

---

# The GRUCON Command Language for Nuclear Data Handling

---

V.Sinitsa  
NRC “Kurchatov Institute”

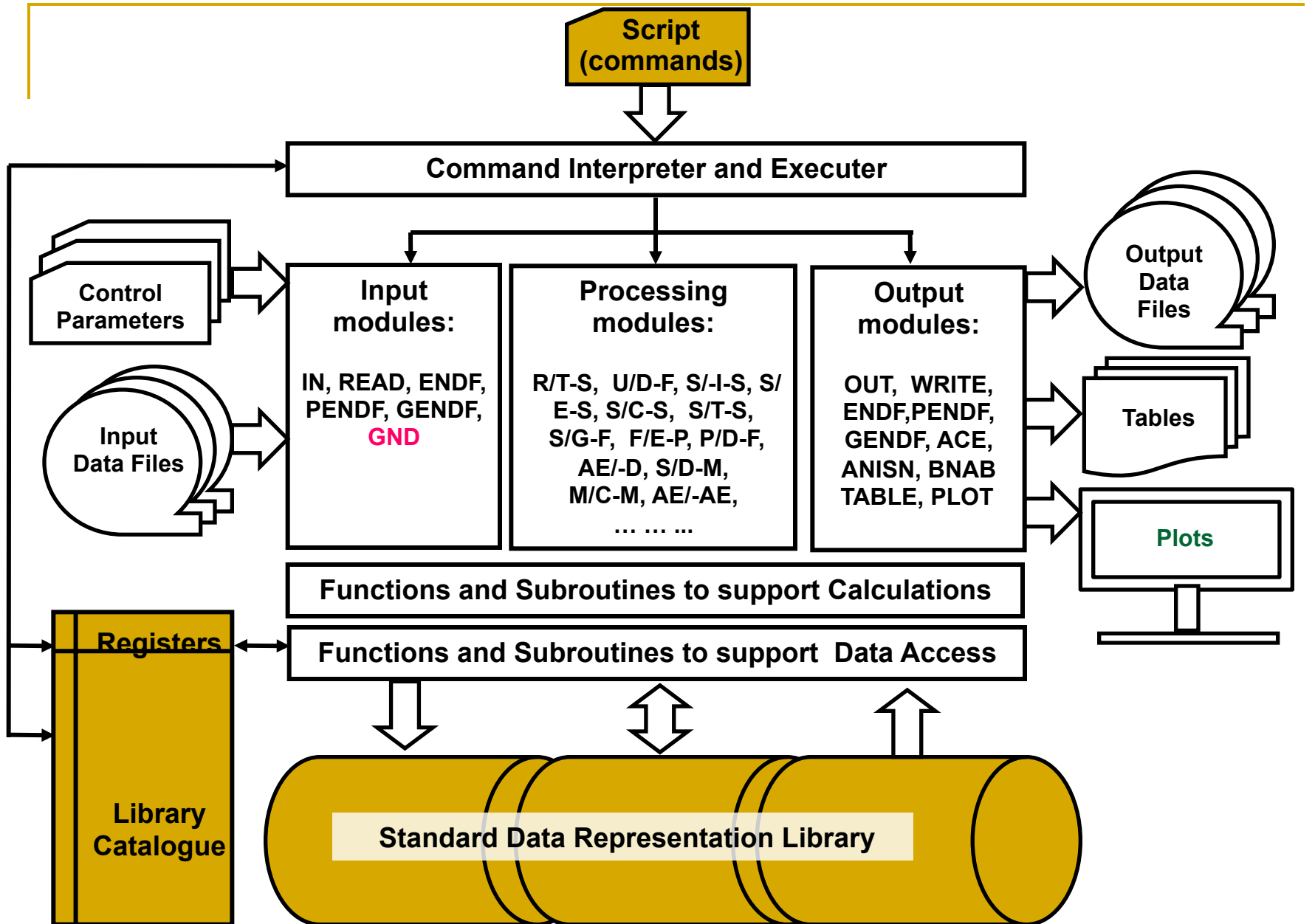
---

# Outline

- The GRUCON Package Architecture
- Library, Catalogue and Commands.  
Similarity with Excel Data Sheets
- Standard Data Structures (SDS)
- Functional Modules and Control Parameters
- Script examples.  
GRUCON/NJOY/FUDGE inter-comparison
- Conclusions

