | | 150 | 71 | | | | | | 166 |
| ^{10}B | | 26 | | | | | | | 26 |
| ^{16}O | | 97 | 14 | 2 | | | | | 98 |
| ^{90}Zr | | 11 | 72 | 4 | | | | | 72 |
| ^{91}Zr | | 27 | 30 | 2 | | | | | 40 |
| ^{92}Zr | | 27 | 20 | 2 | | | | | 33 |
| ^{94}Zr | | 2 | 8 | 2 | | | | | 8 |
| ^{96}Zr | | 2 | 6 | | | | | | 6 |
| ^{234}U | 1 | 6 | 2 | | | | | | 6 |
| ^{235}U | 104 | 174 | 13 | | | 276 | | 142 | 371 |
| ^{236}U | | 1 | | | | | | | 1 |
| ^{238}U | 29 | 165 | 83 | 38 | 18 | 32 | 9 | | 195 |
| Total | 108 | 303 | 137 | 39 | 18 | 277 | 9 | 142 | 470 |



Generation of TSL covariances

Table 7. Example of uncertainties on the reactivity (MOX configuration at room temperature) in pcm due to the nuclear data. The contribution of ^1H in H_2O comes from the present work. The other contributions were calculated with the covariance data base COMAC [32] developed at the CEA of Cadarache.

| Isotopes | (n,f) | Capture | (n,n) | (n,n') | (n,xn) | ν_{tot} | χ_{fast} | χ_{th} | Total |
|--------------------------------------|-------|---------|-------|--------|--------|-------------|---------------|-------------|-------|
| ^1H in H_2O | | 46 | 110 | | | | | | 119 |
| ^{10}B | | 8 | | | | | | | 8 |
| ^{16}O | | 114 | 24 | 4 | | | | | 117 |
| ^{90}Zr | | 11 | 24 | 7 | | | | | 27 |
| ^{91}Zr | | 13 | 16 | 4 | | | | | 21 |
| ^{92}Zr | | 8 | 22 | 4 | | | | | 24 |
| ^{94}Zr | | 2 | 59 | 3 | | | | | 59 |
| ^{96}Zr | | 2 | 13 | 1 | | | | | 14 |
| ^{235}U | 2 | 6 | 3 | 1 | | 5 | | 4 | 9 |
| ^{238}U | 114 | 88 | 80 | -60 | 25 | 35 | 12 | | 160 |
| ^{238}Pu | 1 | 70 | -20 | 1 | | 9 | 1 | | 67 |
| ^{239}Pu | 278 | 371 | 26 | 5 | | 57 | 0 | 126 | 484 |
| ^{240}Pu | 42 | 178 | -16 | -5 | 1 | 2 | 9 | | 182 |
| ^{241}Pu | 108 | 96 | 8 | | | 88 | 58 | | 179 |
| ^{242}Pu | 3 | 131 | 10 | 2 | | 2 | 1 | | 131 |
| ^{241}Am | -3 | 47 | 2 | 29 | | 1 | | | 47 |
| Total | 322 | 475 | 156 | -59 | 25 | 111 | 60 | 126 | 619 |



Future TSL activities for SG48

Future experimental program:

- × Actinide oxides: ThO_2 , NpO_2
- × Low enriched fuels: U_3Si_2 , UMo , UZrH
- × Structural materials: ZrY_4 , Nb

New processing code:

- × CINEL (from Shuqi Xu) in replacement of LEAPR+NCRYSTAL developed in Python with GPU acceleration