NRC "KURCHATOV INSTITUTE"
KURCHATOV NUCLEAR POWER COMPLEX

Verification of GRUCON Modules and Computing Procedures for Group Data Processing

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Topics

1. Last updates of GRUCON package
2. Inter-comparison of group cross sections and matrices, obtained through GRUCON and NJOY
3. Preliminary results of group data integral testing

   Conclusion

1. Last Updates and Developments

GRUCON/SXAEXFM is included to the package to process group neutron transitions and photon production matrices from the MF1, MF4, MF5, MF6, MF12, MF13, MF14, and MF15 ENDF data files

GRUCON/MATXS is included to the package to convert the group vectors and matrices from the internal *F* and *M* representation to **MATXS** input files of **TRANSX** (R.MacFarlane) interface code for **SN** transport calculations

GRUCON/ACTIV module is updated to use yields from the ENDF/B-VIII.0 MF6 file (in addition to MF3, MF8, MF9 and MF10 files) for activation cross section processing

GRUCON/ENDF input module is updated to perform check during reading data from the ENDF files and, optionally, to correct revealed inconsistencies (for example, inconsistent energy range of energy distribution and cross section definition)

2. Inter-comparison of group cross sections and matrices, obtained through GRUCON and NJOY

Verification conditions

Evaluated Data Library: ENDF/B-VIII.0

Processing Codes: GRUCON-2019.6,
NJOY-2016 (June 2019), PREPRO-2018

Auxiliary codes: PLOTTAB (D.Cullen)

Group data parameters: N199/G42/P7 (VITAMIN-B6)
T(K)=293.6
SIGZ (barns)= 1.e-10, 1., 10., 30., 100., 300., 1.e3, 1.e4,
1.e5, 1.e10

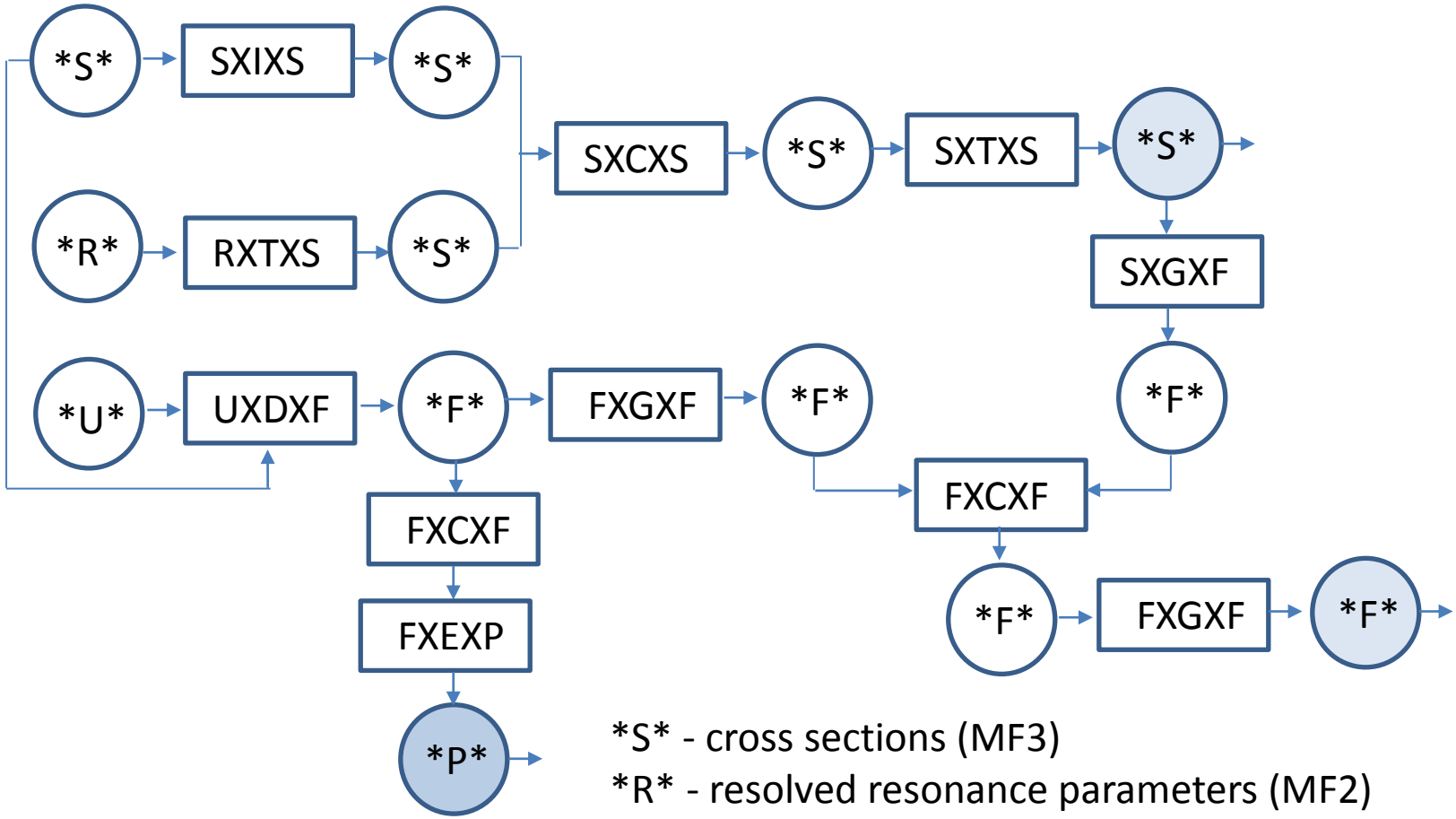
EPS=0.001 (GRUCON),

EPS=0.0001 (NJOY)

Compared data

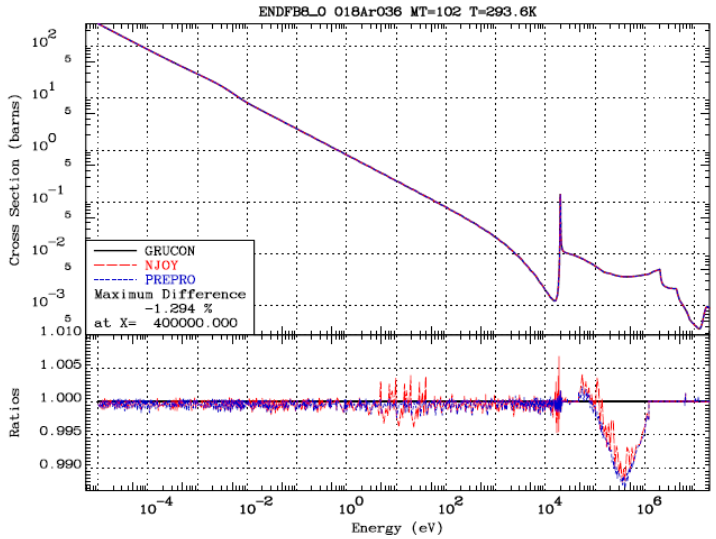
- Neutron point-wise cross sections
- Neutron group averaged cross sections
- Self-shielding factors
- Neutron group transition matrices
- Thermal scattering matrices for bound nuclide
- Free gas scattering matrices
- Photon production cross sections
- Photon production matrices
- Photo-atomic interaction cross sections
- Photo-atomic scattering matrices

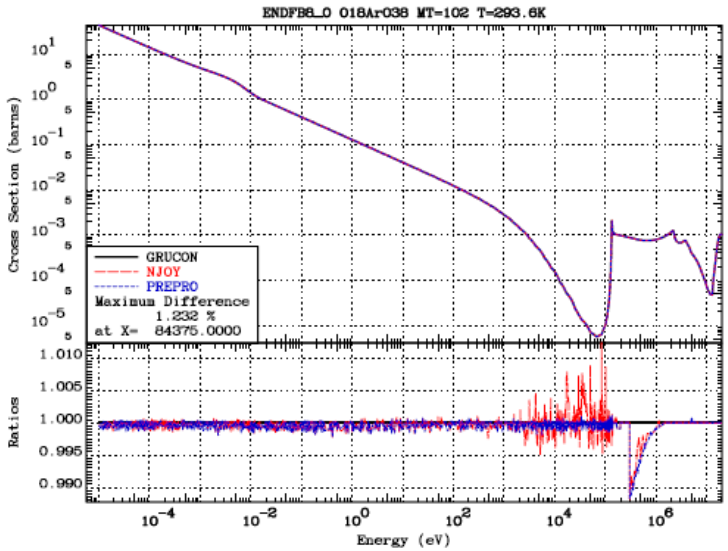
Cross section moments (*F*) and subgroup parameters (*P*) computing procedure

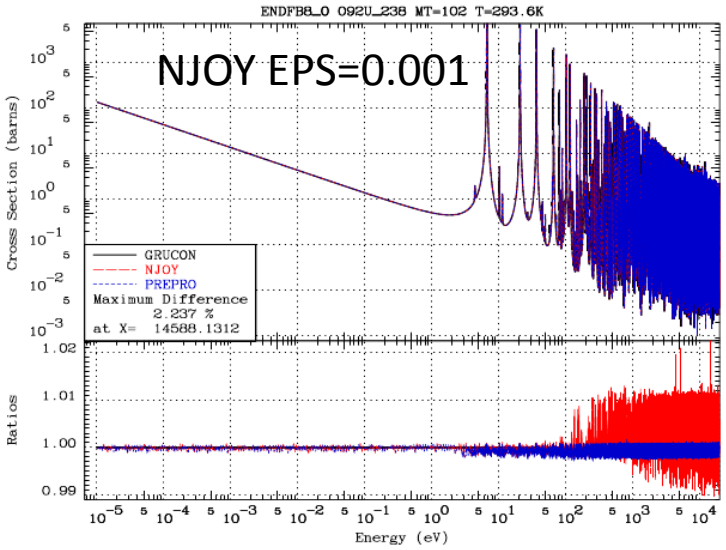


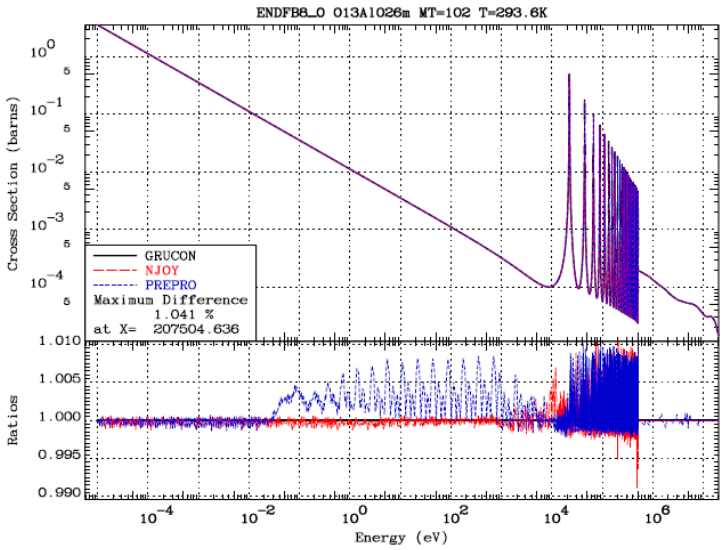
S - cross sections (MF3)
R - resolved resonance parameters (MF2)
U - unresolved resonance parameters (MF2)

Revealed cases of discrepancies

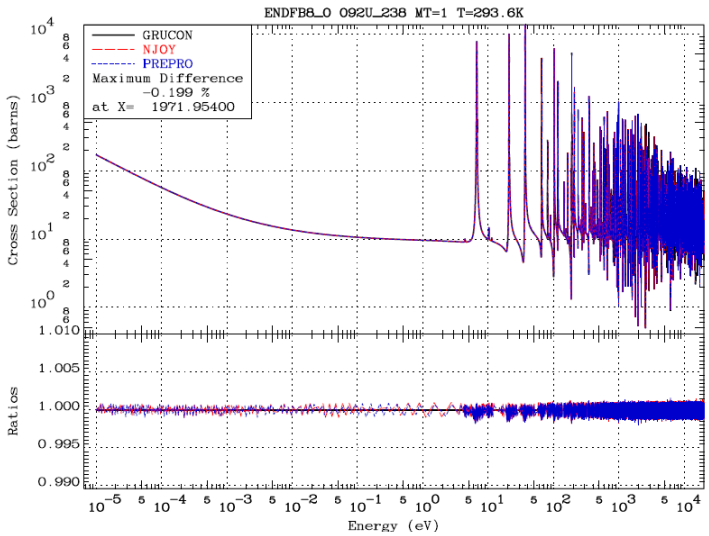


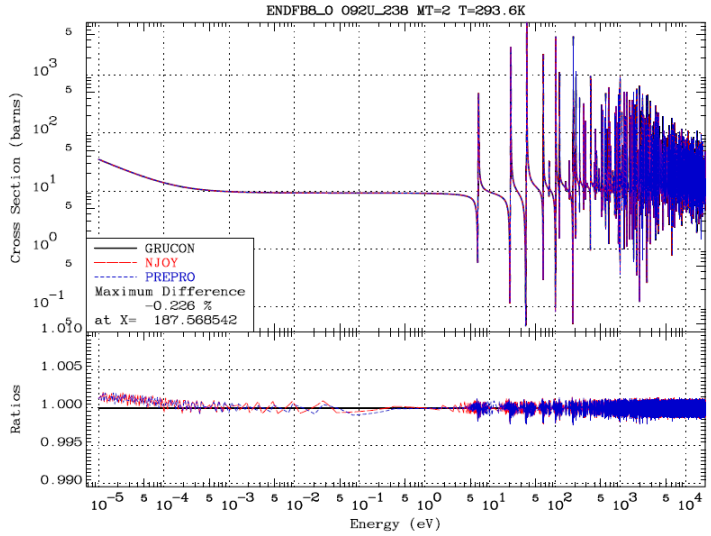


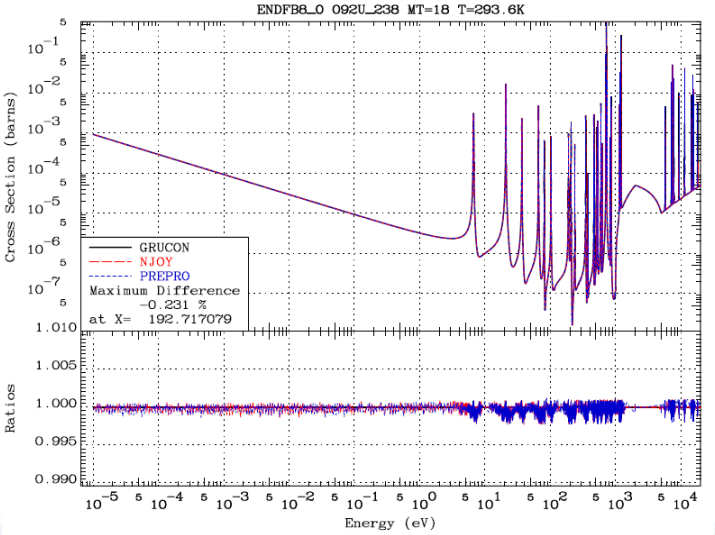


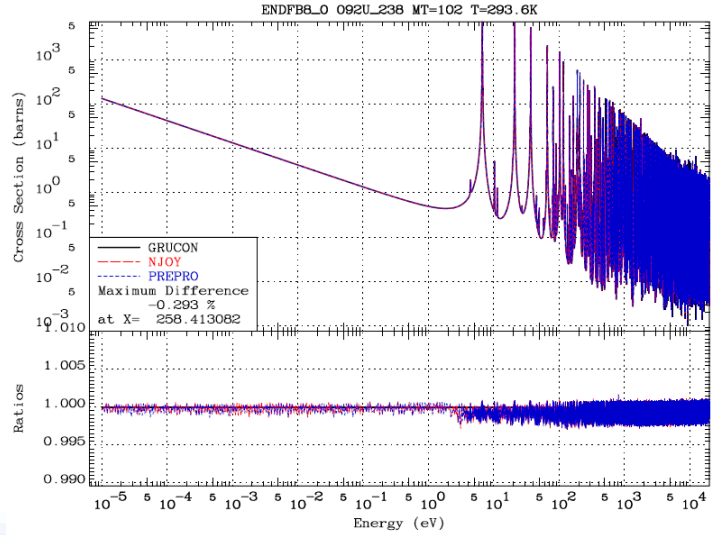


U238: Reconstructed point-wise cross sections (resolved resonance range)

