Potential of GRUCON Package and GND Structures

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- Architecture
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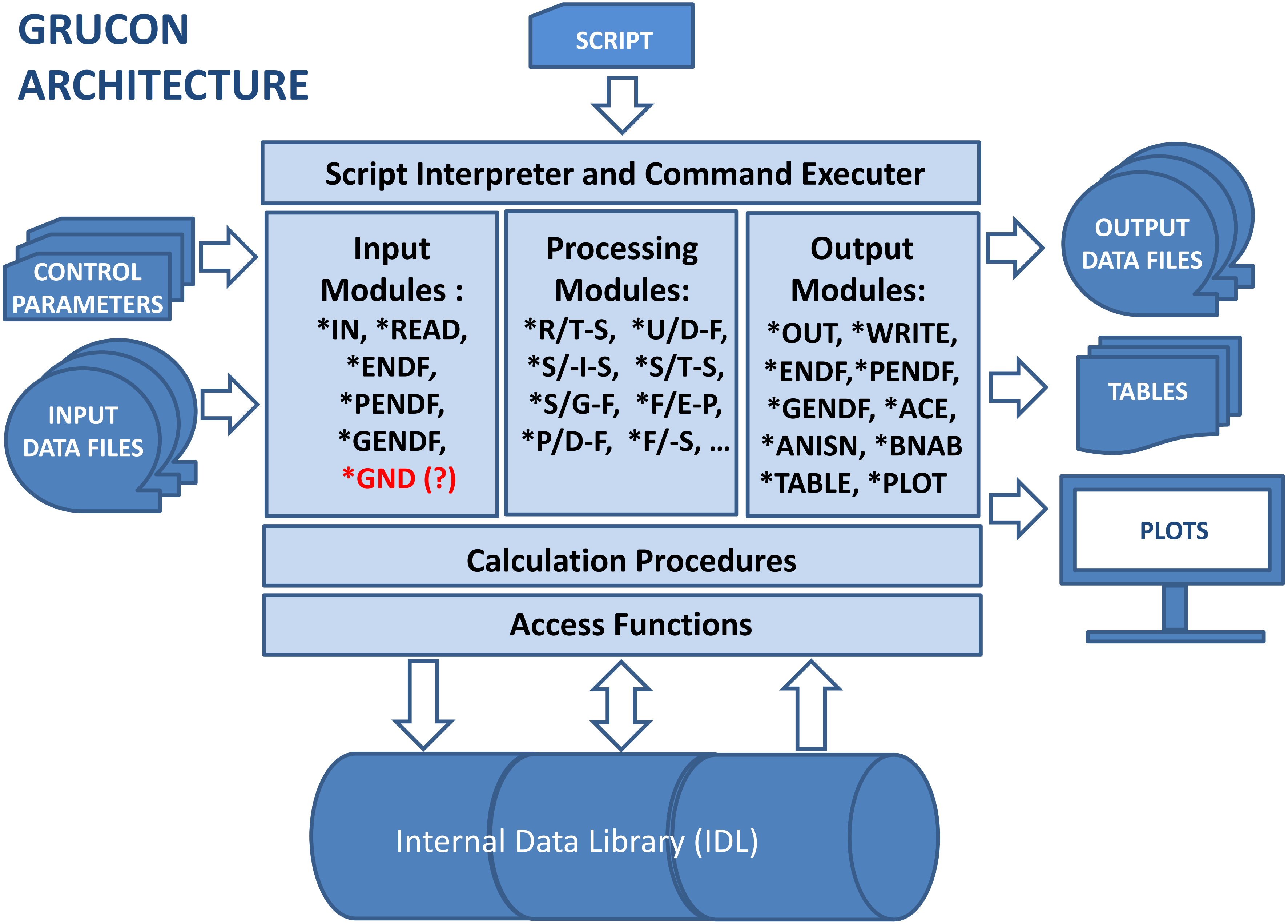
Purpose

- to show potential of the GRUCON package
- to compare the GRUCON and NJOY calculation results
- to consider including of the GND structures to the GRUCON package