---

# The GRUCON Package Architecture



---

# **Library, Catalogue and Commands. Similarity with Excel Data Sheets**

## Definitions

- “Standard Data Representation” (SDR) is any data (nuclear data or control parameters, needed for processing) , structured as follows:

<SDR> = <HDS> <MAT> <MZAS> <MZAP> <LHA> <LIA> <LRA> <HA> <IA> <RA>

where

<HDS> - unique name of structure

<MAT> - data identification number

<MZAS> - target nuclide mass-charge-state flag

<MZAP> - projectile mass-charge flag

LHA,LIA,LRA – total lengths of Character, Integer and Real Arrays

HA(1:LHA),IA(1:LIA),RA(1:LRA) – Character(4), Integer(4) and Real(8) Arrays, containing texts, parameters, and data values.

- “SDR Library” – set of direct access files, or “Segments”, for SDR placing
- “SDR Fascicle” (SDRF) - Any sequence of SDR’s placed on one segment
- “SDR Library Catalogue” – table of rows containing:
  - <NAME> - SDRF mnemonic name
  - <N> - library segment number,
  - <M> - the SDRF first word position on segment
  - <L> - the SDRF length (number of words)

## Commands

Nuclear data handling in the GRUCON package is controlled by the sequence of commands (script).

In general case the command contains seven fields as follows:

<I>, <J>, <K>, <NAME>, <N>, <M>, <L>

where

<I>, <J> - the position numbers of catalogue rows, in which  
the input data and control parameters are registered

<K> - the position number of catalogue row, in which  
the obtained results should be registered

<NAME> - the registration name of results and

<N>, <M>, <L> - the recommended address for placing the obtained SDRF  
( if necessary; it is enough usually to use default values)

There are commands with empty fields, depending from their destination:

,,,INIT,<N>,<M>,<L> - segment creating,

,<J>,<K> ,<NAME> - data reading from the external data file,

<I>,<J> - data writing to the external data file,

<I> - printing of catalogue contents, and so on.

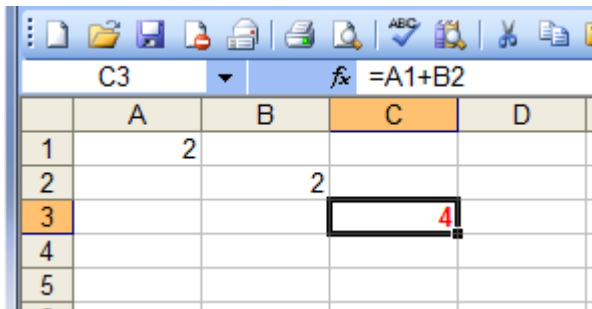
Several commands contain on the <J> field the module name directly:

,IN,<K>,<NAME> - reading control parameters in input flow after commands,

<I>,TAB - printing SDR and so on.

## Similarity with Excel Data Sheets

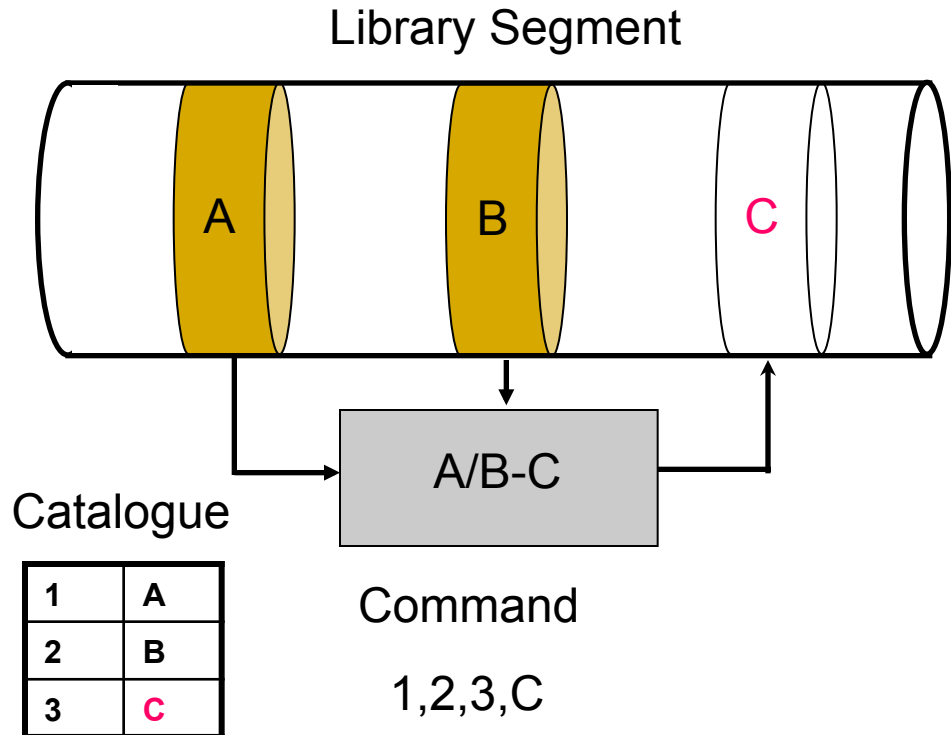
The logic of data handling in the GRUCON package can be compared with calculations in Excel, where role of cells coordinates in Excel Data Sheet play row position numbers in the catalogue.