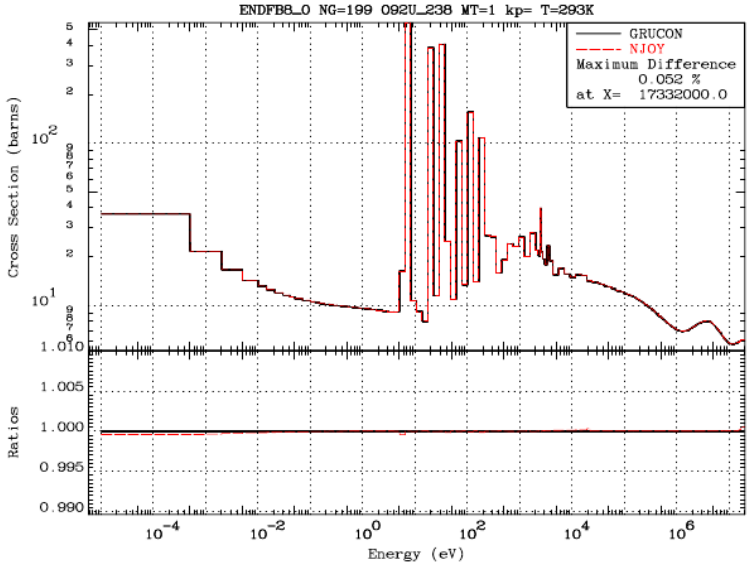


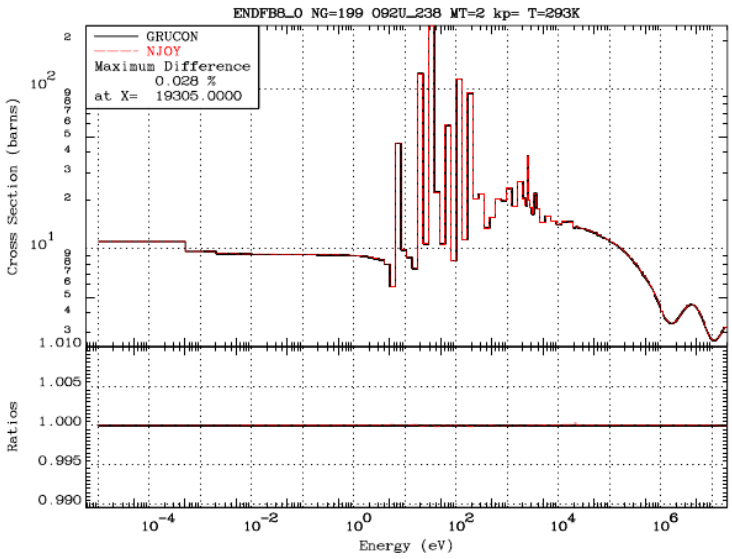


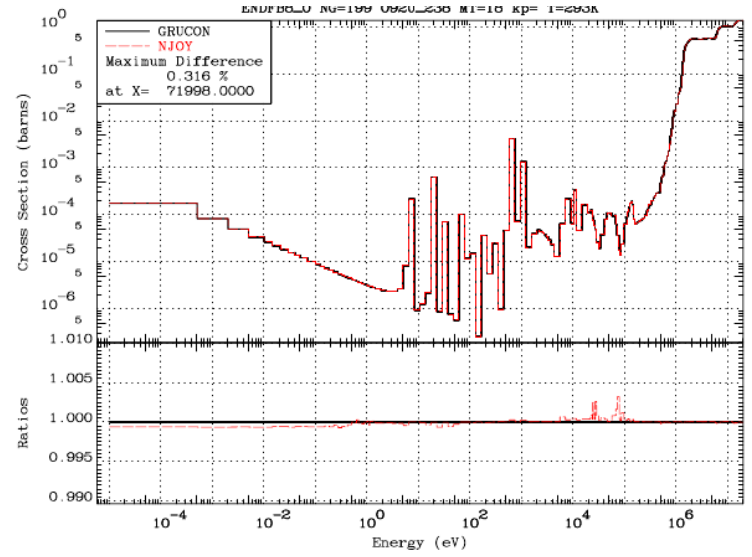


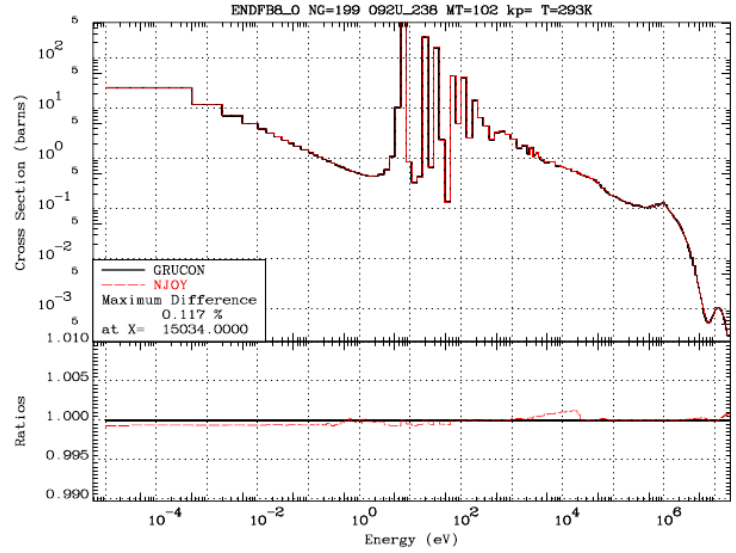


U238: Group Cross Sections

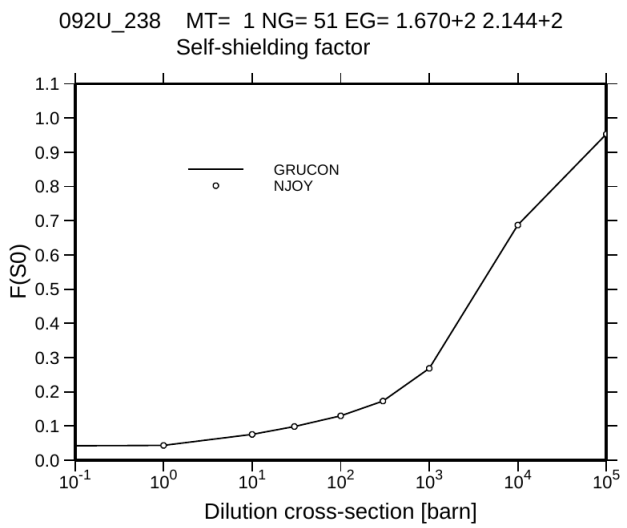


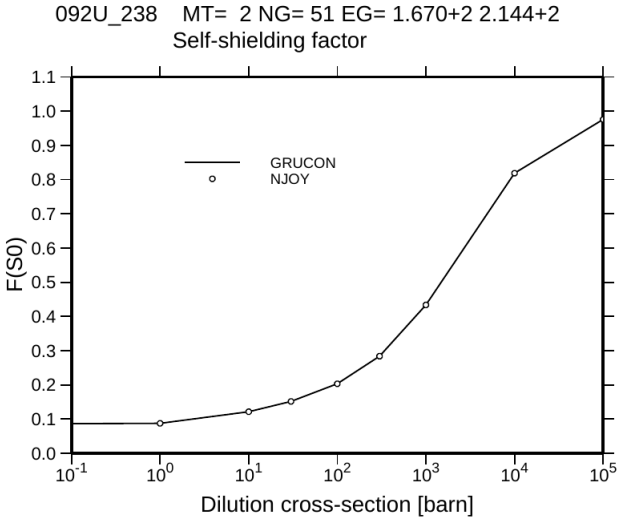


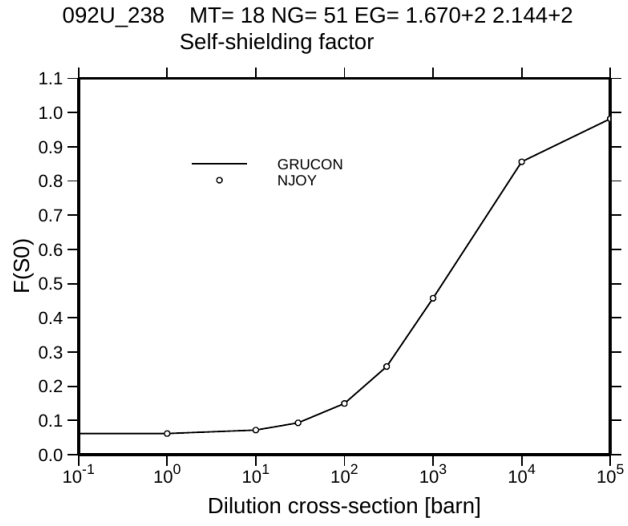


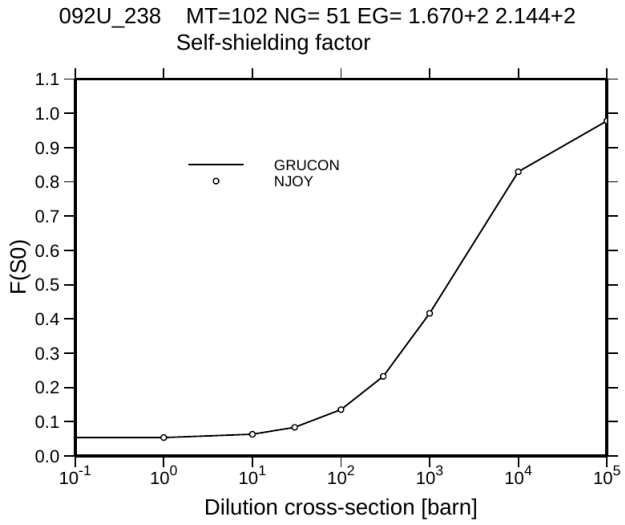


U238: Self-shielding factors (RRR)

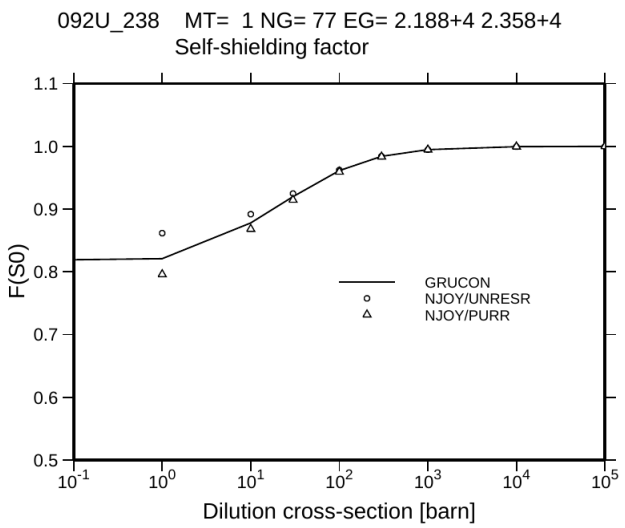


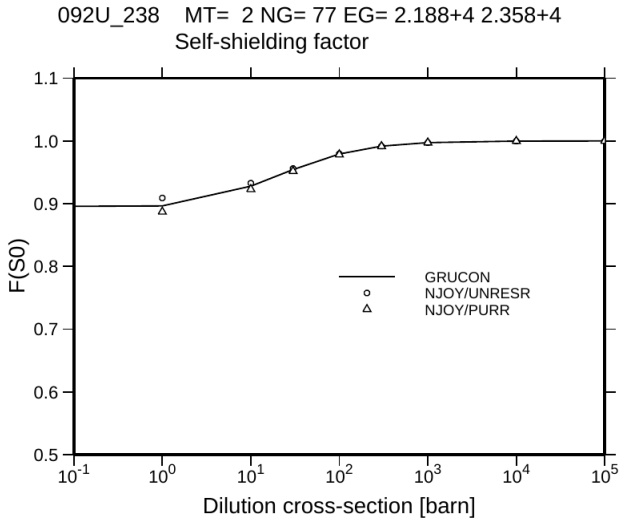


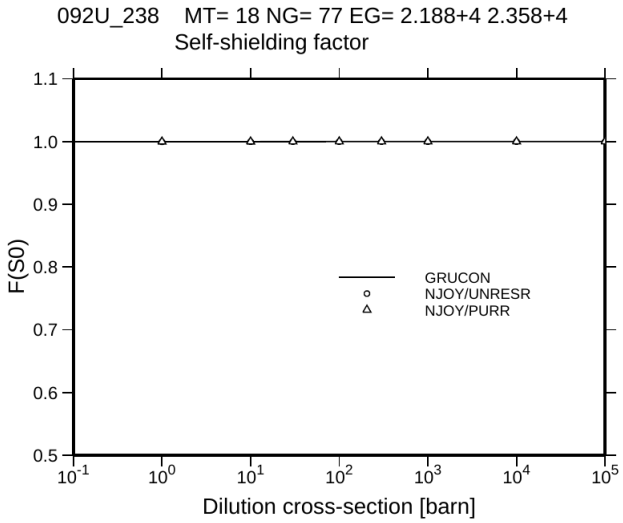


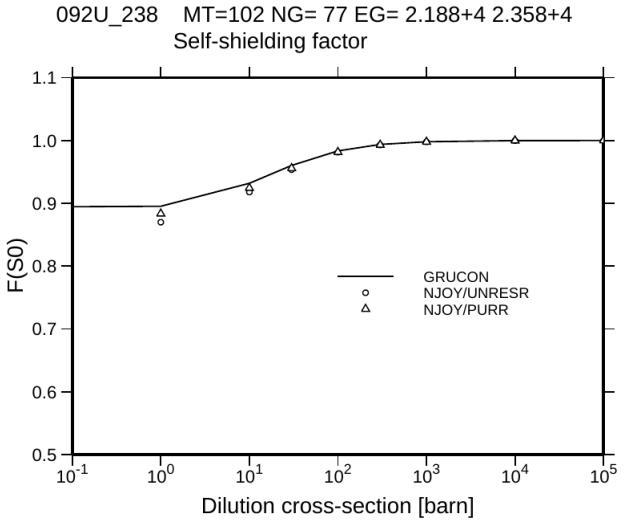


U238: Self-shielding factors (URR)