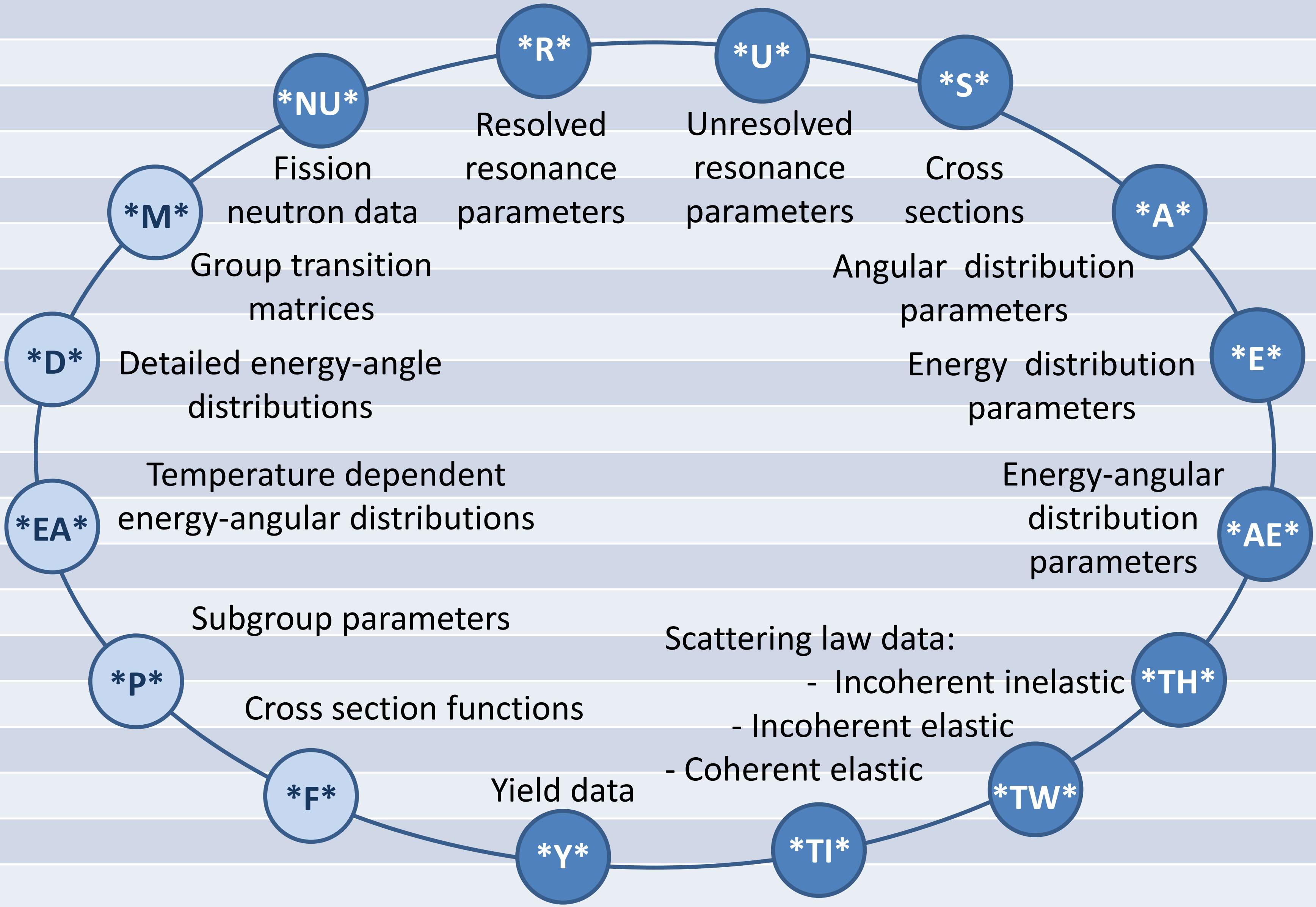
GRUCON History

- **1970-1980: SOKRATOR format, ALGOL-60, M-220**
  Data processing problem.
  Predecessors: URAN+MUF+ NERPA+ PRUSSAK+SOM+ +UMBLOCK+MANNERS=GRUCON (complex)
  (L.P.Abagyan, N.O.Bazazyanz, M.N.Nikolaev)
- **1980-1985: ENDF format, BESM-6 , Fortran-BESM.**
  GRUCON-1 (package): /MF=2,3/ =>
  group cross-sections, self-shielding factors, subgroup parameters
- **1985-1990: EC computer machines, Fortran-77**
  GRUCON-2: /+MF=4,5,6,12,13,14,15/=>
  group transition and photon production matrices (A. Rineiski),
  Padé-II approximation technique, convolution procedure (S.Badikov)
- **1990- 1993: Personal Computers (Windows,Linux)**
  GRUCON-3/+MF= 23,27/ photo-atomic cross-sections
- **1994-2007** **Pause**
- **2008- till now:** **GRUCON-3 /+MF=23,27,7/ photo-atomic cross-sections, thermal scattering matrices, free-gas scattering in resonance energy region (M.Malkov, A.Rineiski)**

GRUCON ARCHITECTURE



Nuclear Data Structures



Control Parameters

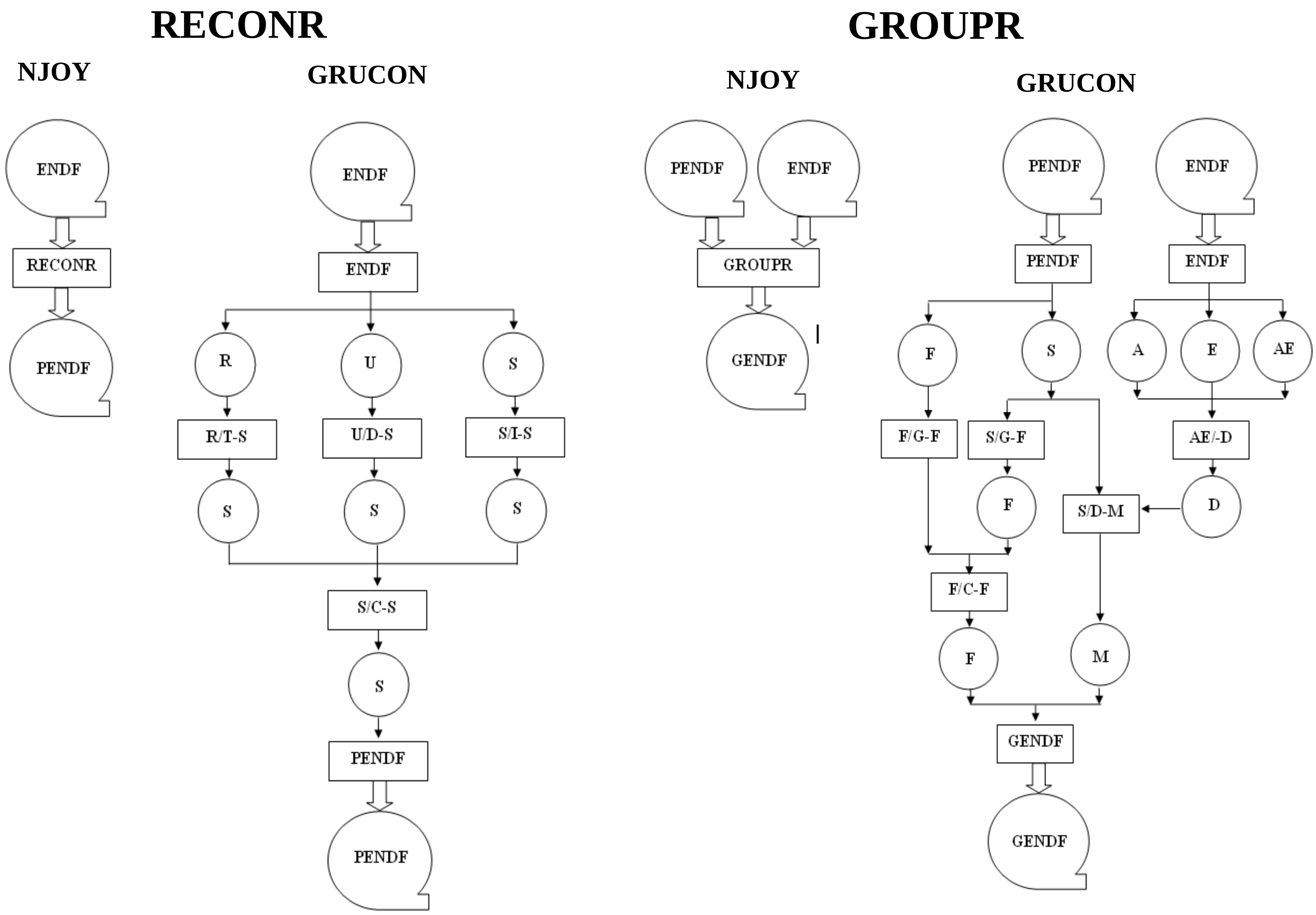
*IN	*OUT	*READ	*WRITE	*CP	*CC	*CON	*TAB
*ENDF	*PENDF	*GENDF	*GND (?)	*BNAB	*ACE	*ANISN	*PLOT
*R/T-S	*U/D-F	*U/D-S	*S/A-S	*S/C-S	*S/E-S	*S/I-S	*S/P-S
*S/T-S	*S/Y-S	*S/NU-S	*S/P-P	*S/G-F	*S/T-EA	*S/D-M	*S/G-MF
*S/-S	*S/-A	*S/-P	*S/-E	*S/O-S	*F/C-F	*F/E-F	*F/G-F
*F/S-S	*F/I-S	*F/C-S	*F/E-P	*F/O-F	*F/-F	*F/-P	*F/-S
*A/-A	*A/-S	*AE/-D	*AE/-AE	*EA/-D	*EA/-EA	*E/-S	*E/G-E
*M/C-M	*M/D-S	*P/D-F	*P/C-S	*P/-P	*TH/-EAS		
*ARITH	*DISTU	*EXTRA	*ORDER	*SELECT	*CATLG		