The screenshot shows an Excel spreadsheet with the following data:

	A	B	C	D
1	2			
2		2		
3			4	
4				
5				

The formula bar shows the formula  $=A1+B2$  for cell C3.



---

# Standard Data Structures (SDS)

## Evaluated Data Standard Structures

<b>*S*</b>	<b>Cross section tables</b>
<b>*R*</b>	<b>Resolved resonance parameters</b>
<b>*U*</b>	<b>Unresolved resonance parameters</b>
<b>*A*</b>	<b>Angle distribution parameters</b>
<b>*E*</b>	<b>Secondary energy distribution parameters</b>
<b>*AE*</b>	<b>Energy-angle distribution parameters</b>
<b>*TH*</b>	<b>Scattering functions in thermal energy region</b>
<b>*NU</b>	<b>Fission neutron data</b>
<b>*Y*</b>	<b>Reaction product yields</b>
<b>*D*</b>	<b>Group-angle distributions</b>
<b>*F*</b>	<b>Group averaged cross section functions</b>
<b>*M*</b>	<b>Group transition matrices with angle dependences</b>
<b>*P*</b>	<b>Subgroup parameters ("probability tables")</b>
<b>*EA*</b>	<b>Energy-angle distributions</b>

## Multigroup Data Standard Structures

<b>*EA*</b>	<b>Modifications of energy-angle distributions</b>
<b>*D*</b>	<b>Group-angle distributions</b>
<b>*F*</b>	<b>Group averaged cross section functions (moments, exponents)</b>
<b>*M*</b>	<b>Group transition matrices</b>
<b>*P*</b>	<b>Subgroup parameters ("probability tables")</b>

### Representations of angular dependency:

- 0 - Tabulated function
- 1 - Distribution averaged in equal cosine intervals
- 2 - Legendre expansion coefficients
- 3 - Equal probable cosine boundaries
- 4 - Equal probable cosine values

## Example: the GRUCON \*S\* standard structure

<b>NE</b>	<b>Number of energy points</b>
<b>NS</b>	<b>Number of reaction types</b>
<b>NT</b>	<b>Number of temperatures</b>
<b>±KINT</b>	<b>Interpolation law flag for cross section energy dependency. KINT&lt;0 - number of interpolation ranges</b>
<b>LS(NS)</b>	<b>List of reaction types</b>
<b>LIN(2,-KINT)</b>	<b>Interpolation ranges table (KINT&lt;0): LIN(1,I) - serial number of separating point for I<sup>th</sup> and (I+1)<sup>th</sup> ranges, LIN(2,I) - interpolation scheme in I<sup>th</sup>-range</b>
<b>EL</b>	<b>Lower limit for energy range (eV)</b>
<b>EH</b>	<b>Upper limit for energy range (eV)</b>
<b>EPS</b>	<b>Tolerance parameter value</b>
<b>AW</b>	<b>Nuclear mass ( C<sup>12</sup> units)</b>
<b>Q(NR)</b>	<b>Reaction Q-value (eV)</b>
<b>TEM(NT)</b>	<b>Temperature values (°K)</b>
<b>TAB(*)</b>	<b>(E(IE),((XS(IT,IS,IE),IT=1,NT),IS=1,NS),IE=1,NE) - data table</b>