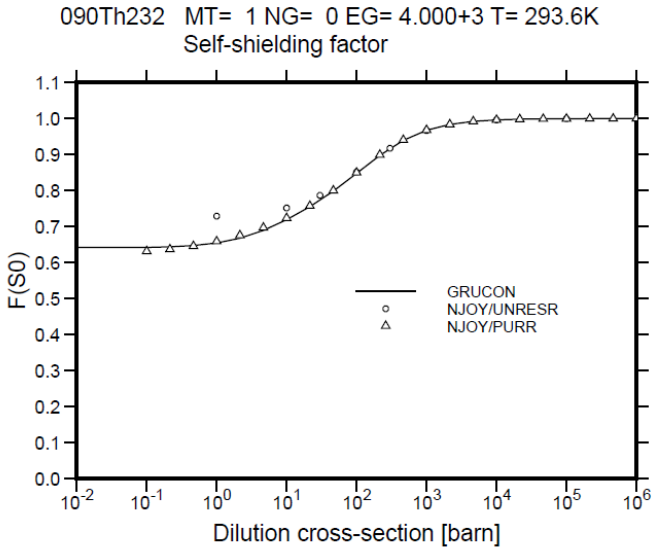


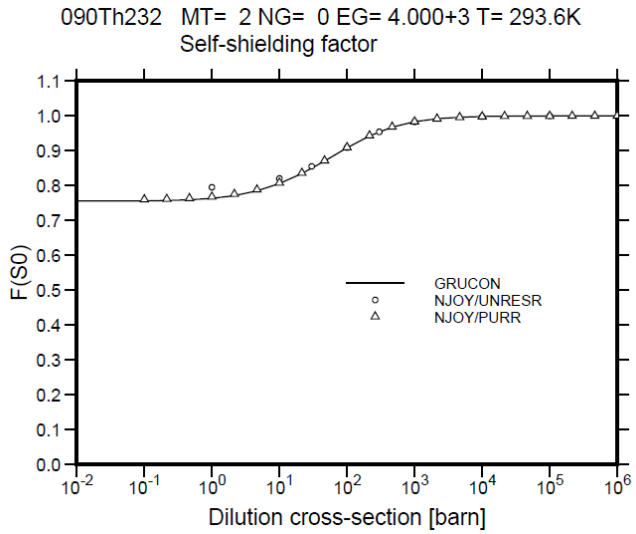


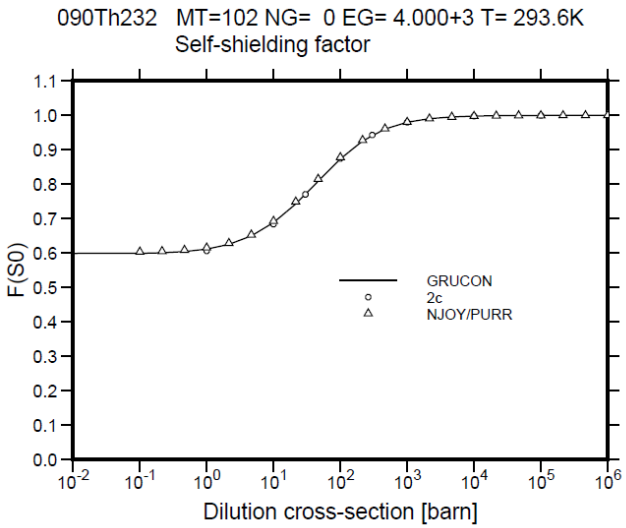




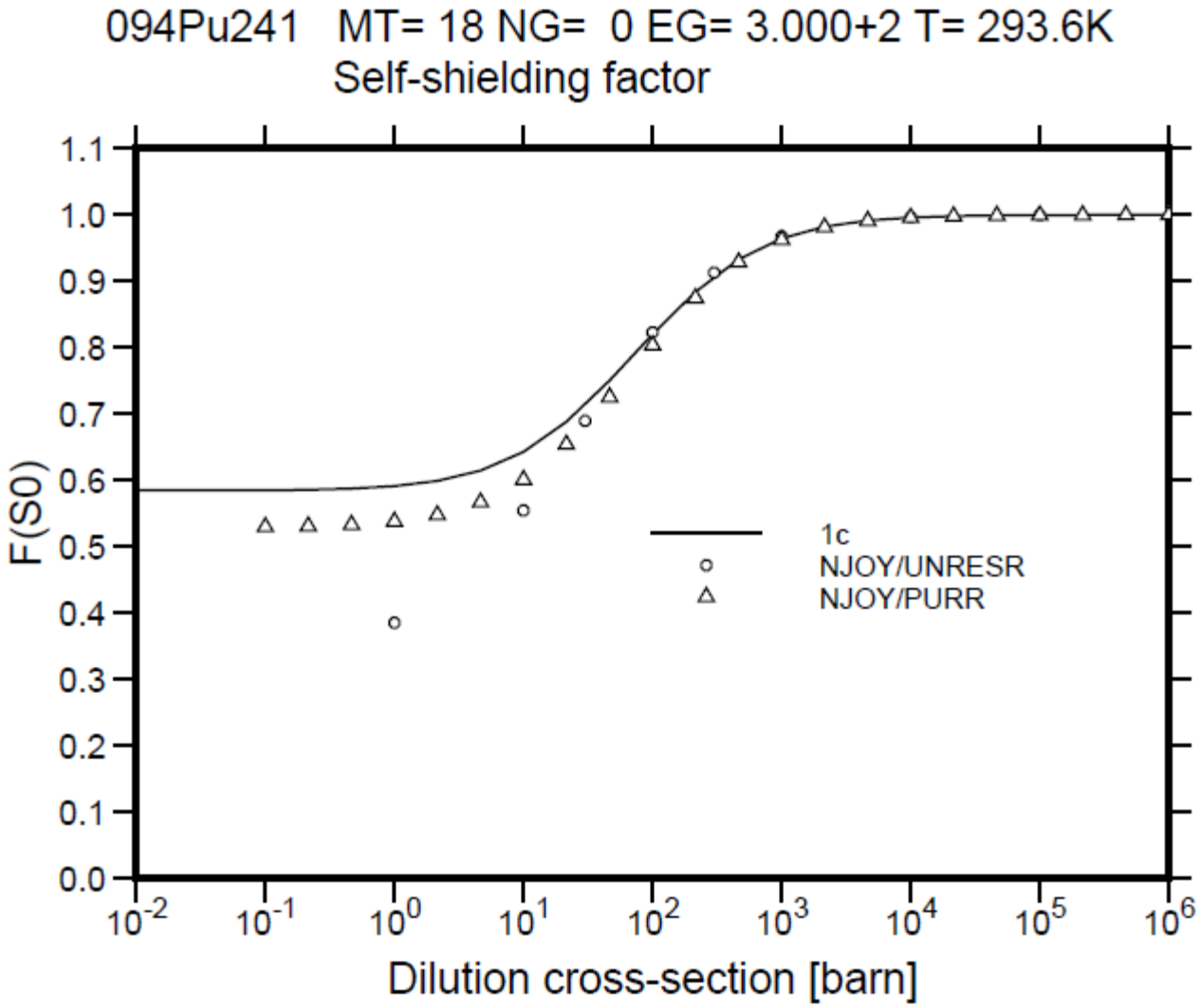
Th232: Self-shielding factors (URR)



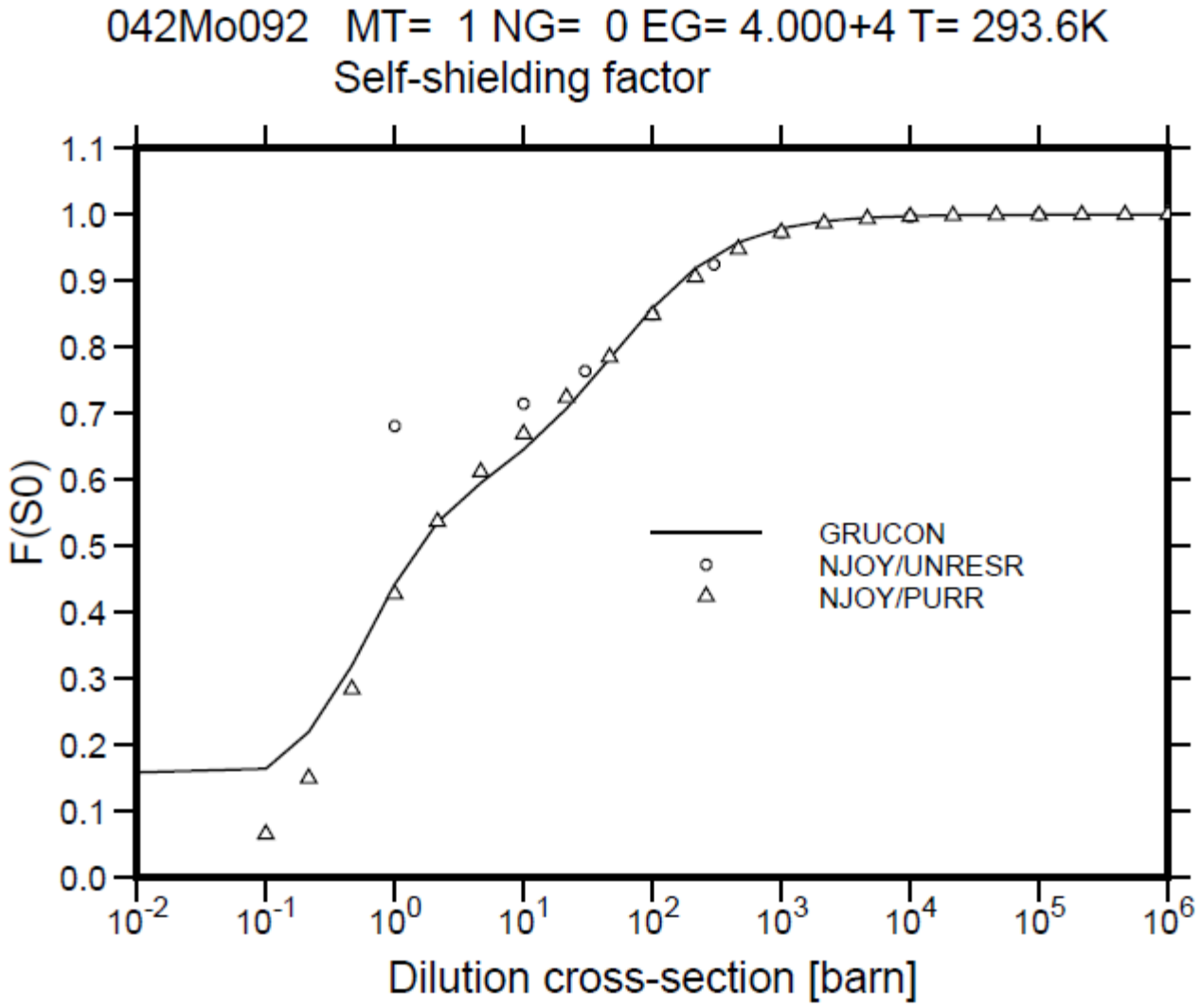




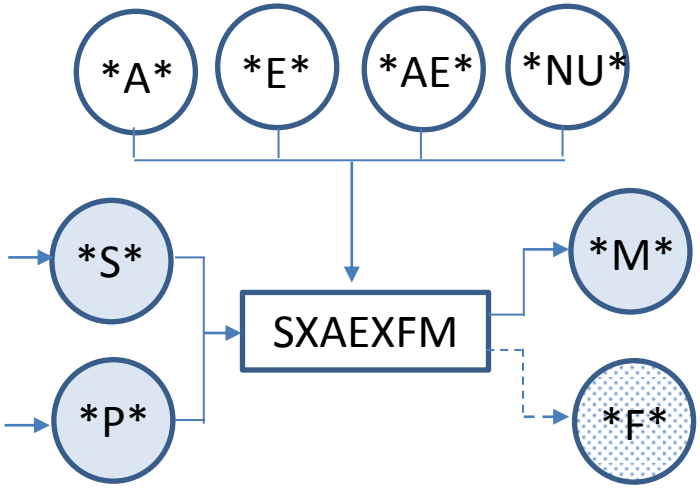
Pu241: Self-shielding factor for fission XS (URR)



Mo-92: Self-shielding factor for total XS (URR)

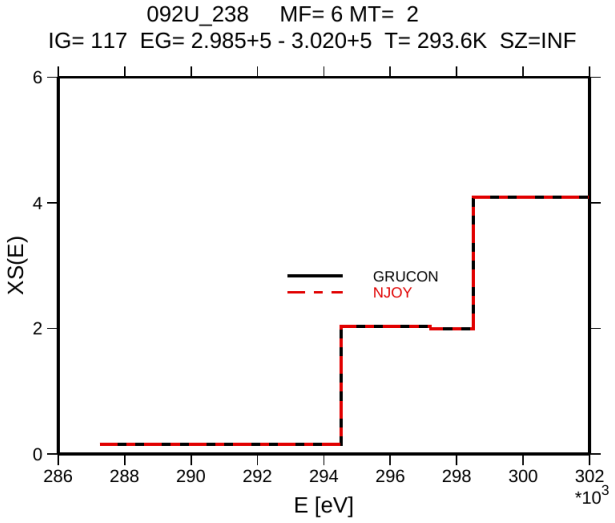


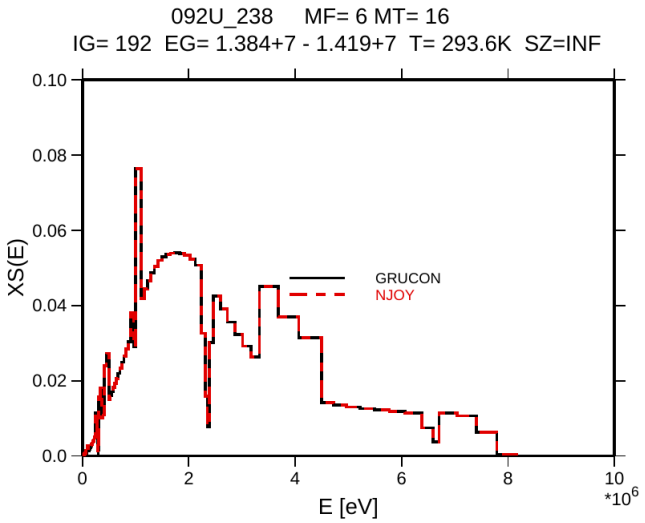
Neutron group transition and fission matrices (*M*) computing module