External Data and Convertors

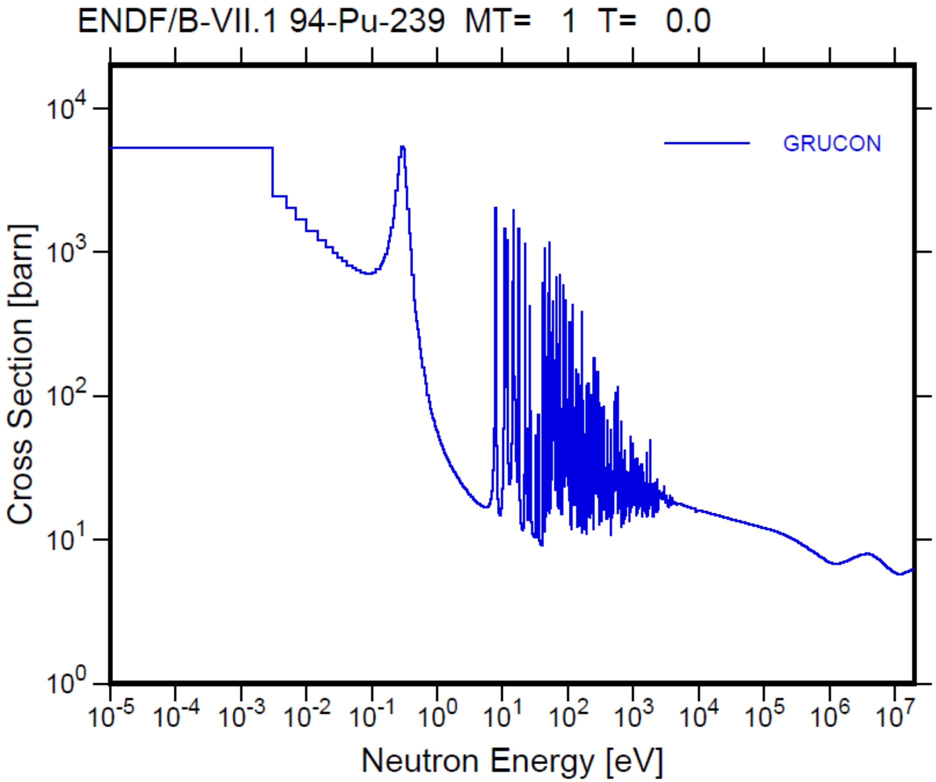
- **External Data Formats:**
  ENDF, PENDF, GENDF, BNAB, ACE, ANISN
  GND (?)

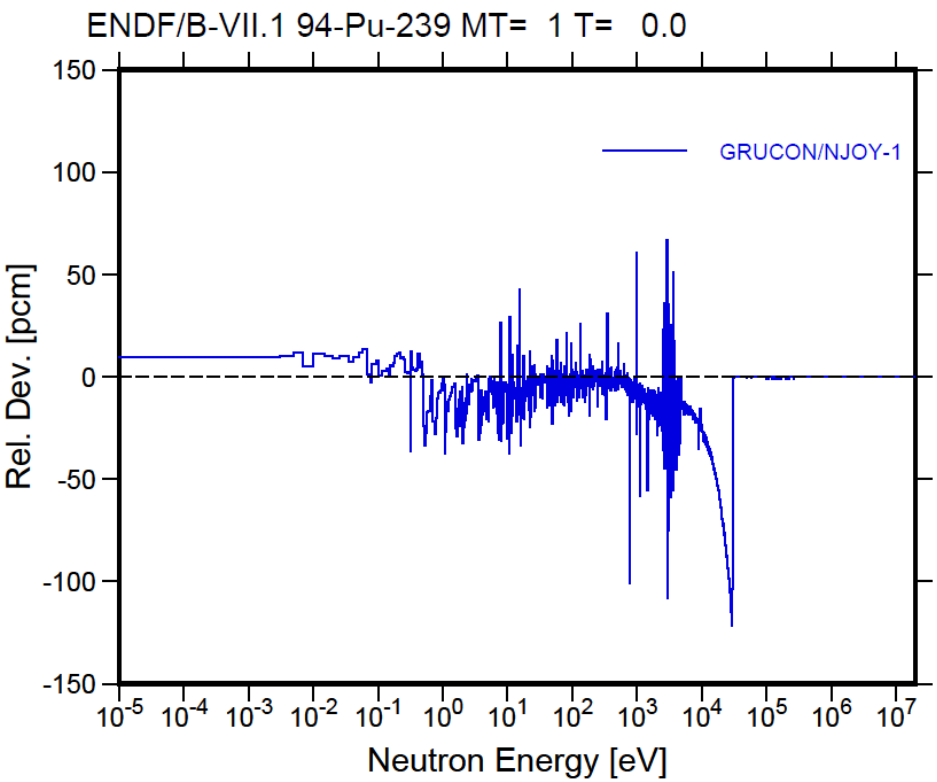
- **GRUCON Converters:**
  *ENDF : ENDF => GIR, GIR => ENDF
  *PENDF: PENDF => GIR, GIR => PENDF
  *GENDF: GENDF => GIR, GIR => ENDF
  *BNAB: GIR => BNAB
  *ACE: GIR => ACE
  *ANISN: GIR => ANISN
  *GND: GND => GIR (?)

