

COVARIANCE DATA GENERATION IN THE RESONANCE REGION

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TOOLS

- **EVALUATION TOOLS: SAMMY**
 - **Evaluation code used for data and uncertainty evaluations in the resonance region**
 - **Used also to check the results of data processing codes (average cross sections)**
- **PROCESSING TOOLS: NJOY/ERRORJ and AMPX/PUFF**
 - **ERROJ is now part of the NJOY code system**
 - **PUFF is the ORNL tool for processing covariance data**

Covariance Evaluation Procedure

Use the SAMMY code

Retroactive covariance: Obtained when no experimental data exist.
Educated guess on “pseudo” experimental data generation;

Direct generation of covariance: Done in the flow of the evaluation;

SAMMY to ENDF

SAMMY generated resonance covariance can be converted into the ENDF format (FILE 32 SECTION 2151)

LCOMP=1 existing ENDF format

LCOMP=2 new compact format. There are still some issues with this option. Nancy Larson will talk about that !!

Covariance Evaluation Procedure (cont'd)

1. Memory Allocation for SAMMY

Dominant contribution to the SAMMY array (sensitivity matrix):

Number of resonances N_{res}

Number parameters per resonance N_{par}

Number of experimental data points N_{dat} (auxiliary grid**)**

SAMMY requested memory size:

Mem= $(N_{\text{res}} \times N_{\text{par}} \times N_{\text{dat}}) \times 8$ bytes

SAMMY computation of the Resonance Parameter Covariance Matrix (RPCM) requires a memory size of approximately

$2 \times \text{Mem}$

Covariance Evaluations

3. Evaluations

- a) **Resonance covariance evaluations have been done for ^{233}U , ^{235}U , ^{238}U , ^{239}Pu , and ^{232}Th**
- b) **LCOMP=1 format used**
- c) **High energy covariance provided by LANL for ^{235}U , ^{238}U and ^{239}Pu were merged with ORNL resonance evaluations**
- d) **Evaluation for ^{232}Th done under IAEA/CRP**
- e) **New cross section and covariance evaluation for ^{239}Pu**
- f) **Resolved and unresolved covariance for ^{233}U (No high energy covariance)**

NOTE:

- **Memory allocation:**

8 bytes/word

- **ASCII file allocation:**

11 bytes/word

²³³U Covariance Matrix

Full covariance has been generated in the energy range from 10^{-5} to 600 eV (RR) and from 600 to 40 keV (UR)