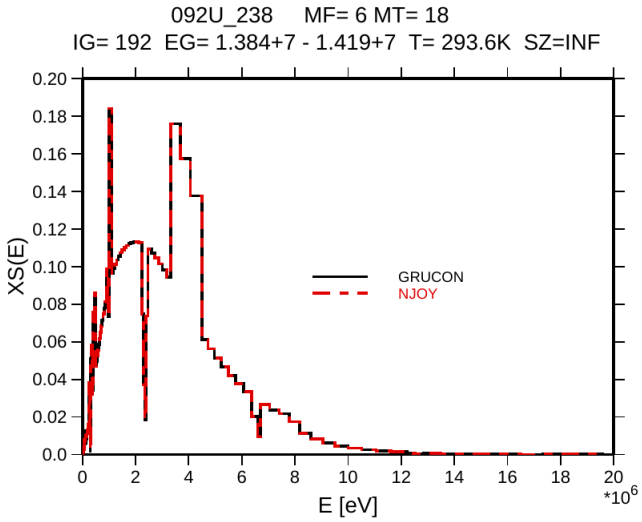


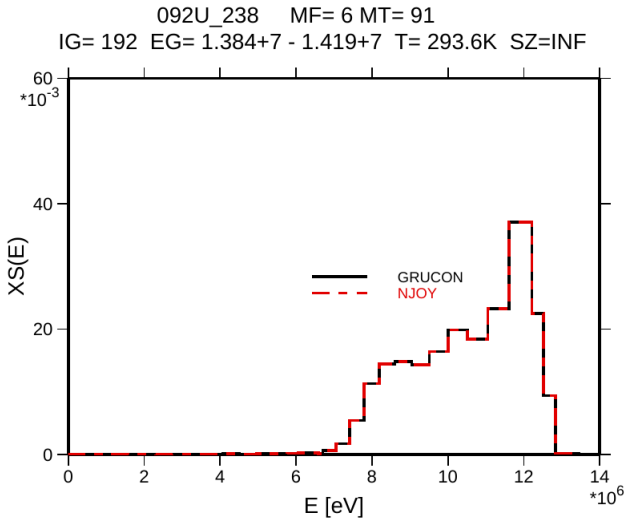
S - reconstructed cross sections
P - probability tables
A - angular distribution parameters (MF4)
E - energy distribution parameters (MF5)
AE - energy-angular distribution parameters (MF6)
NU - nu-bar (MF1)

U238: Neutron energy distributions in reactions with secondary neutrons

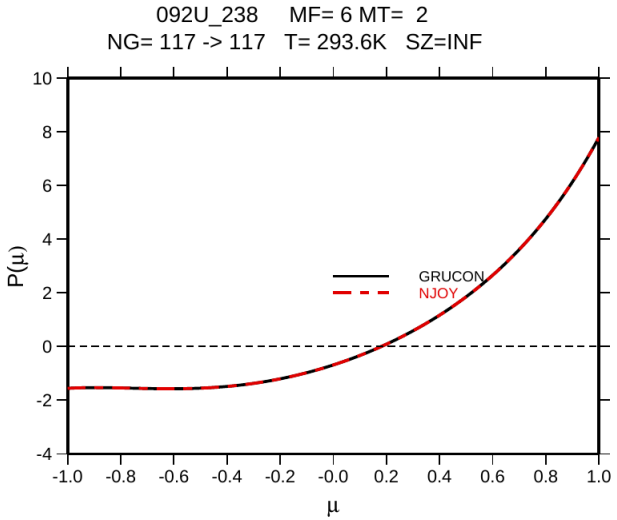


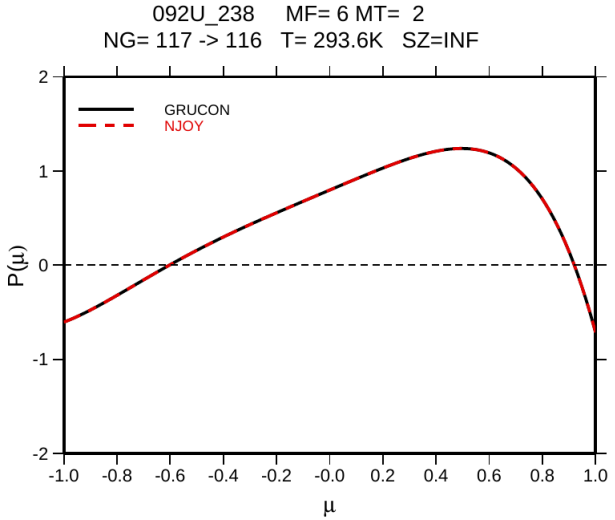


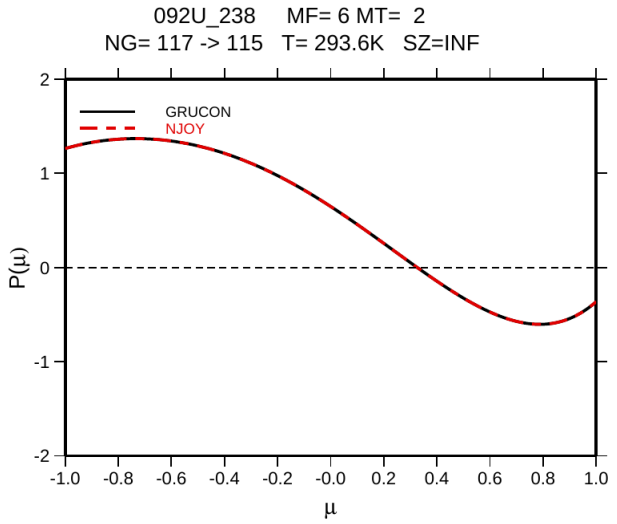


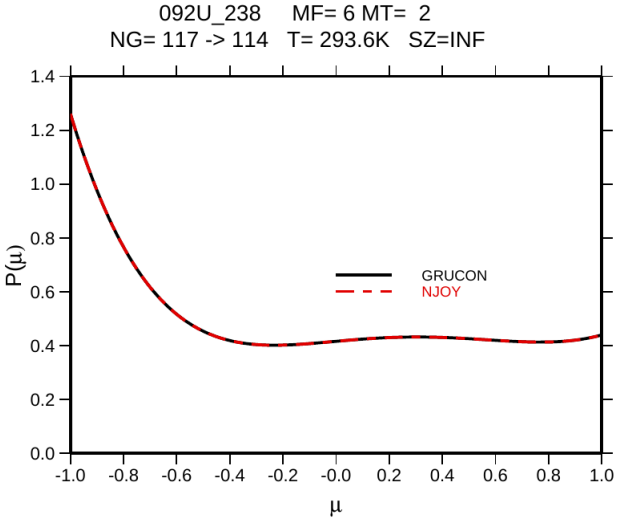


U238: Neutron angular distribution in elastic scattering

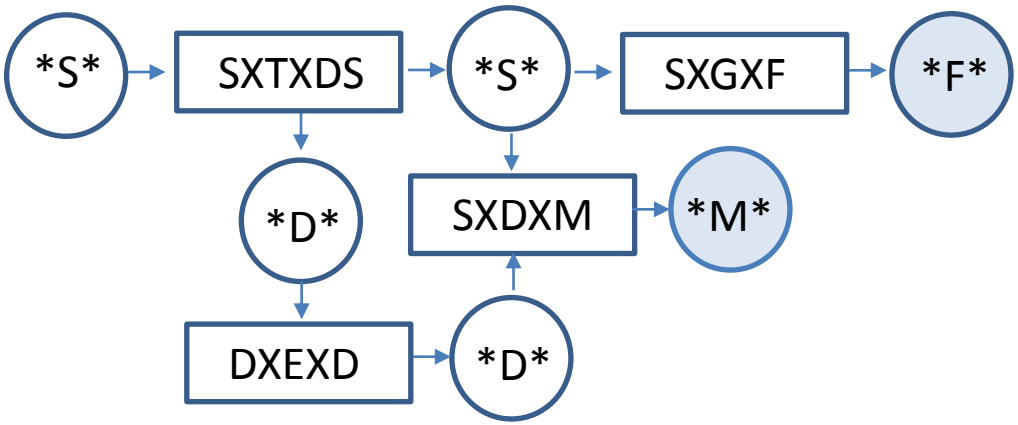








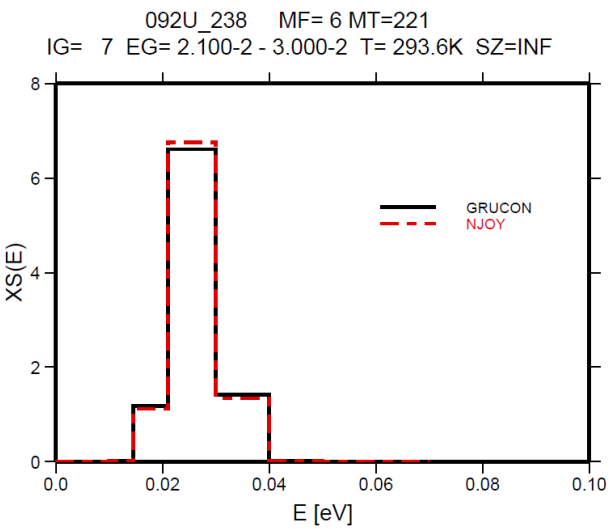
Free gas and resonance scattering group cross sections (*F*) and matrices (*M*) computing procedure

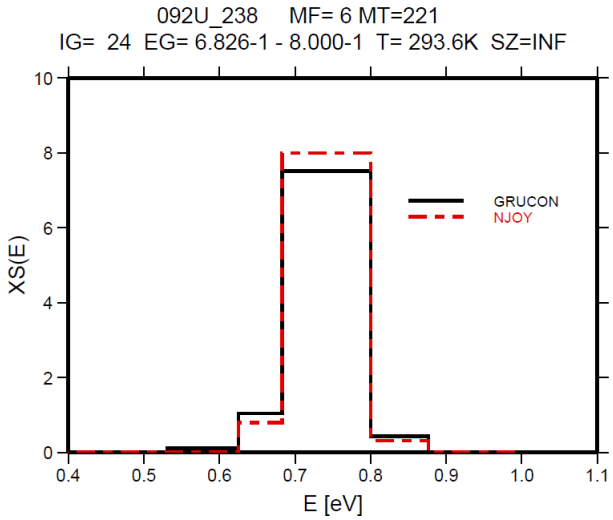


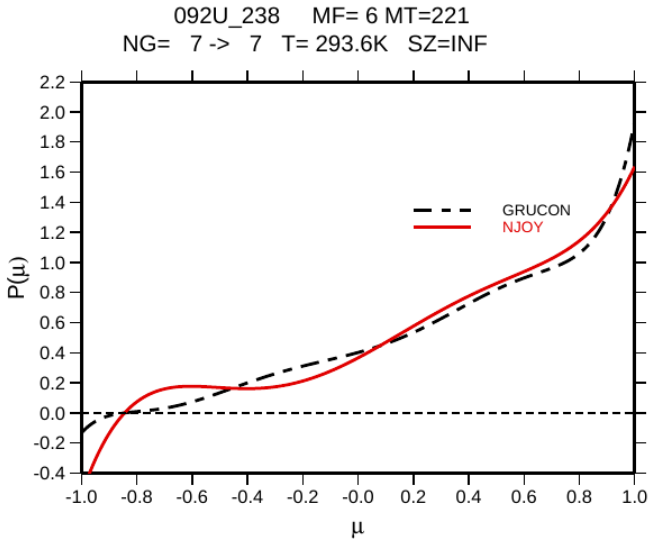
S input data is elastic scattering cross sections prepared preliminary at zero and desired temperatures.

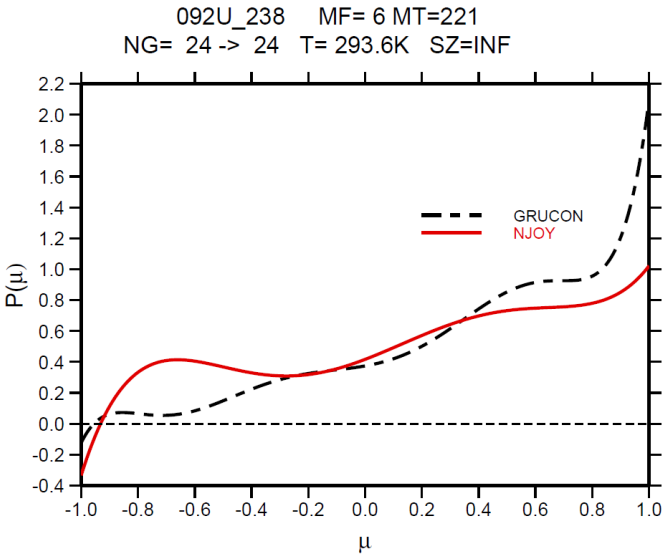
For free gas matrices, the SXTXDS time-consuming module (due to Monte Carlo integration) can be replaced by THXXDS .