Simulation of NJOY Modules



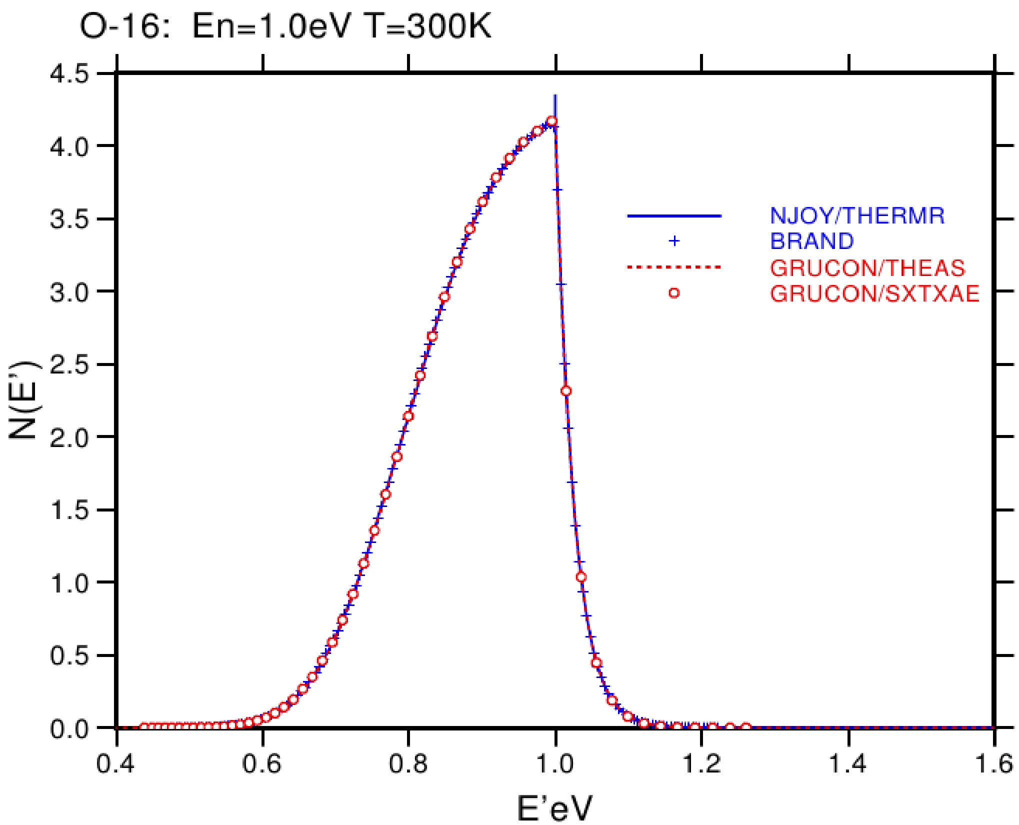
GRUCON vs NJOY/RECONR+GROUPR





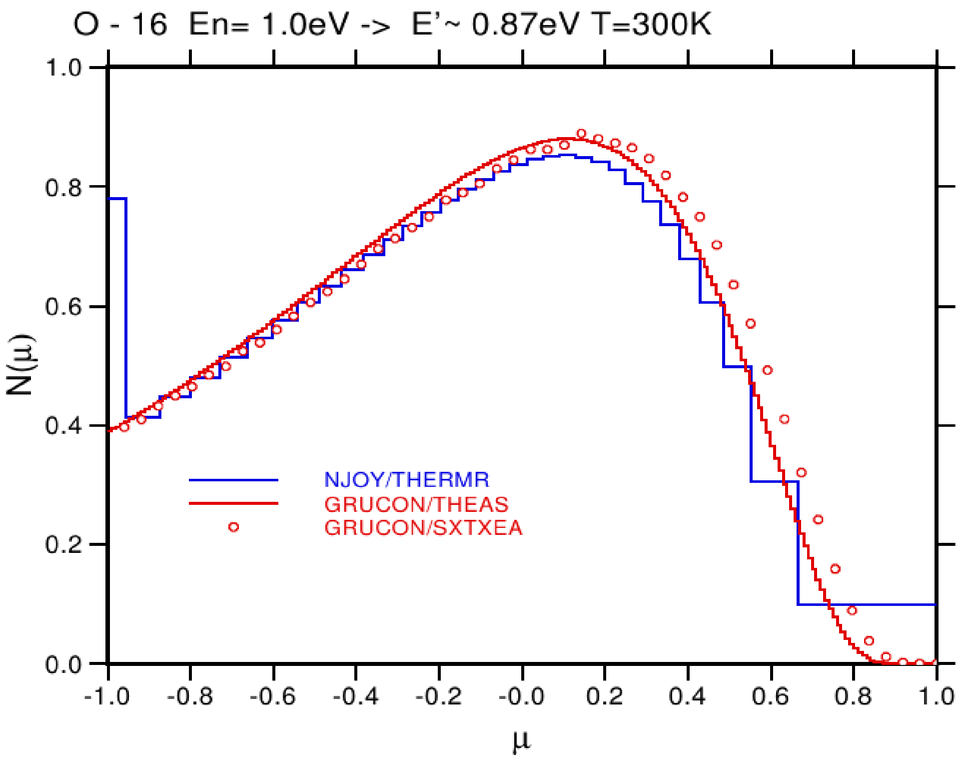
Pu-239: Total cross-sections, ECCO-1968 group structure (eps=0.001)