---

# Functional Modules and Control Parameters

## The GRUCON Reading/Writing Modules

<b>*IN</b>	<b>Reading Control Parameters</b>
<b>*READ</b>	<b>Reading SDR file ( BCD or Binary)</b>
<b>*ENDF</b>	<b>Reading ENDF file (MF=1,2,3,4,5,6,7,8,9,10,13,14,23,27)</b>
<b>*PENDF</b>	<b>Reading PENDF file ( the NJOY pointwise format )</b>
<b>*GENDF</b>	<b>Reading GENDF file ( the NJOY groupwise format )</b>
<b>*GND</b>	<b>Reading GND file ( for *S* structures) – trial version</b>

<b>*OUT</b>	<b>Printing SDR</b>
<b>*WRITE</b>	<b>Writing SDR file (BCD or Binary)</b>
<b>*TABLE</b>	<b>Printing SDS annotated table</b>
<b>*PLOT</b>	<b>Plotting SDS</b>
<b>*ENDF</b>	<b>Writing SDS to ENDF file</b>
<b>*PENDF</b>	<b>Writing SDS to PENDF file</b>
<b>*GENDF</b>	<b>Writing SDS to GENDF file</b>

## The GRUCON Processing Modules ( 15 most common, with total number ~ 50 )

<b>*R/T-S</b>	<b>Reconstructing cross sections from resonance parameters</b>
<b>*S/I-S</b>	<b>Changing interpolation law</b>
<b>*S/C-S</b>	<b>Joining cross section tables to one table</b>
<b>*S/NU-S</b>	<b>Multiplying fission cross-section on the neutron multiplicity</b>
<b>*S/Y-S</b>	<b>Multiplying cross section on the correspond product yield</b>
<b>*S/T-S</b>	<b>Doppler broadening of cross sections (the SIGMA-1 algorithm)</b>
<b>*S/G-F</b>	<b>Group averaging of cross section functions</b>
<b>*U/D-F</b>	<b>Reconstructing functions from unresolved resonance parameters</b>
<b>*F/C-F</b>	<b>Collapsing group cross section function</b>
<b>*F/E-P</b>	<b>Preparing subgroup parameters</b>
<b>*AE/-D</b>	<b>Group averaging of secondary energy distributions</b>
<b>*S/D-M</b>	<b>Calculating group transition matrices</b>
<b>*THEAS</b>	<b>Reconstructing energy-angular distribution in thermal energy region</b>
<b>*S/T-EA</b>	<b>Calculating energy-angular distribution in resonance energy region</b>
<b>*S/G-MF</b>	<b>Calculating group cross-sections and matrices for photo-atomic data</b>

## Example: the R/T-S module control parameters

<b>*R/T-S</b>	<b>Reconstructing cross sections from resonance parameters</b>	
	<b>NFOR</b>	<b>Formula number:</b> <b>0 –Take from *R* input data</b> <b>1 - Single-level Breit-Wigner</b> <b>2 - Multilevel Breit-Wigner</b> <b>3 - Reich-Moore</b> <b>4 - Adler-Adler</b> <b>13 - Reich-Moore for nonfissile nuclei (Lukyanov)</b> <b>14 - Adler-Adler (Lukyanov-Kolesov)</b>
	<b>NTEM</b>	<b>Number of temperatures</b>
	<b>EL</b>	<b>Lower limit for energy range (eV)</b>
	<b>EH</b>	<b>Upper limit for energy range (eV)</b>
	<b>EPS</b>	<b>Tolerance parameter value</b>
	<b>TEM(NTEM)</b>	<b>Temperature values (°K)</b>

## Example: the GND module control parameters (trial version)

<b>*GND</b>	<b>Reading GND/XML data</b>	
	<b>NTAPE</b>	<b>Unit for input GND/XML tape</b>
	<b>NS</b>	<b>Number of reactions (NS=0 – all reactions)</b>
	<b>LS(NS)</b>	<b>List of Reactions (ENDF_MT) ( if NS&gt;0 )</b>