U238: Free Gas Scattering Distributions

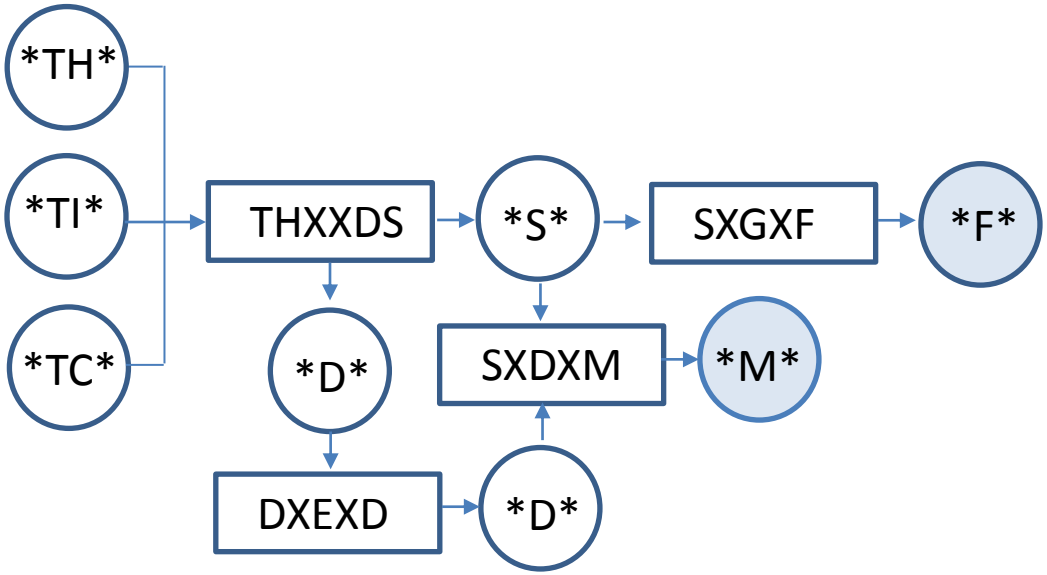








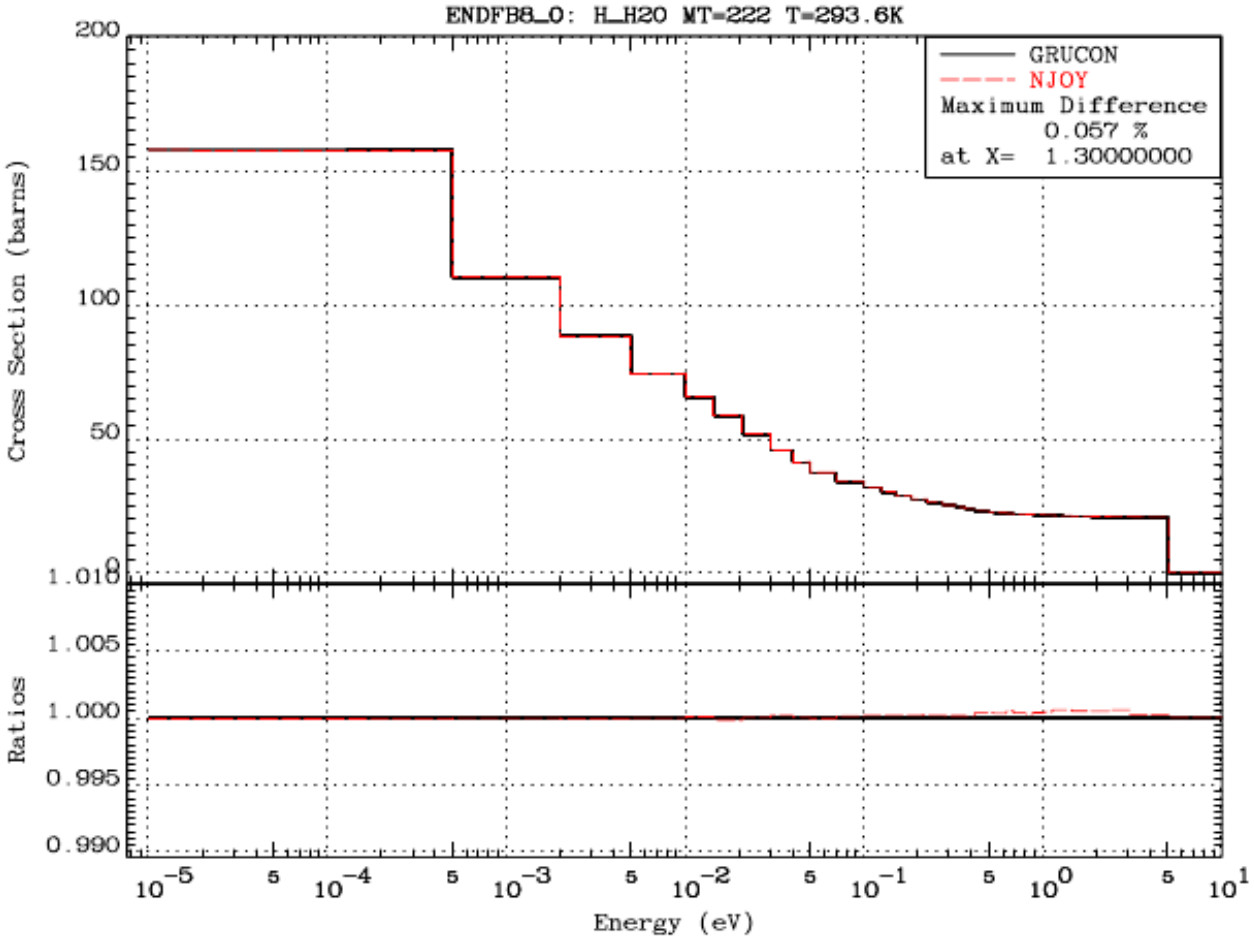
Bound nuclei scattering group cross sections (*F*) and matrices (*M*) computing procedure



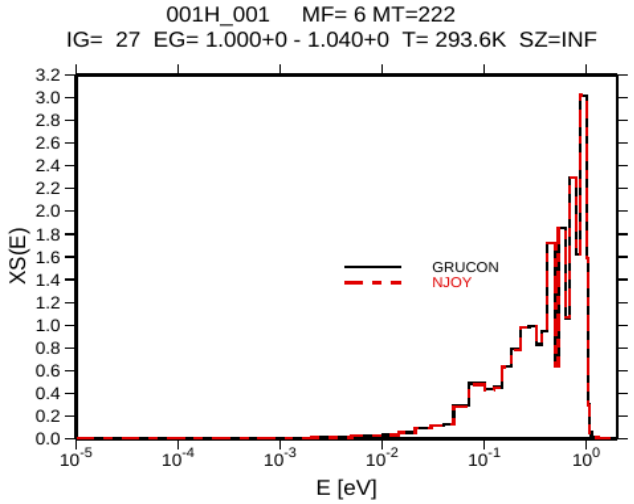
Thermal scattering data (MF7)
TH - incoherent inelastic
TI - incoherent elastic
TC - coherent elastic

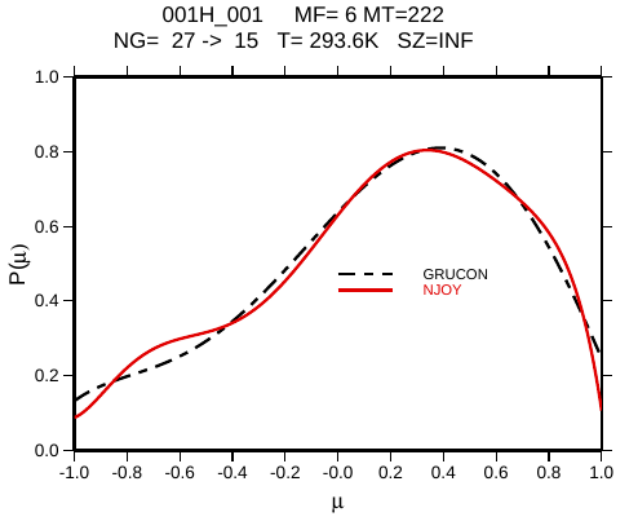
D - tabulated energy-angular distributions
F - group cross sections
M - group transition matrices

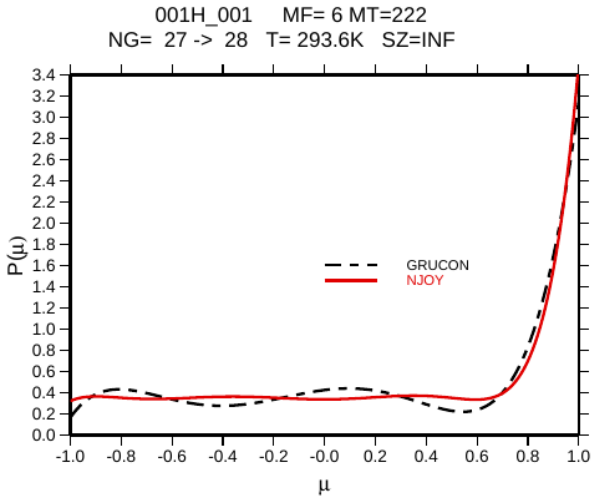
H_H2O: Inelastic incoherent scattering cross section



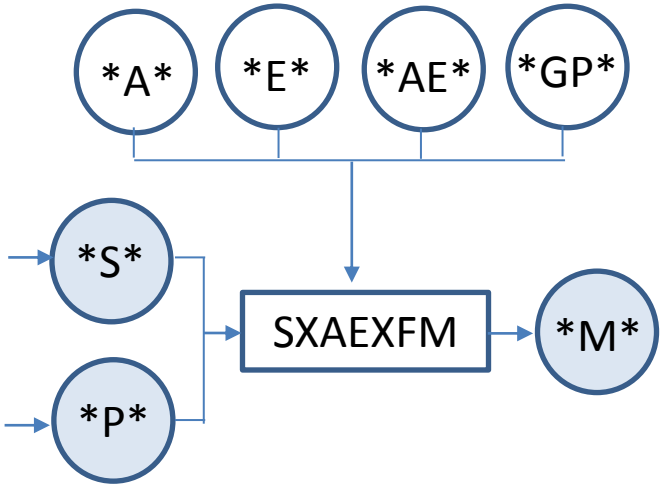
H_H2O: Group transition cross sections and angular distributions





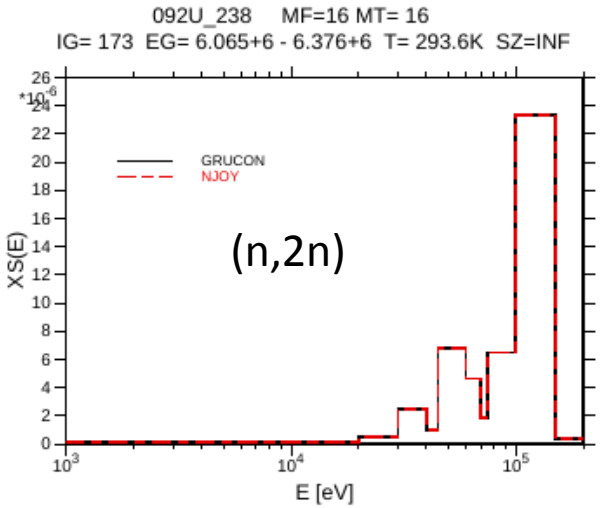


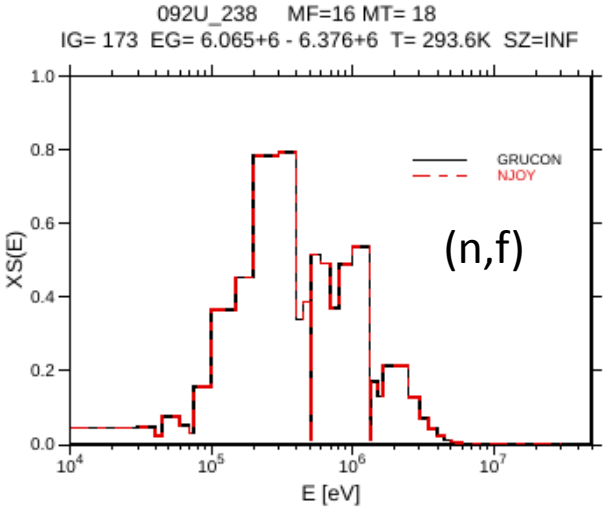
Photon production matrices (*M*) computing module

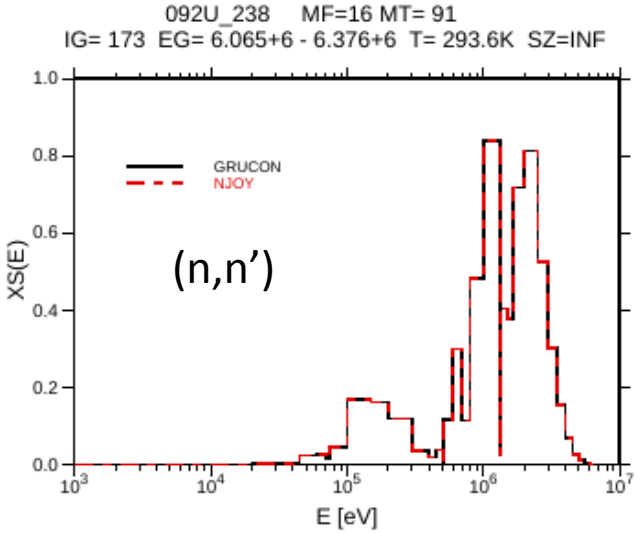


S - reconstructed cross sections
P - subgroup parameters
GP - gamma yields and transition probabilities (MF12,13)
A - angular distribution parameters (MF14)
E - energy distribution parameters (MF15)
AE - gamma yields and energy-angular distribution parameters (MF6)

U238: Energy distribution of photons, emitted in neutron reactions







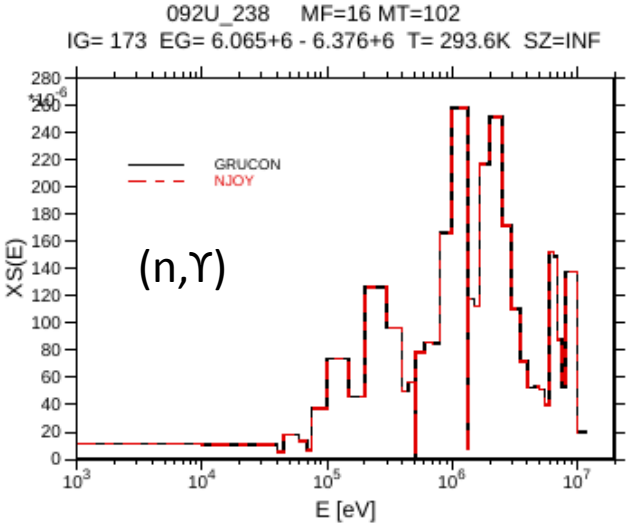
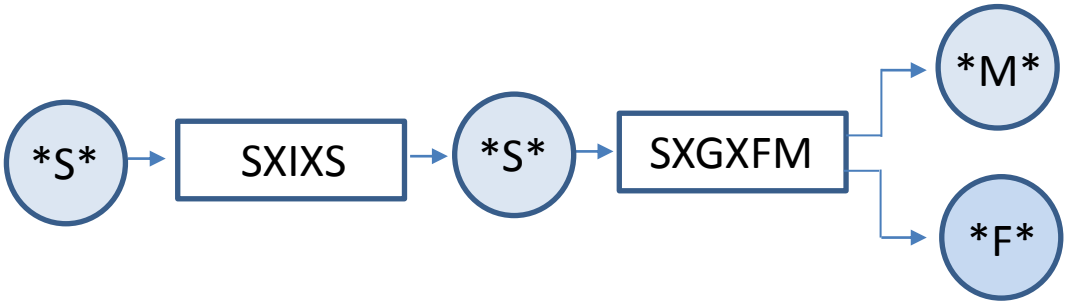
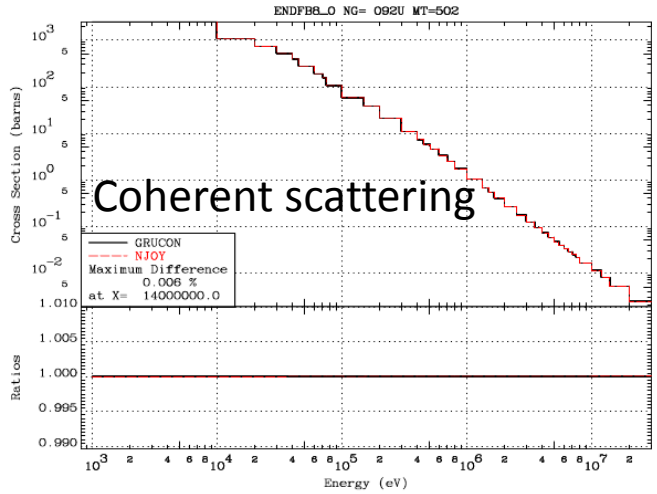