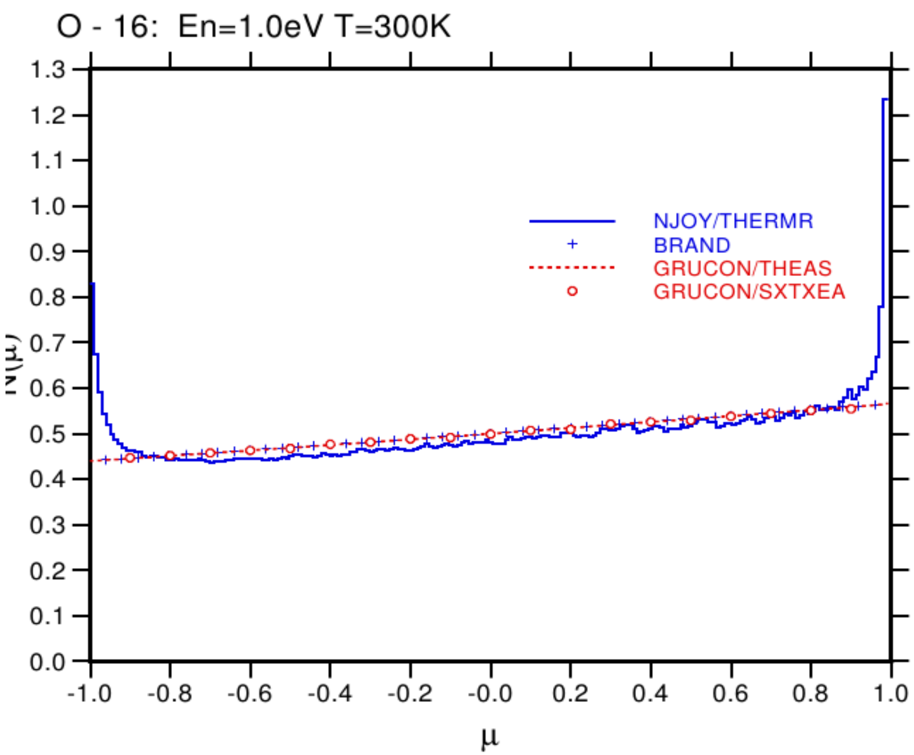
GRUCON vs NJOY/THERMR



O-16: Energy distributions, free gas scattering model

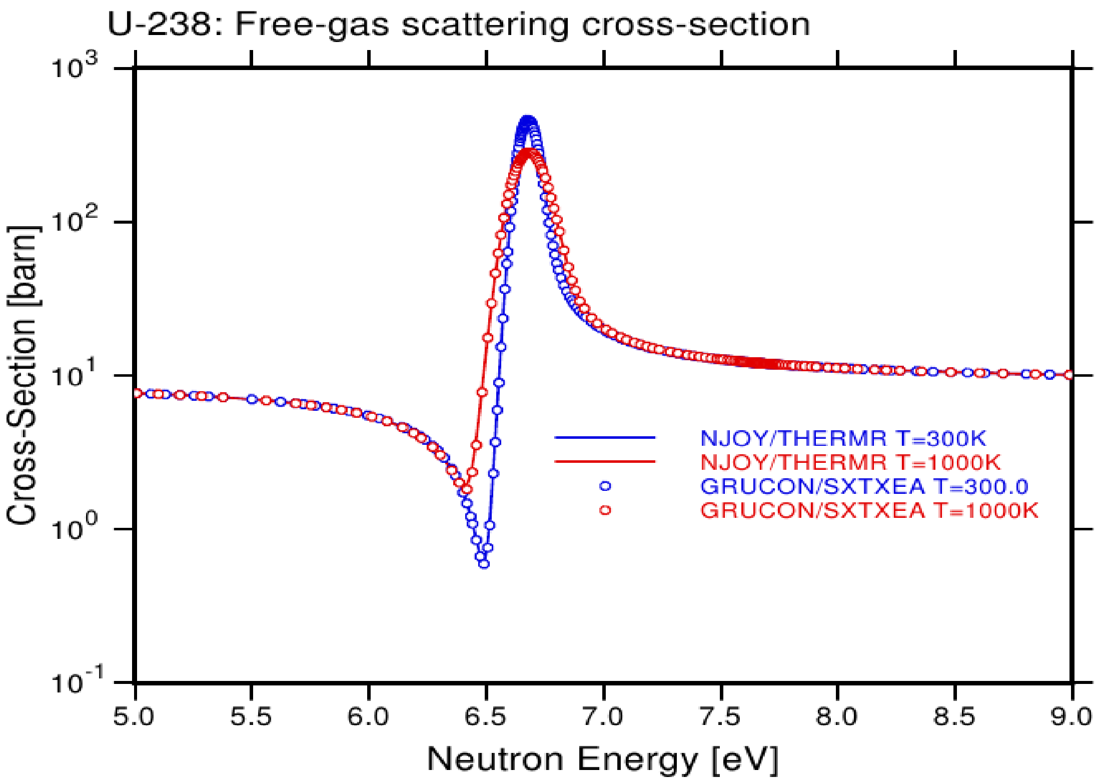
GRUCON vs NJOY/THERMR





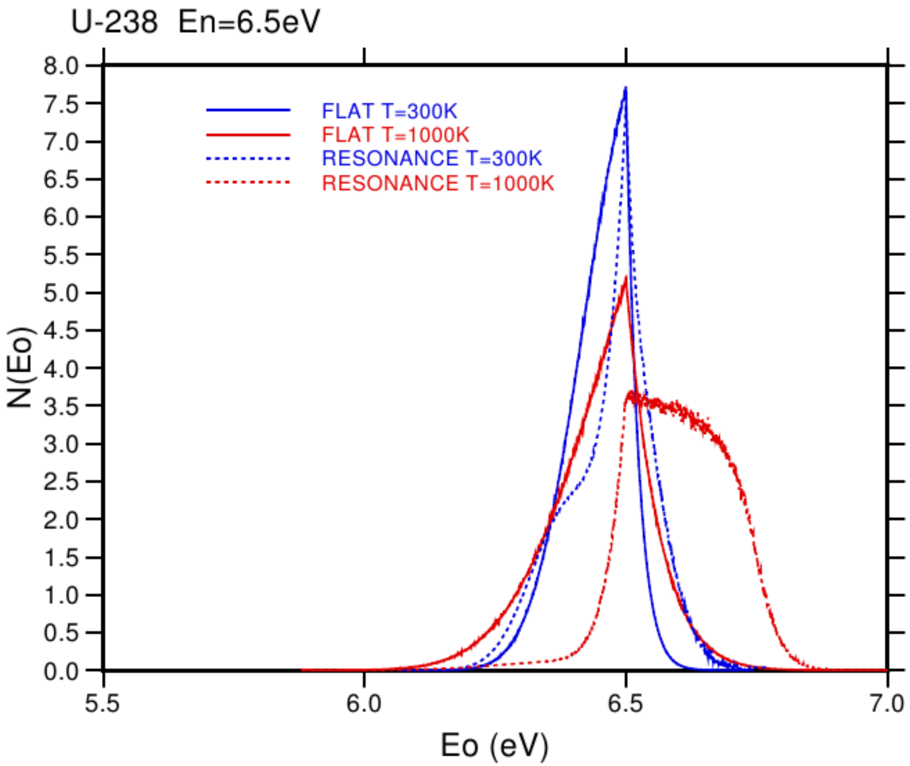
O-16: Angular distributions, free gas scattering model