---

# **Script examples.**

## **NJOY/FUDGE/GRUCON comparison**

## Example: Script for reconstructing cross-sections from any ENDF file

```
,,,init,1,0,10000k ! Prepare segment number 1 for current work
,in ! Enter local parameters ( here: *de - energy range, *eps - tolerance)
,in,1,endf ! Enter control parameters: ENDF, S/I-S, R/T-S,U/D-S, S/C-S, WRITE
,in,2,s/i-s
,in,3,r/t-s
,in,4,u/d-s
,in,5,s/c-s
,in,6,write
,1,20,rus ! Read ENDF data (tape20,bcd)
20,2,21,s ! Linearize x-s tables (s/i-s)
20,3,21 ! Prepare x-s from resonance parameters (r/t-s)
20,4,21 ! Prepare x-s from average resonance parameters (u/d-s)
21,5,22,s ! Join all prepared cross-section tables (s/c-s)
23,6 ! Write cross-section to file (tape30, binary)
,,,end ! End of script
*de: el=1.e5,eh=20.e6,
*eps: eps=0.001
*endf: ntape=20, nmat=0, nmf=2, nmt=4 ,mf=2,3, mt=1,2,18,102
*s/i-s: nint=2,*de,*eps
*r/t-s: nfor=0, nt=1,*de,*eps, tem=0.
*u/d-s: nun=20, nfun=0, nin=2, nt=1, np=0, nl=0, nh=0,*de,*eps, tem=0.
*s/c-s: ncom=0, ns=0,*de,*eps
*write: ntape= -30
```

## Example: Script for cross section plotting

```
,,,init,1,0,1000k  ! Prepare segment
,in                ! Enter local parameters *mt ( reaction type), *de ,*eps
,in,1,read        ! Enter the READ control parameters
,in,2,plot        ! Enter the PLOT control parameters
,1,10, s          ! Read the tape30 binary file ( with cross sections)
10,2              ! Prepare ps-file for plotting
,,,end            ! End of script
```

```
*/ **** local parameters ***
```

```
*mt: mt=?,
```

```
*de: el=1.e-5,20.e6,
```

```
*eps: eps= 0.001
```

```
*/ *** control parameters ***
```

```
*read: ntape=-30
```

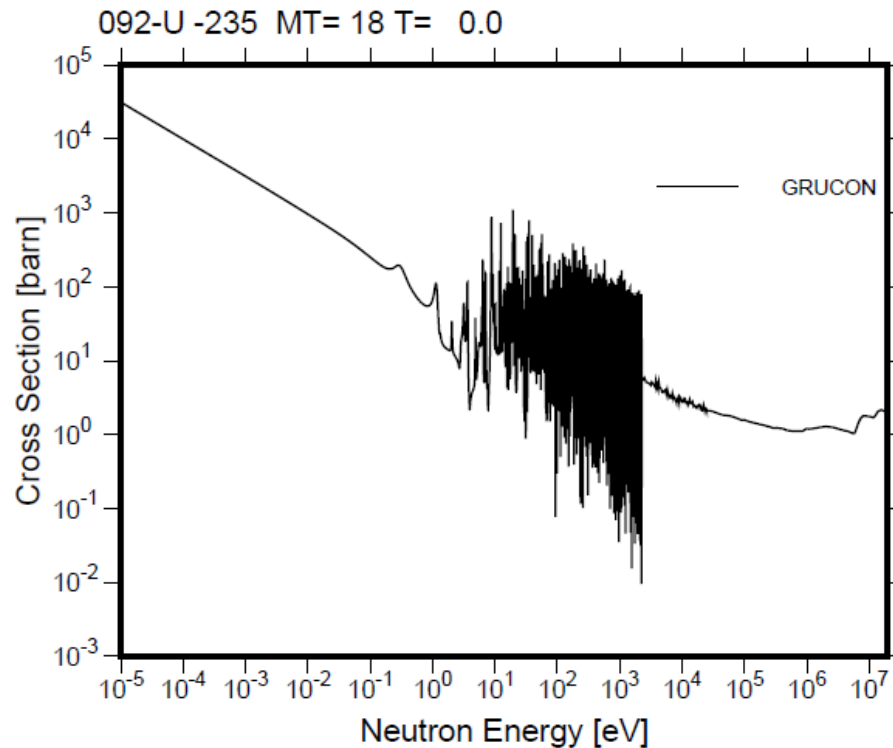
```
*plot: ncur=1, nmod=0,
```

```
nr=1, nt=1, *mt,
```

```
*eps, *de, deo=0.,0.,
```

```
dx=0.,0.,dy=0.,0.,
```

```
tem=0.
```