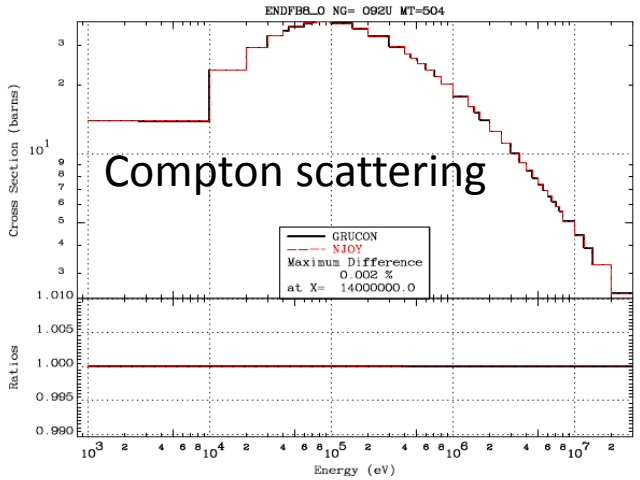
Photo-atomic group cross sections (*F*) and matrices (*M*) computing procedure

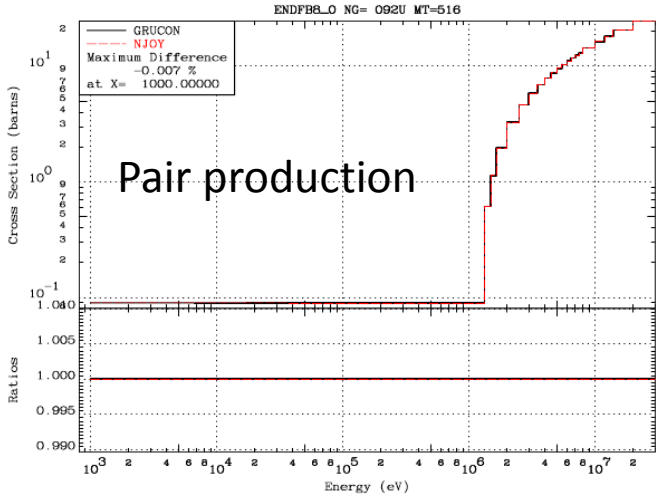


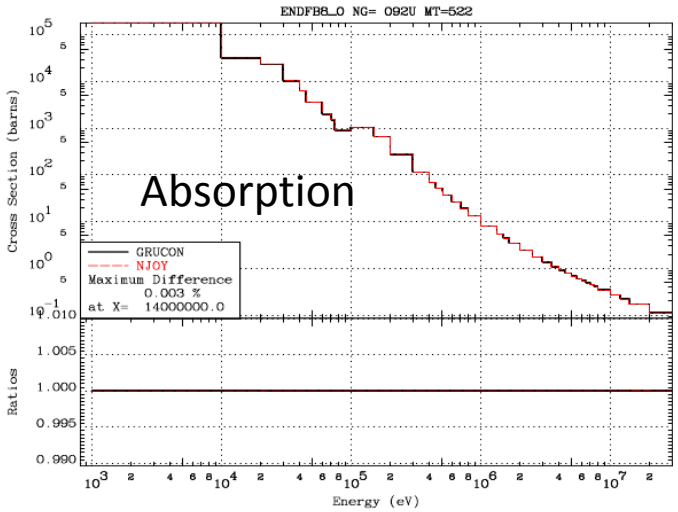
S - smooth photon interaction cross sections (MF23),
atomic form factors or scattering functions (MF27)

092U: Photo-atomic interaction cross sections

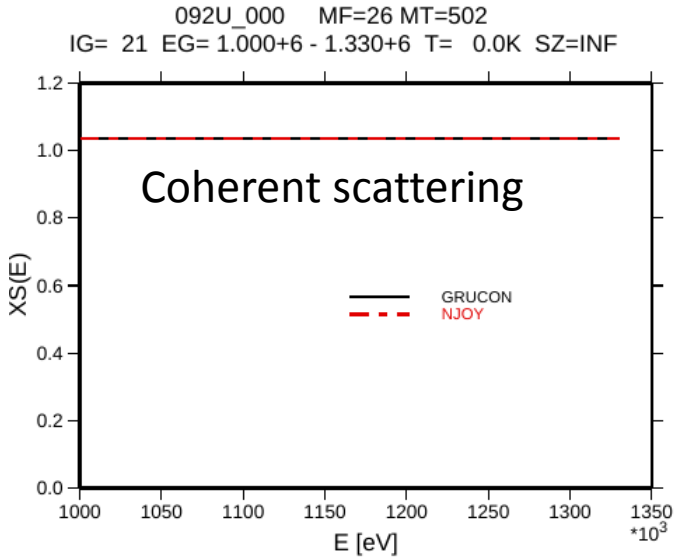


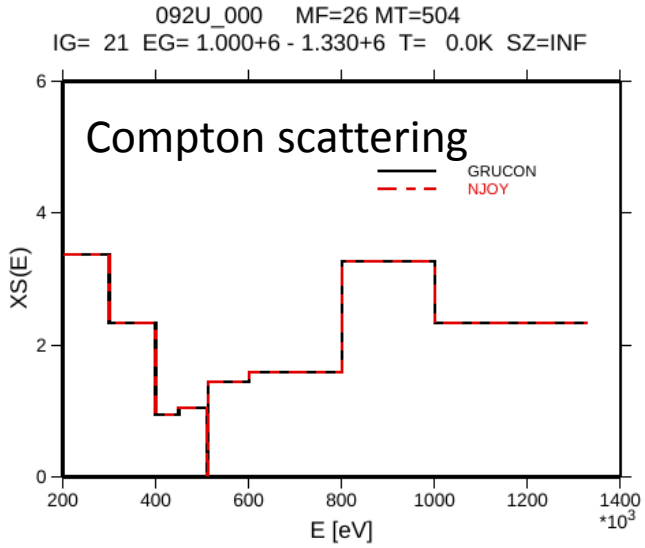


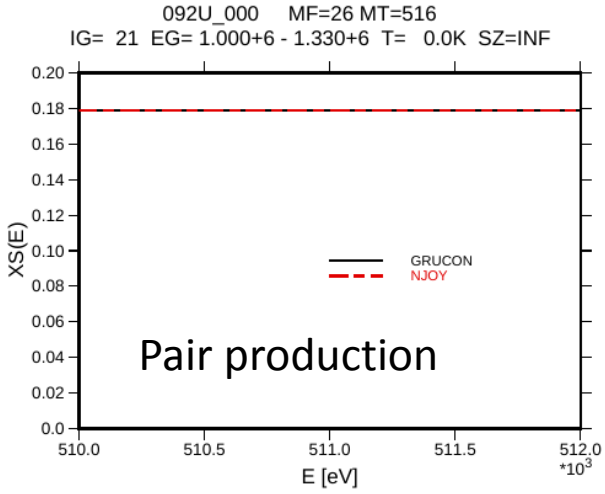




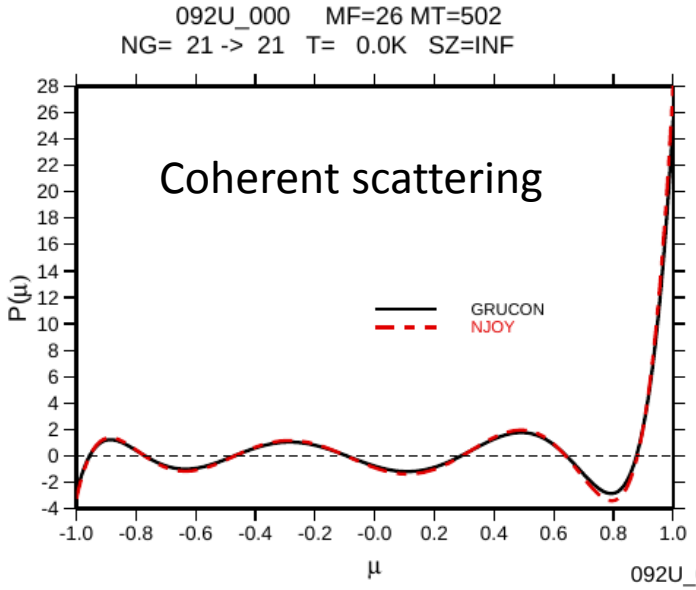
092U: Photon energy distributions

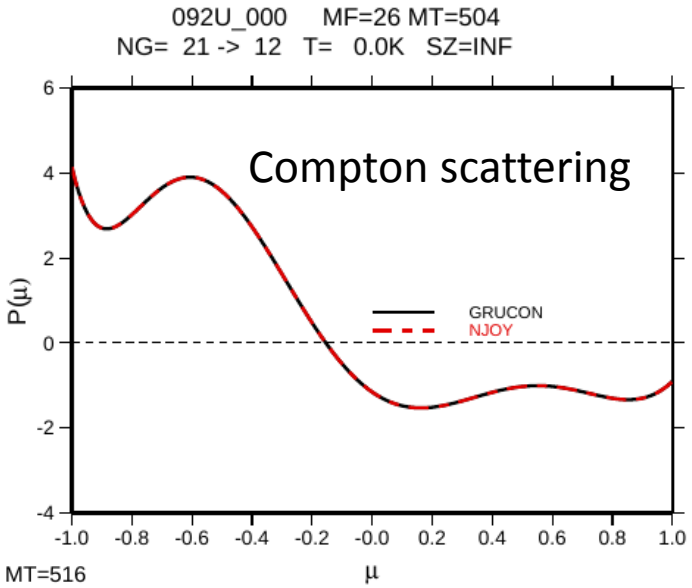


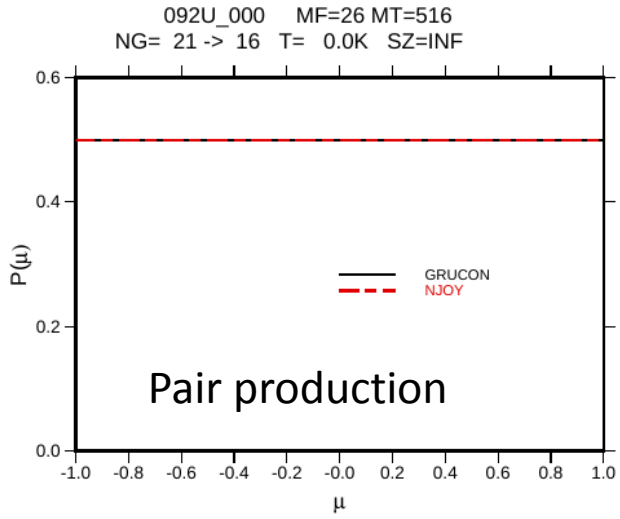




092U: Photon angular distributions

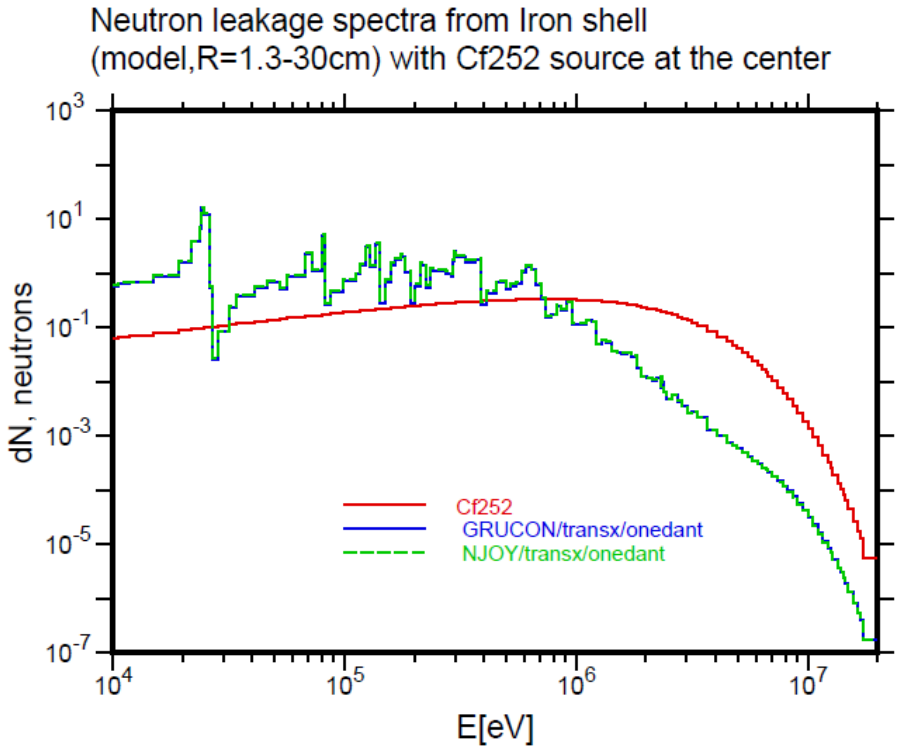


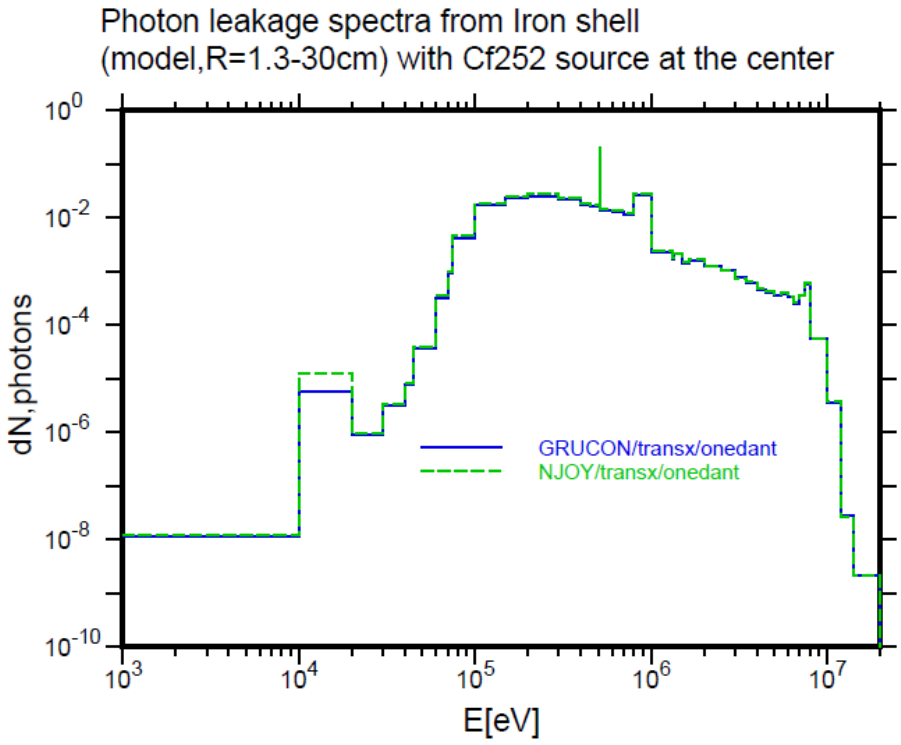




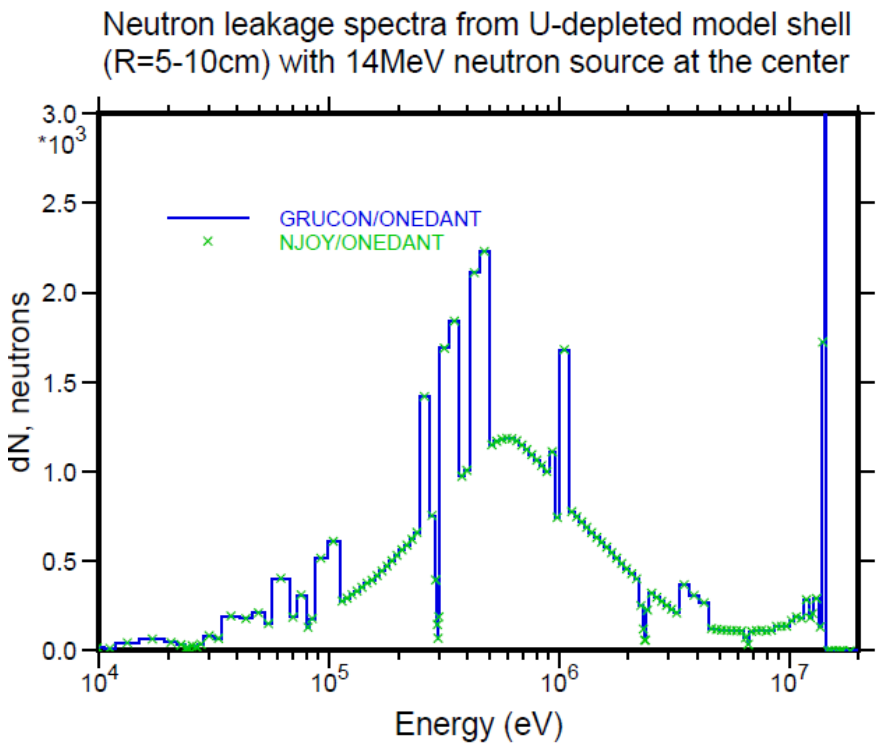
3.1 Integral Testing: comparison of photon and neutron leakage from spheres (model calculations)