GRUCON vs NJOY/THERMR

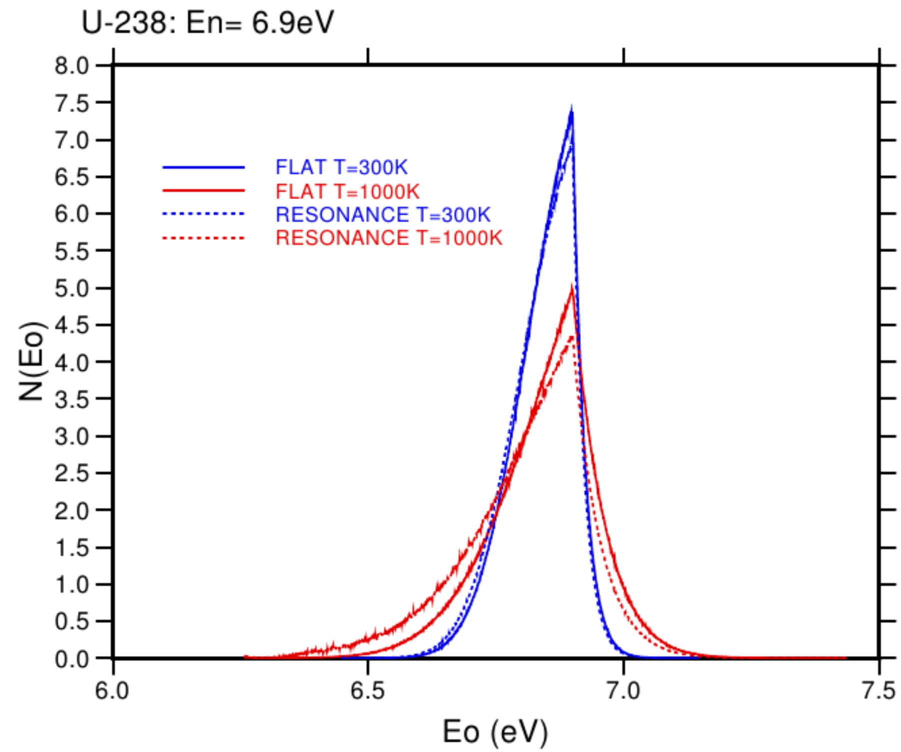


U-238: Scattering cross sections, free-gas model, T=300K and T=1000K

GRUCON vs NJOY/THERMR : Resonance influence



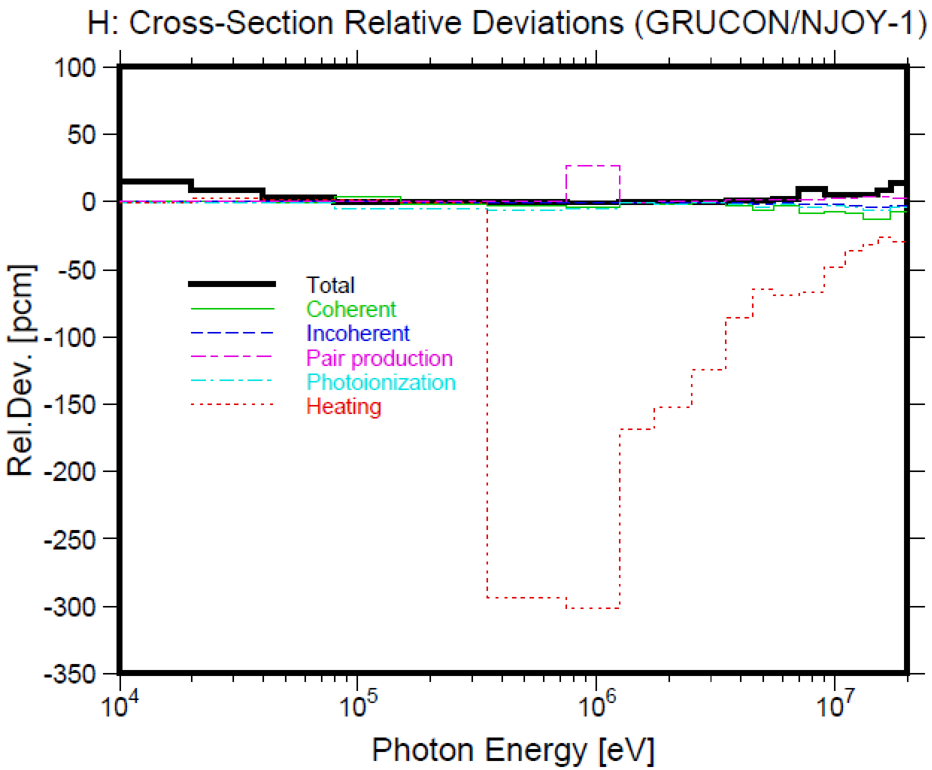
left wing

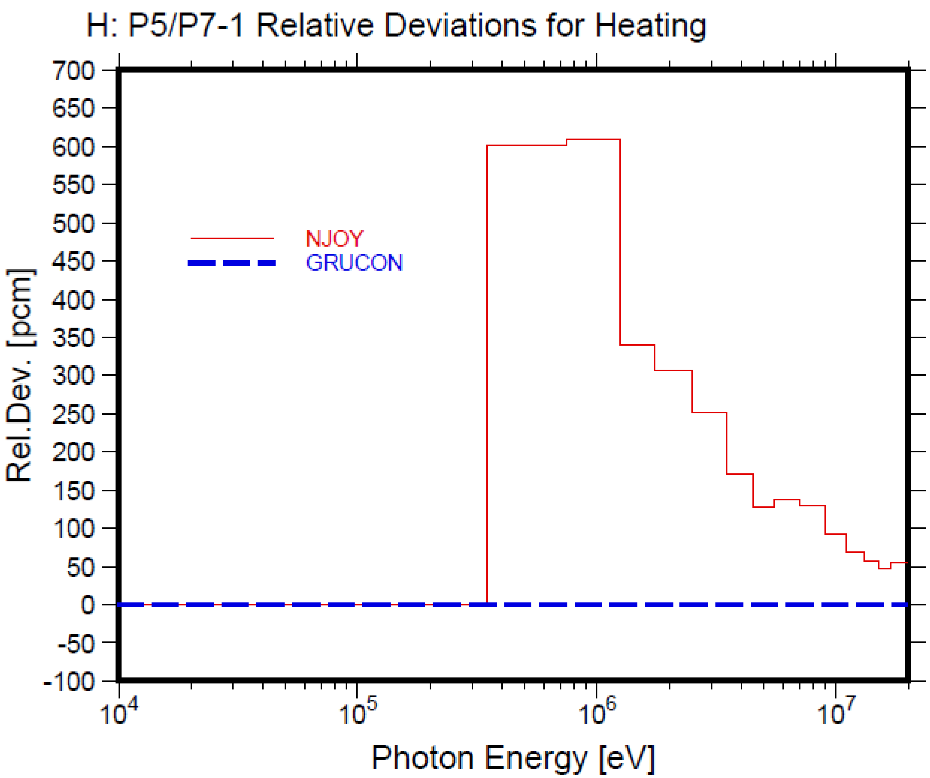


right wing

U-238: Energy distributions, calculated by the THERMR (flat scattering kernel) and SXTXEA (resonance scattering kernel) modules

GRUCON vs NJOY : GAMINR





H: Photo-atomic cross-sections

F/E-P Module: Subgroup (Multiband) Parameters calculation

Subgroup approximation of self-shielding factors (Gauss Quadratures, or *Padé-I*)

$$< 1/(\sigma_t(E)+\sigma_0)^{L-n} >= \sum_{i=1}^{N} a_i/(\sigma_{t,i}+\sigma_0)^{L-n}, n=1,...,2N$$

$$< \sigma_x(E)/(\sigma_t(E)+\sigma_0)^{K-n} >= \sum_{i=1}^{N} a_i\sigma_{x,i}/(\sigma_{t,i}+\sigma_0)^{K-n}, n=1,.., N$$