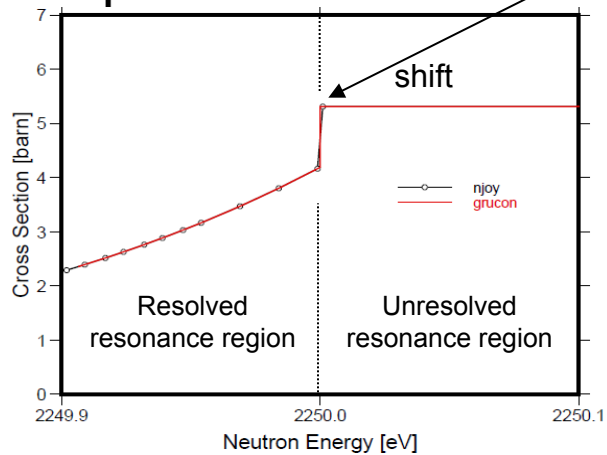
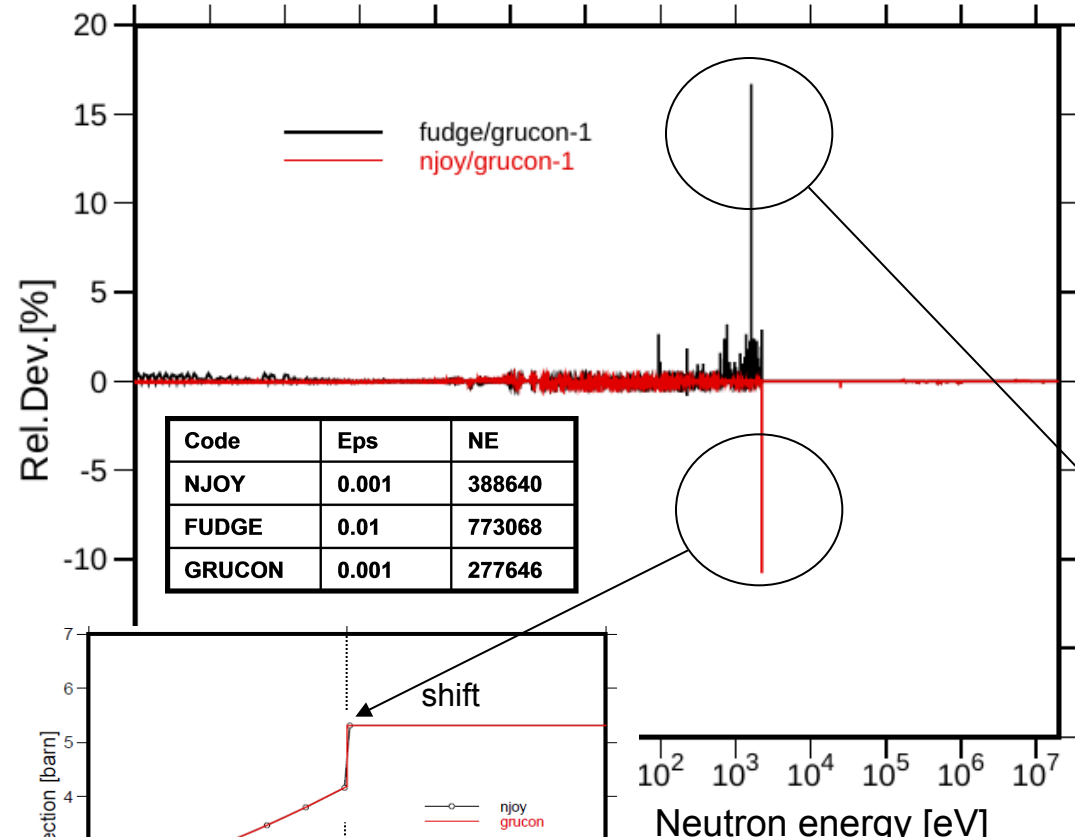