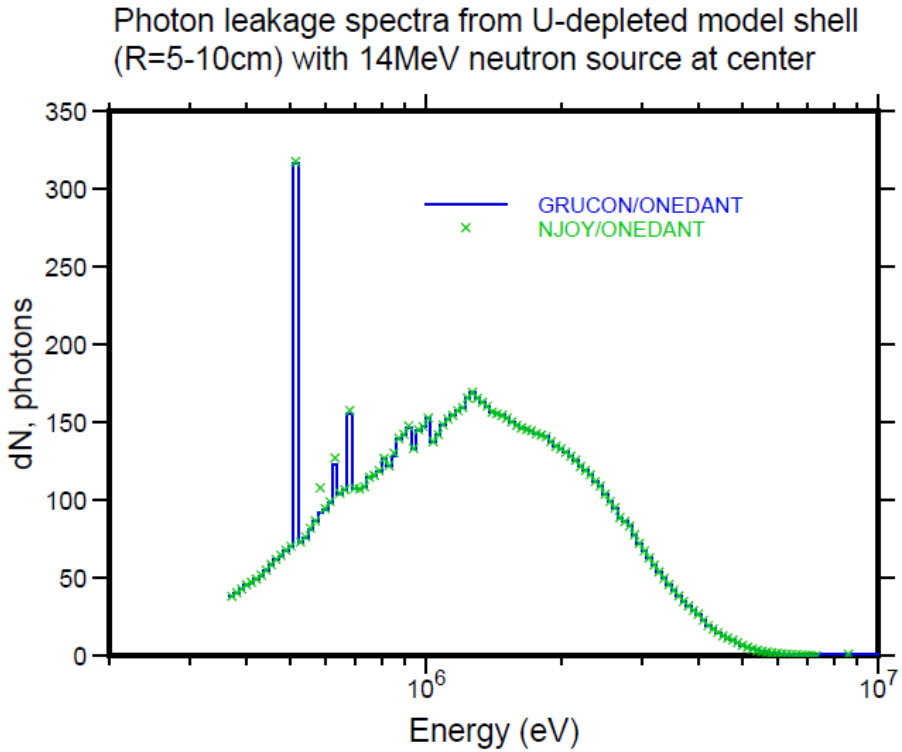
Iron sphere, Cf-252 source



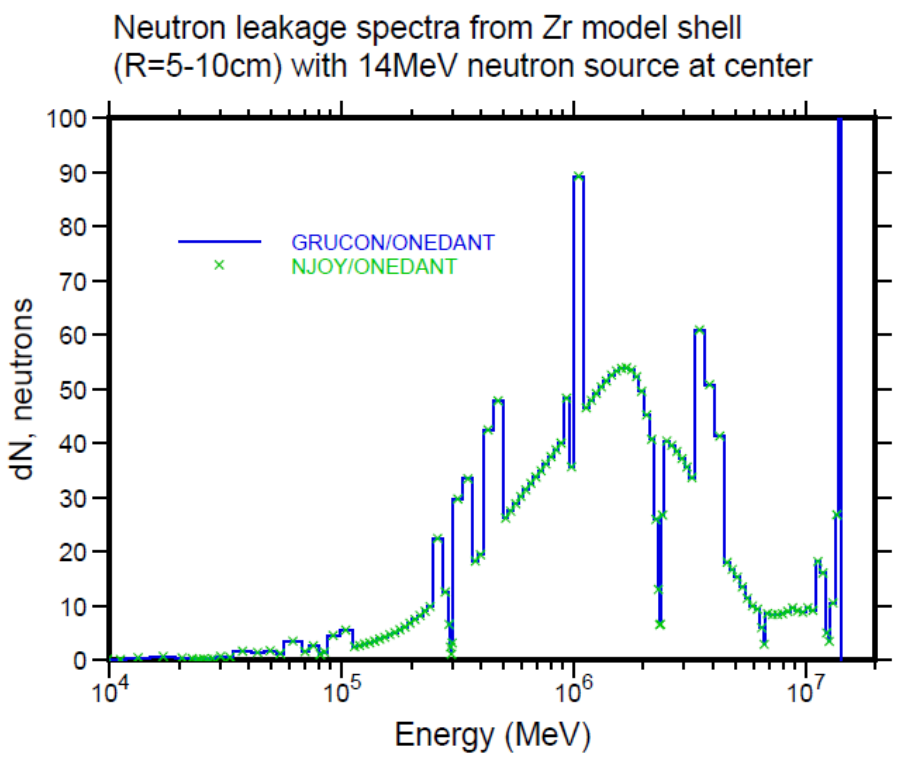


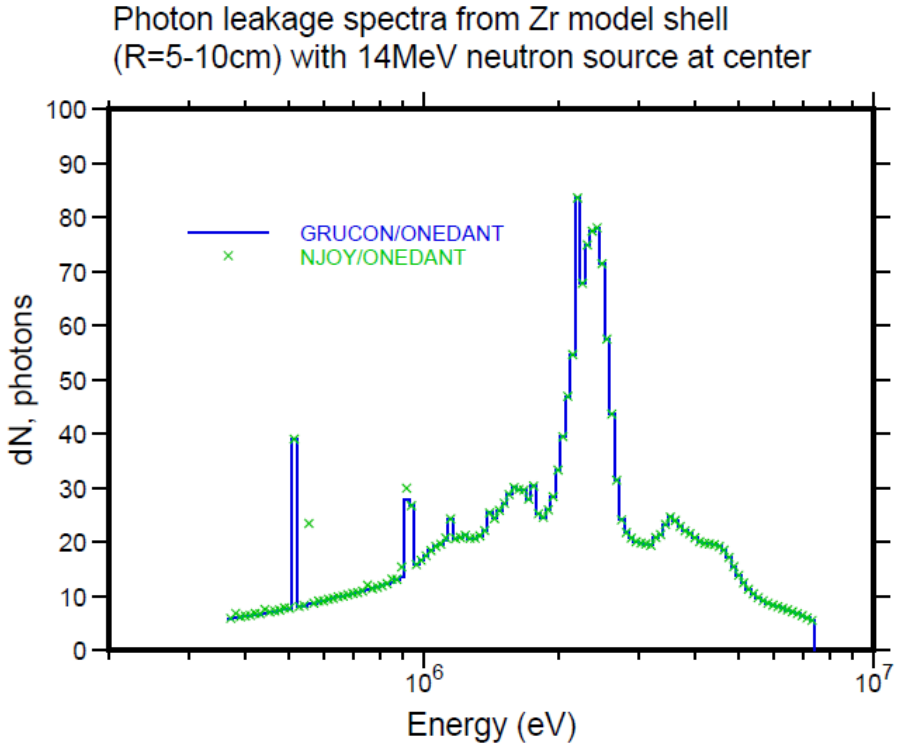
Uranium sphere, 14MeV source





Zirconium sphere, 14MeV source

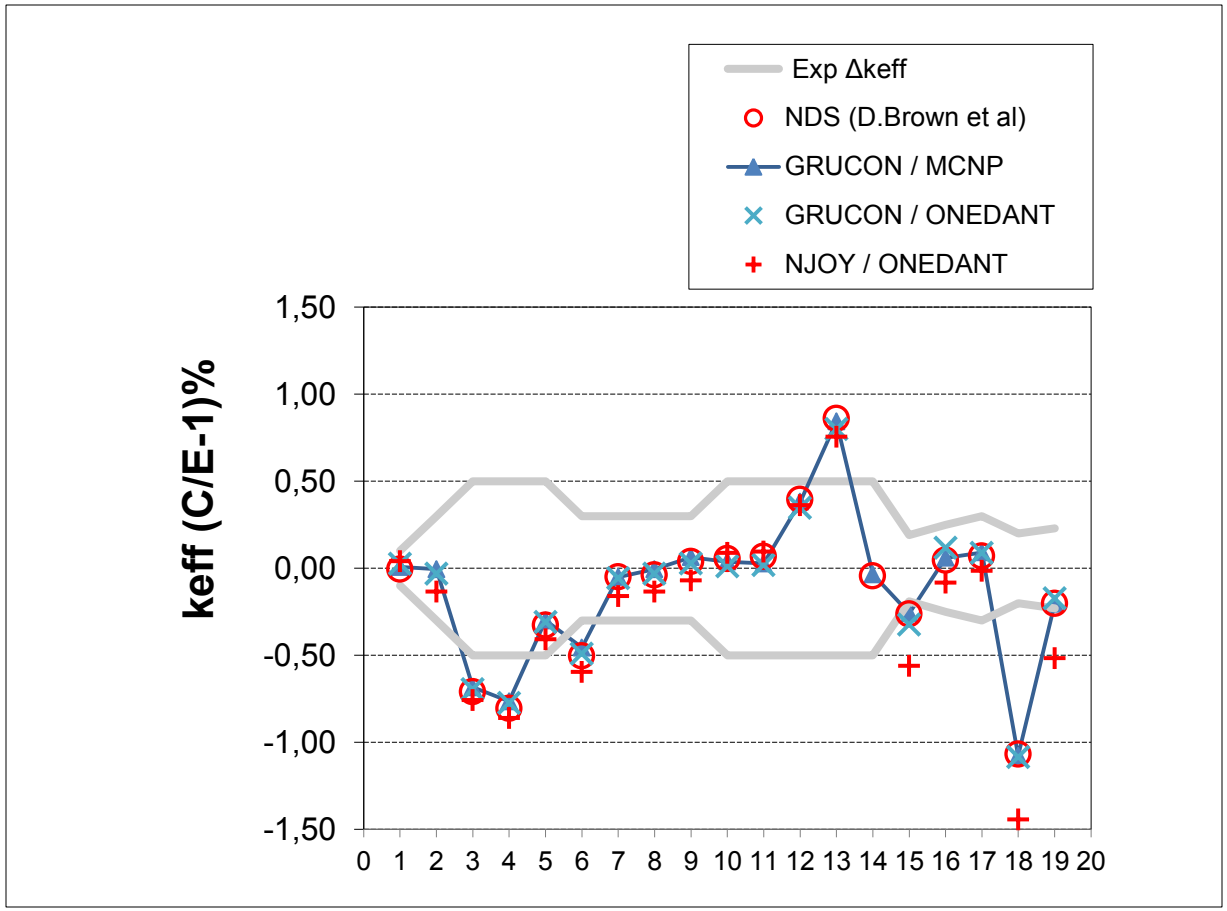




3. 2 Integral Testing: comparison of Keff for critical benchmark experiments (preliminary results)

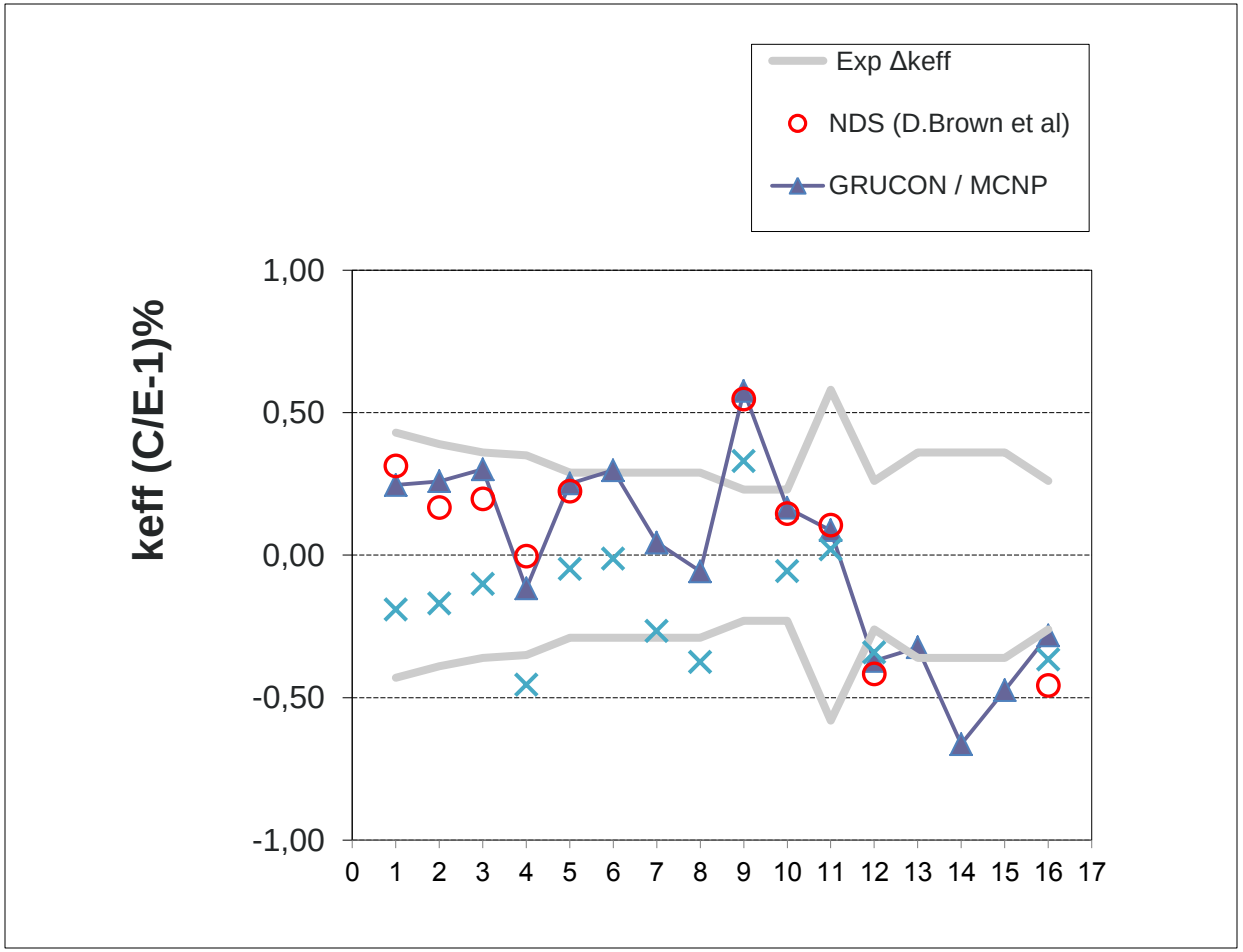
HEU-MET-FAST

1	hmf-001-001
2	hmf-002-001
3	hmf-003-001
4	hmf-003-002
5	hmf-003-003
6	hmf-003-004
7	hmf-003-005
8	hmf-003-006
9	hmf-003-007
10	hmf-003-008
11	hmf-003-009
12	hmf-003-010
13	hmf-003-011
14	hmf-003-012
15	hmf-022-001
16	hmf-027-001
17	hmf-028-001
18	hmf-057-001
19	hmf-057-002