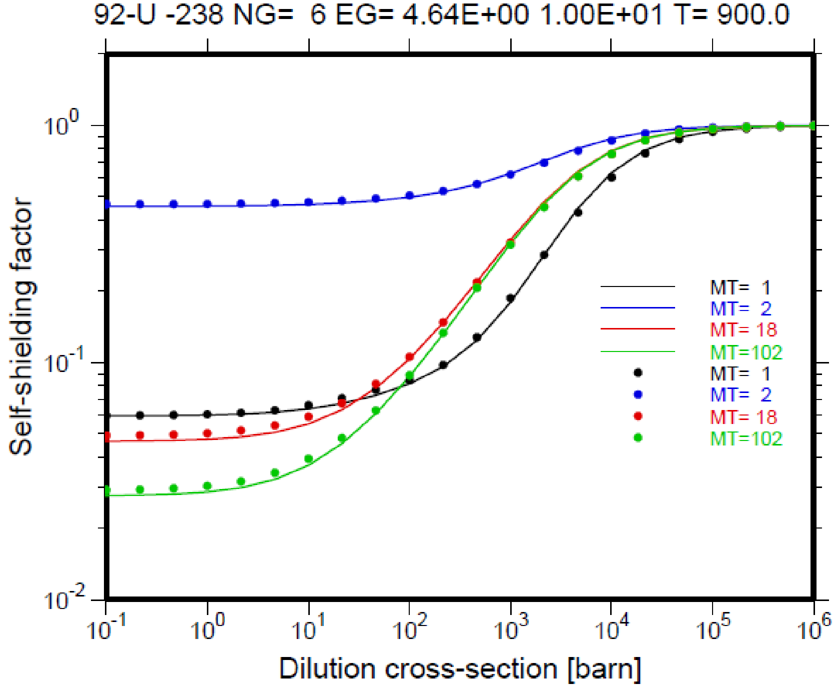
Where L,K, σ_0- parameters, defined to satisfy constraints:

$$\sum_{i=1}^{N} a_i = 1$$

$$\sum_{i=1}^{N} a_i\sigma_{x,i} = < \sigma_x >$$

$$\sum_{x\neq t} \sigma_{x,i} = \sigma_{t,i}, i=1,..., N$$

$$a_i, \sigma_{x,i} > 0$$



V.V.Sinitsa,M.N.Nikolaev, Analityc Determination of Subgroup Parameters, Atomic Energy, 35, No.6 (1973) pp. 429-430

F/C-F Module of GRUCON: Convolution Procedure

Self-shielding factors for mixtures.
“Extended” subgroup parameters

$$F_r(T,\sigma_0)=\frac{M_r(\sigma_0)}{M(\sigma_0)}$$

Where:

$$M(\sigma_0)=\sum_{\vec{i}} a_{\vec{i}}\frac{1}{(\sum_c \rho^{(c)}\sigma_{i(c)}^{(c)}+\sigma_0)}$$

$$M_r(\sigma_0)=\sum_{\vec{i}} a_{\vec{i}}\sum_c\frac{a_{r,i(c)}^{(c)}}{a_{i(c)}^{(c)}(\rho^{(c)}\sigma_{r,i(c)}^{(c)}+\sum_{c'\neq c}\rho^{(c')}\sigma_{i(c')}^{(c')}+\sigma_0)}$$