## Example: Script for U-235 cross section comparison

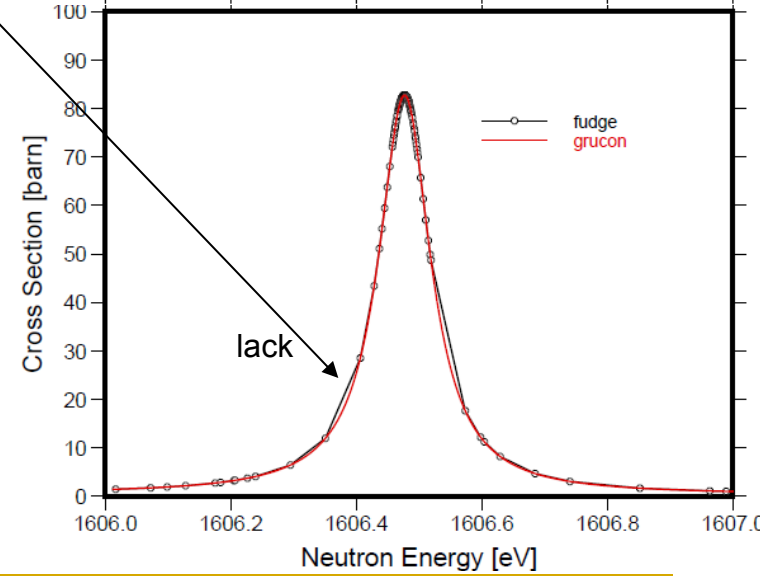
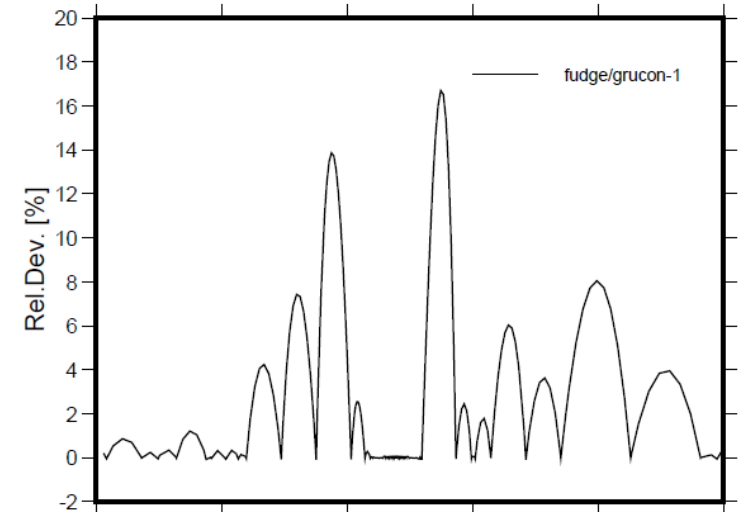
```
,,,init,1,0,100000k ! Prepare segment
,in                ! Enter local parameters
,in,1,read        ! Enter control parameters for modules: READ, PENDF, GND, S/-S, PLOT
,in,2,gnd
,in,3,pendf
,in,4,s/-s
,in,5,plot
,1,20, s          ! Read tape30 ( the GRUCON results)
20,4,21,dev       ! Extract cross-section MT=18 and use for Rel. deviations
,2,22,s          ! Read tape40 (the GND/XML file with FUDGE results)
,3,23,s          ! Read tape50 ( the PENDF binary file with NJOY results)
22,21,24,s       ! Calculate FUDGE/GRUCON-1 relative deviation
23,21,24         ! Calculate NJOY/GRUCON-1 relative deviation
24,5             ! Plot
,,,end           ! End of script
*mt: mt=?       ! Local parameter; the symbol "?" means "interactive inquire"
*read: ntape=-30
*gnd: ntape=40,mat=9228,nmt=1, *mt
*pendf: ntape=50,ktem=0,nmat=0,nmf=0,nmt=1,mf=3, *mt
*s/-s: ns=1,nt=0, *mt
*plot: ncur=2,imod=2,kint=3,nr=1,nt=1, *mt,
eps=0.001,dei=1.e-5,20.e6,deo=0.,0.,dec=0.,0.,dy=0.,0.,tem=0.
```

# U235: Cross-section comparison

092-U -235 MT= 18 T= 0.0



092-U -235 MT= 18 T= 0.0



# Conclusions

- **The GRUCON Command Language and nuclear data Standard Representation Types allow to handle data in large variety of applications.**
- **The new GND module opens possibility to handle GND/SML data structures.**
- **The comparison of cross-sections, reconstructed from resonance parameters, reveals cases of insufficiency and non-optimality in the selection of reference energy points.**