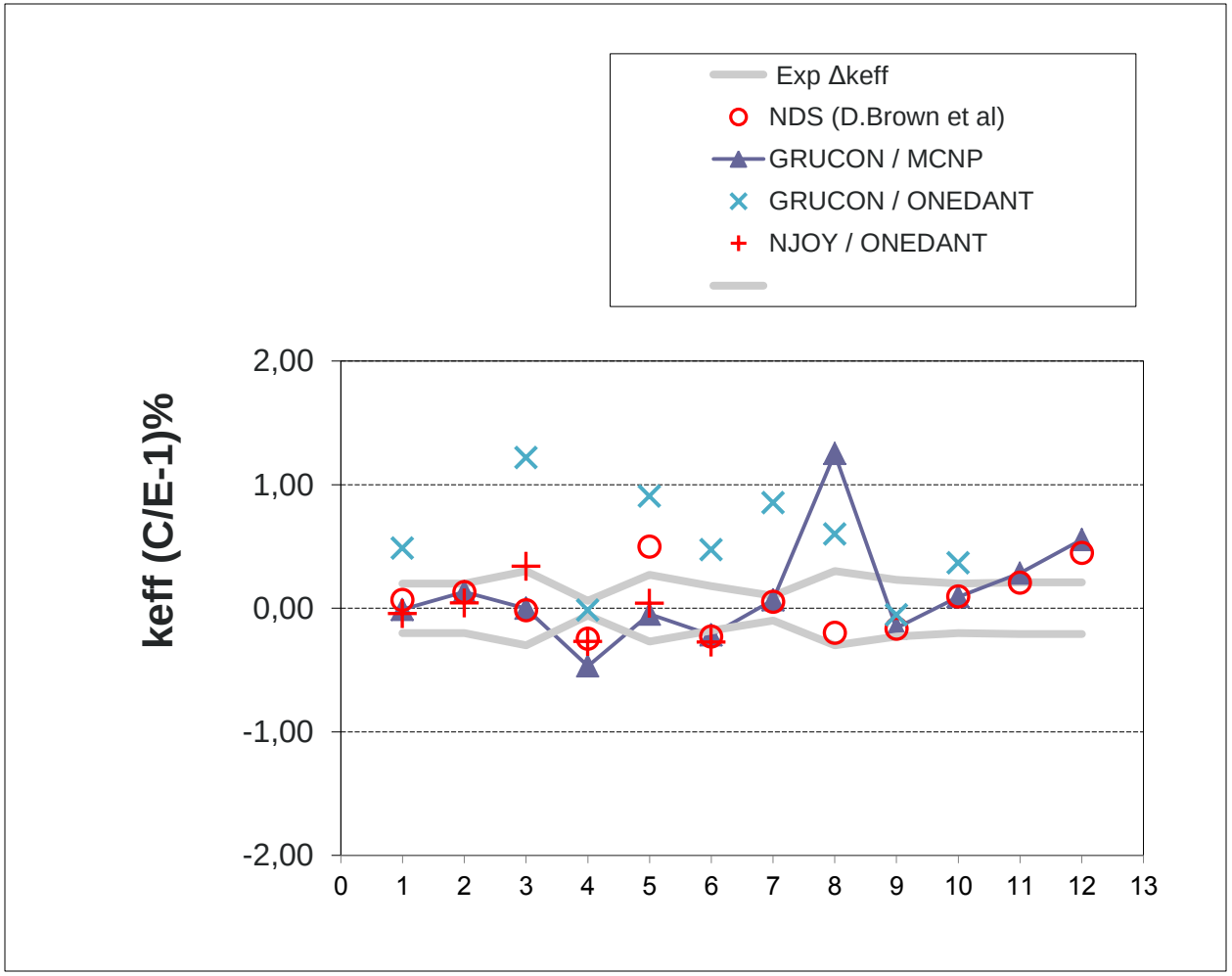
HEU-SOL-THERM

1	hst-009-001
2	hst-009-002
3	hst-009-003
4	hst-009-004
5	hst-010-001
6	hst-010-002
7	hst-010-003
8	hst-010-004
9	hst-011-001
10	hst-011-002
11	hst-012-001
12	hst-013-001
13	hst-013-002
14	hst-013-003
15	hst-013-004
16	hst-032-001



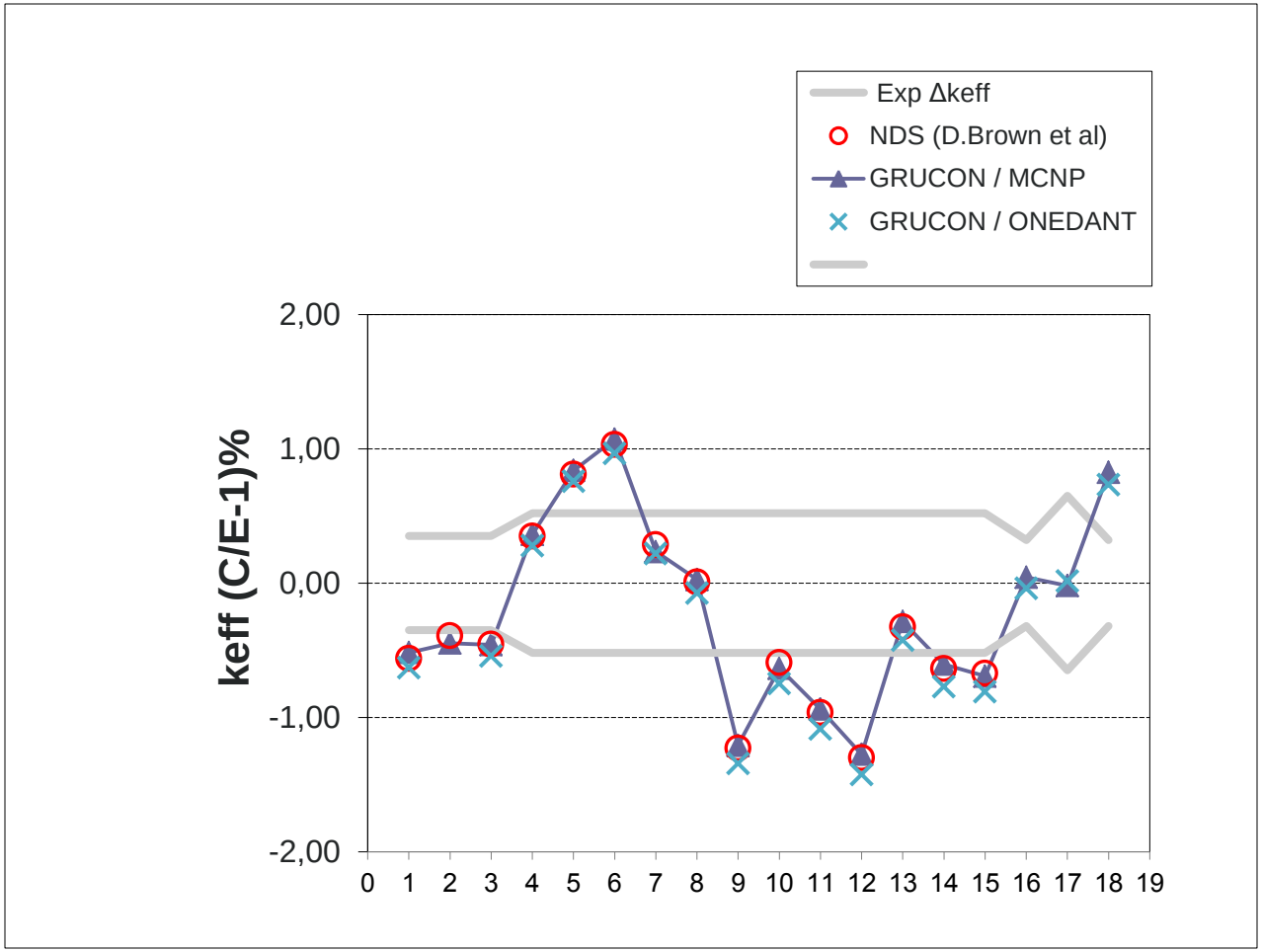
PU-MET-FAST

1 pmf-001-001
2 pmf-002-001
3 pmf-006-001
4 pmf-008-001
5 pmf-009-001
6 pmf-010-001
7 pmf-011-001
8 pmf-018-001
9 pmf-023-001
10 pmf-024-001
11 pmf-030-001
12 pmf-031-001



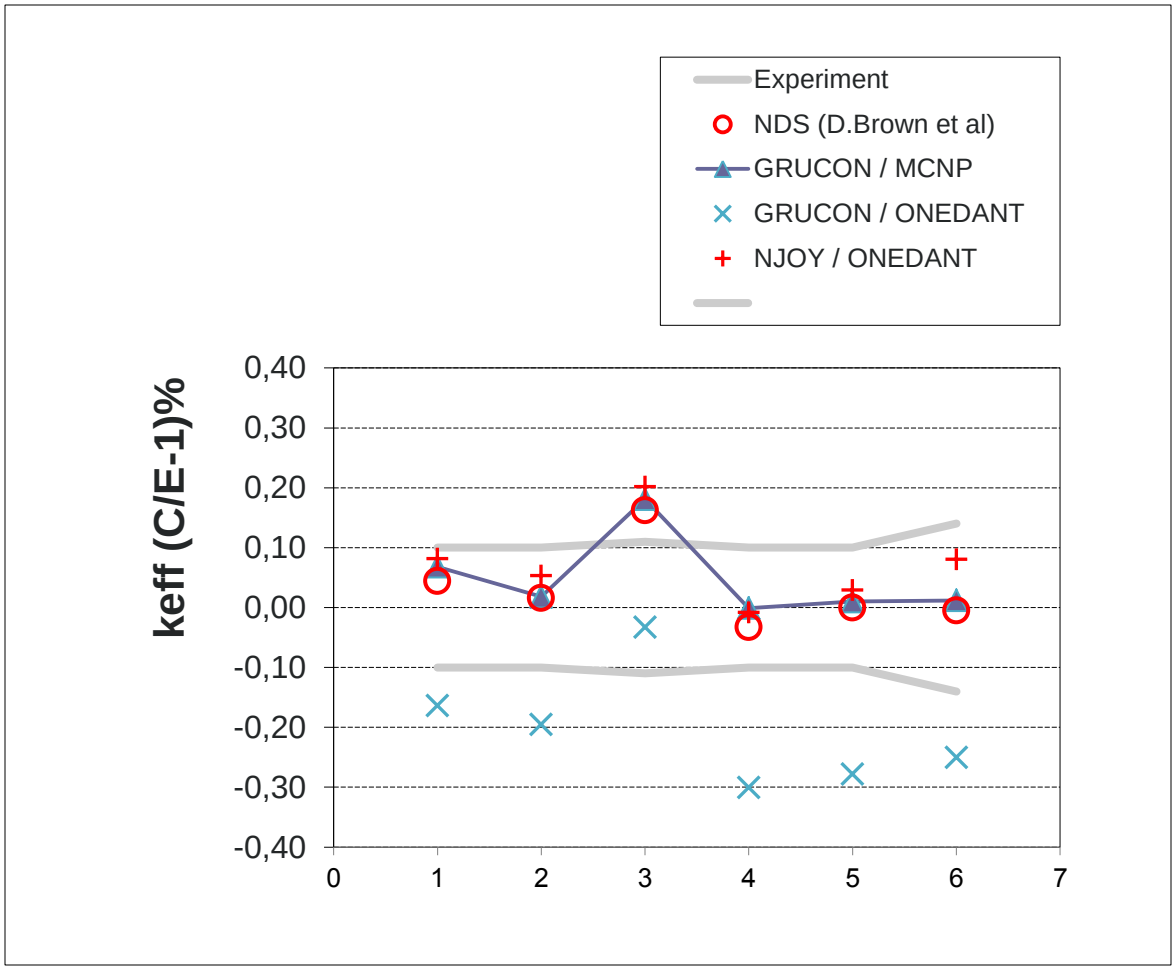
PU-SOL-THERM

1	pst-006-001
2	pst-006-002
3	pst-006-003
4	pst-011-001
5	pst-011-002
6	pst-011-003
7	pst-011-004
8	pst-011-005
9	pst-011-006
10	pst-011-007
11	pst-011-008
12	pst-011-009
13	pst-011-010
14	pst-011-011
15	pst-011-012
16	pst-021-007
17	pst-021-008
18	pst-021-009



U233-MET-FAST

1 umf-001-001
2 umf-002-001
3 umf-002-002
4 umf-003-001
5 umf-003-002
6 umf-006-001



4. CONCLUSION

A new version of GRUCON package - GRUCON-2019.6 - allows to prepare a coupled neutron-gamma group data and convert them to the GENDF and MATXS formats.

Comparison of reconstructed point-wise cross sections has revealed a few non-essential discrepancies between GRUCON, N JOY and PREPRO codes, but they disappear in group data due to compensation.

Resonance structure functions completely agree in the RRR, but reveal remarkable inconsistency in the URR (especially for fissile nuclides - up to ~10% at $\sigma_0 \leq 1$ barn).

Comparison of other group vectors and matrices (group-transition and fission matrices, thermal scattering data, photo-production and photo-atomic interaction cross sections and matrices) has demonstrated a good agreement.

As for integral testing, in spite of good agreement of some results, they can not be considered as final. Problems, revealed in comparison of Keff values, obtained from data prepared by GRUCON and NJOY, both with each other and with reference values (*), are casting doubts in reliability of MATXS / ONEDANT interface, fulfilled through TRANSX. Additional study should be performed to understand, is it processing problem, or interface one, or in transport SN calculation (poor convergence).

(*) D.A.Brown, M.B.Chadwick, et all **ENDF/B-VIII.0: The 8th Major Release of the Nuclear Reaction Data Library with CIELO-project Cross Sections, New Standards and Thermal Scattering Data,** Nuclear Data Sheets , Volume 148, February 2018, Pages 1-142

Acknowledgments

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Thank you for attention!