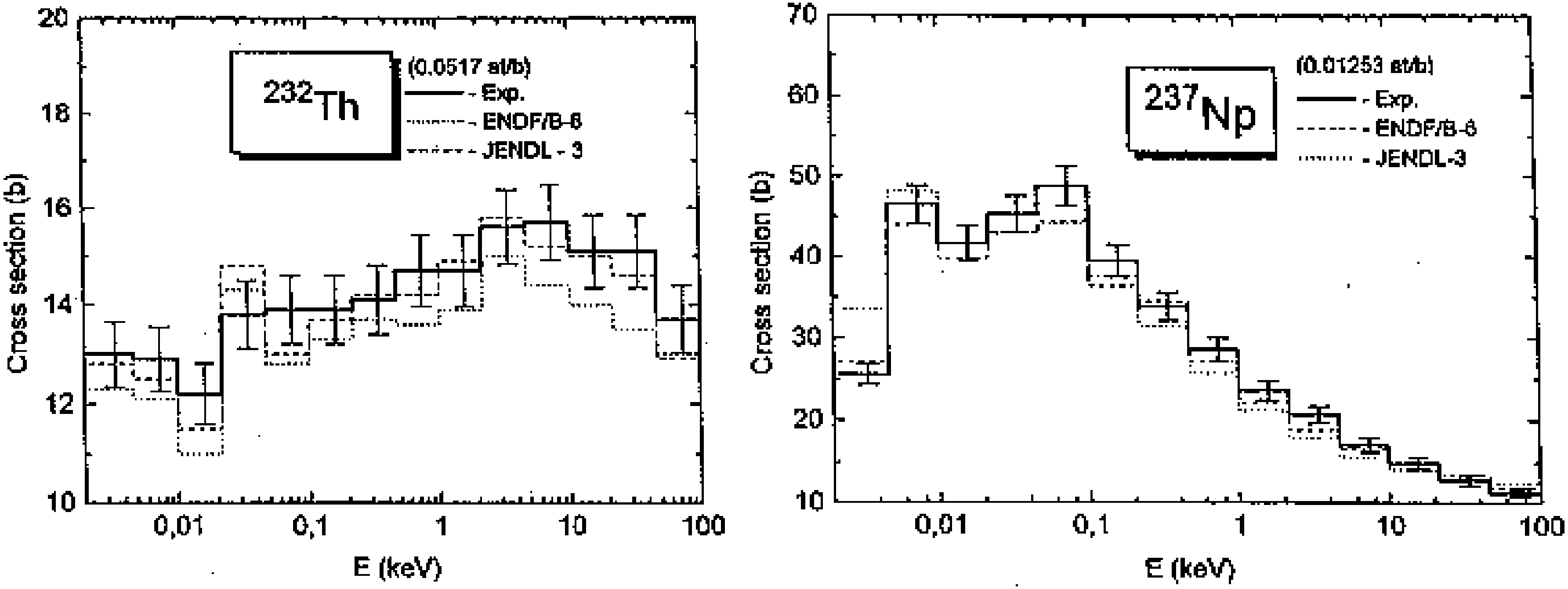
$\rho^{(c)}$ - nuclear density, $\quad a_{\vec{i}}\equiv\prod_{c=1}^{NC}a_{i(c)}^{(c)},\quad \sum_{\vec{i}}\{...\}\equiv\sum_{i(1)=1}^{I(1)}\sum_{i(2)=1}^{I(2)}...\sum_{i(NC)=1}^{I(NC)}\{...\}$

$a_{i(c)}^{(c)},\sigma_{i(c)}^{(c)},a_{r,i(c)}^{(c)},\sigma_{r,i(c)}^{c}$ - “extended” subgroup parameters, defined by *Padé-II* approximation of microscopic moments:

$$m_r^{(c)}(\sigma_0)\approx\sum_{i(c)}^{I(c)}\frac{a_{r,i(c)}^{(c)}}{(\sigma_{r,i(c)}^{(c)}+\sigma_0)},\quad m^{(c)}(\sigma_0)\approx\sum_{i(c)}^{I(c)}\frac{a_{i(c)}^{(c)}}{(\sigma_{i(c)}^{(c)}+\sigma_0)}$$

A. Rineiski and V. Sinitsa, "Extended Probability Tables for Approximating Neutron Multigroup Cross-Sections”, *M&C 2003, Gatlinburg, Tn, April 6-11, (2003).*

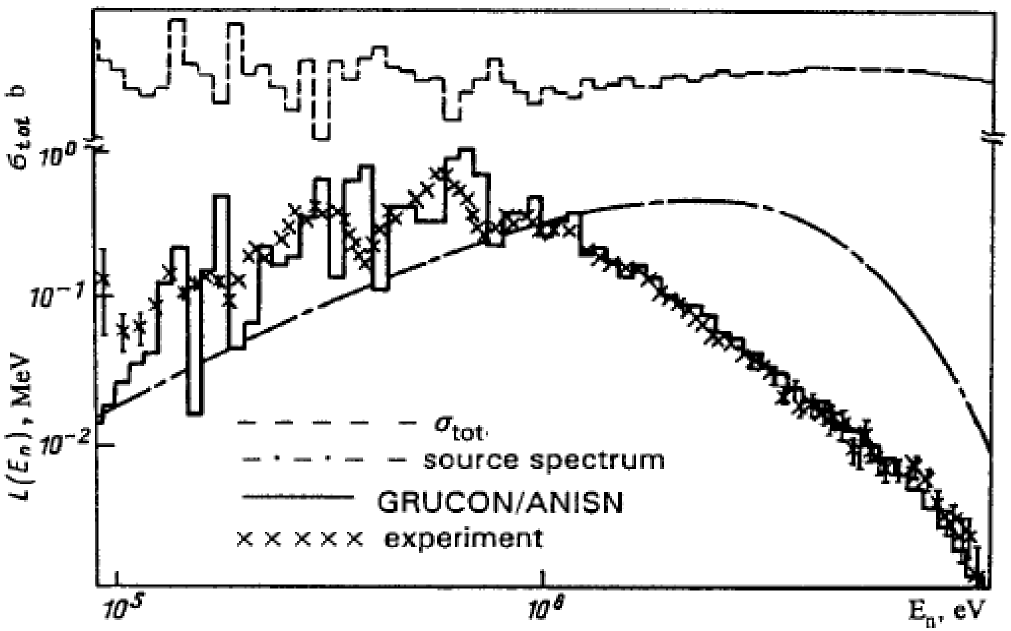
Transmission Function Calculations



Experimental and calculated observed total cross-sections of Th^{232} (left) and Np^{237}(right)

Grigoriev, Yu.V., Sinitsa,V.V., Gundorin, N.A.,Popov, Yu.,P., Investigations of the Resonance Structure of Neutron cross-Sections for Thorium-232 and Neptunium-237 in the 2eV-100keV Energy Region, VANT, *Nucl.Data*, 1, (1998) p.9

Neutron Leakage Spectra Calculations



Spectrum of leakage neutrons from iron sphere with a californium source

Zhuravlev, B.V., Lychagin, A.A., Trykova,V.I.,Demenkov,V.G.,Androsenko,P.A.,Sinitsa,V.V., Spectrum of Leakage Neutrons from an Iron Sphere with a Californium Neutron Source, Atomic Energy, 76,No.3,(1994) pp. 229-234

CURRENT STATE, INTENTIONS

After a long pause (~15 years), the works under the GRUCON package are continued. The Fortran texts and documentation are revising and updating (~70%).

Intentions exist to extend the GRUCON possibilities in different applications, such as preparation of special data libraries, verification of processing algorithms, evaluation and validation of nuclear data.

The possibility of inclusion the GND structures to the GRUCON package is under consideration. Due to absence of any explicit dependency the GRUCON processing modules from “external” formats, it will not require, apparently, extensive rework.

Thank you for attention!