SAMMY memory size estimation

No. of resonances = 770

No. of varied parameters per resonance = 5

No. of data points = 20,000

Mem = $(770 \times 5 \times 20,000) \times 8$

Memory needed = $2 \times \text{Mem} \sim 1.3$ Gbytes

Resonance Covariance for ^{233}U

Space storage needed for ^{233}U covariance

$$N_{\text{res}}=770$$

$$N_{\text{par}}=5$$

$$N=N_{\text{res}} \times N_{\text{par}}$$

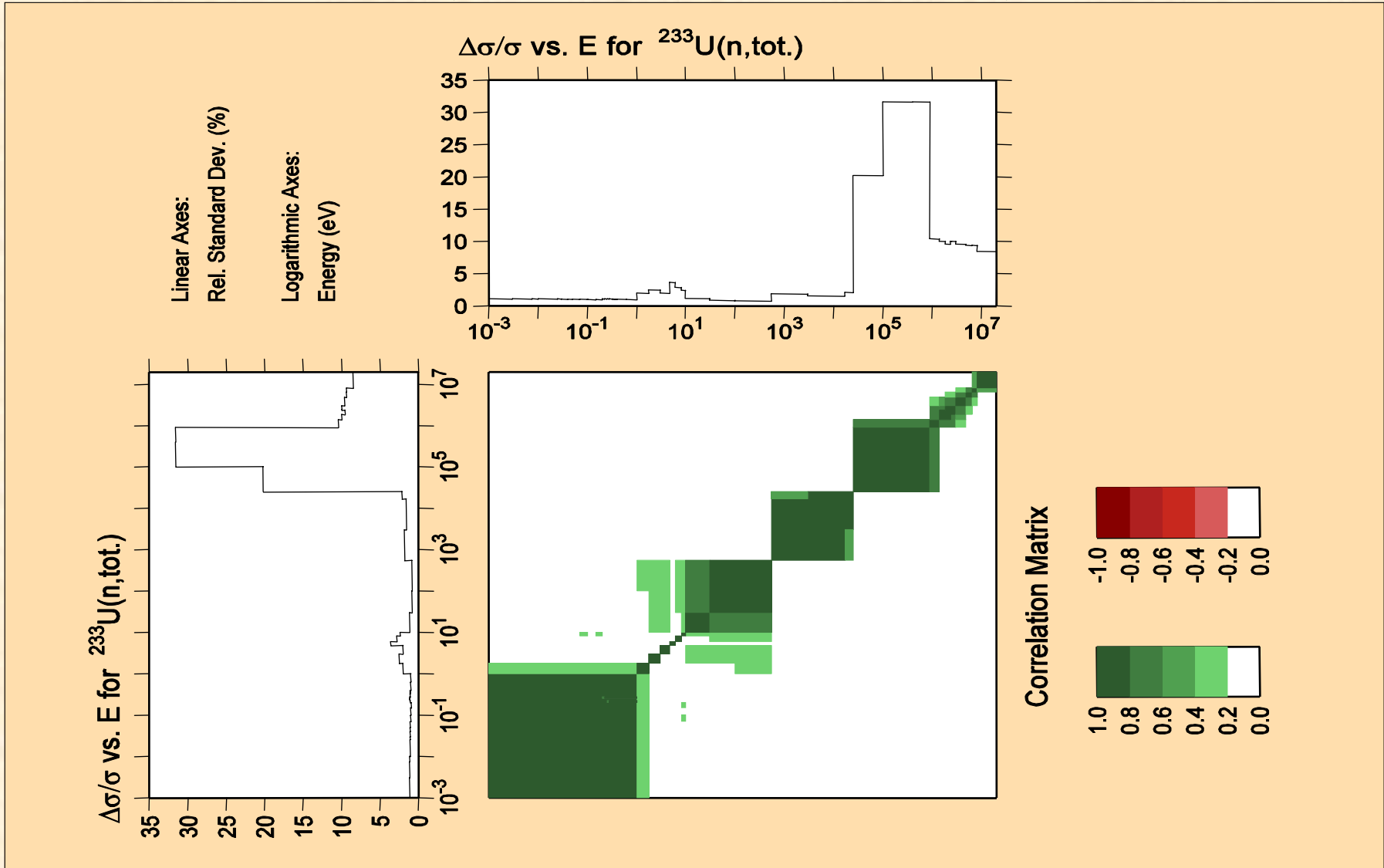
$$N_s = (N^2/2 + N/2) \times 14^*$$

$$N_s \sim 100 \text{ Mbytes}$$

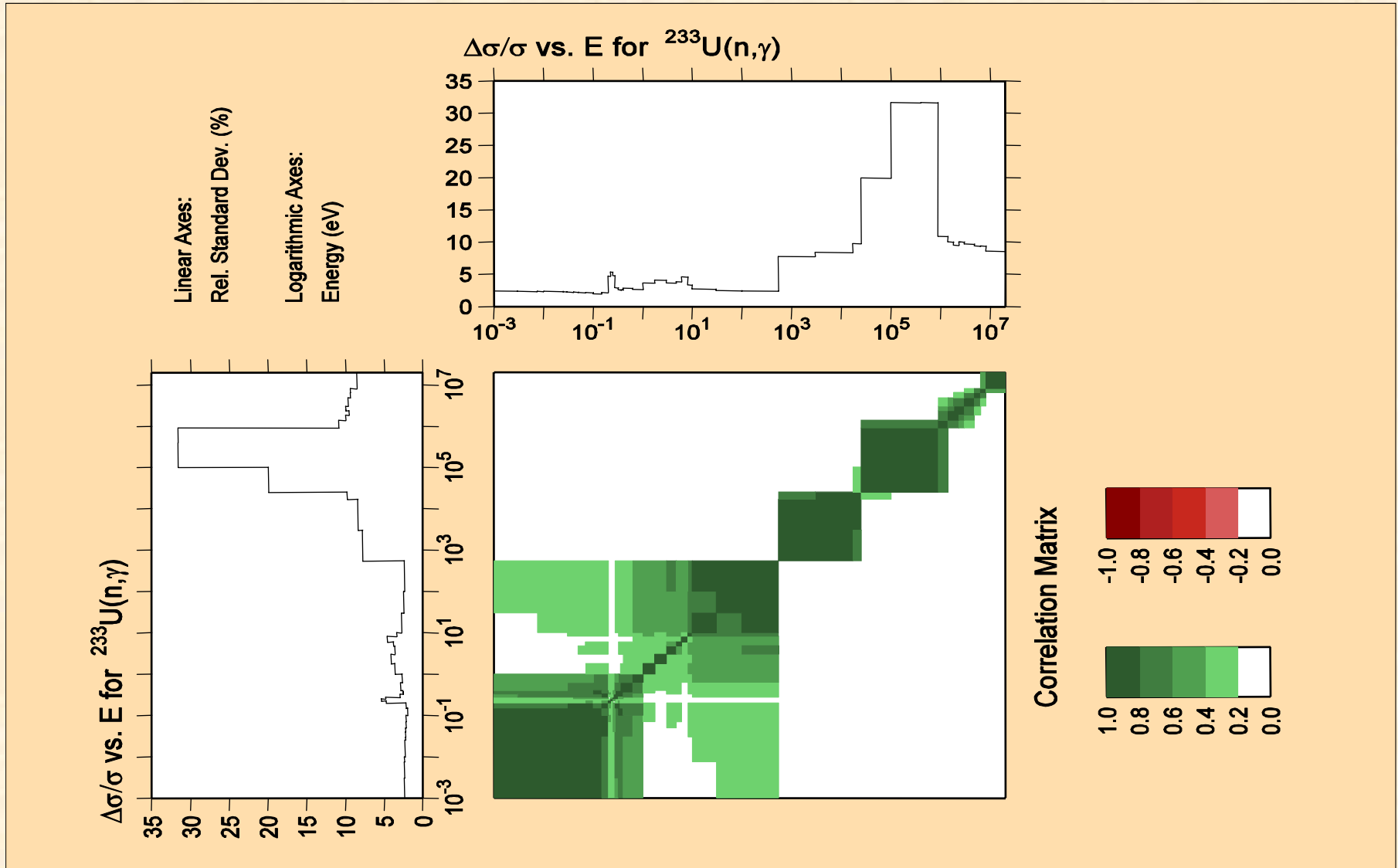
Clearly LCOMP=1 is not ideal !!

***some overhead added to the ASCII/bytes conversion**

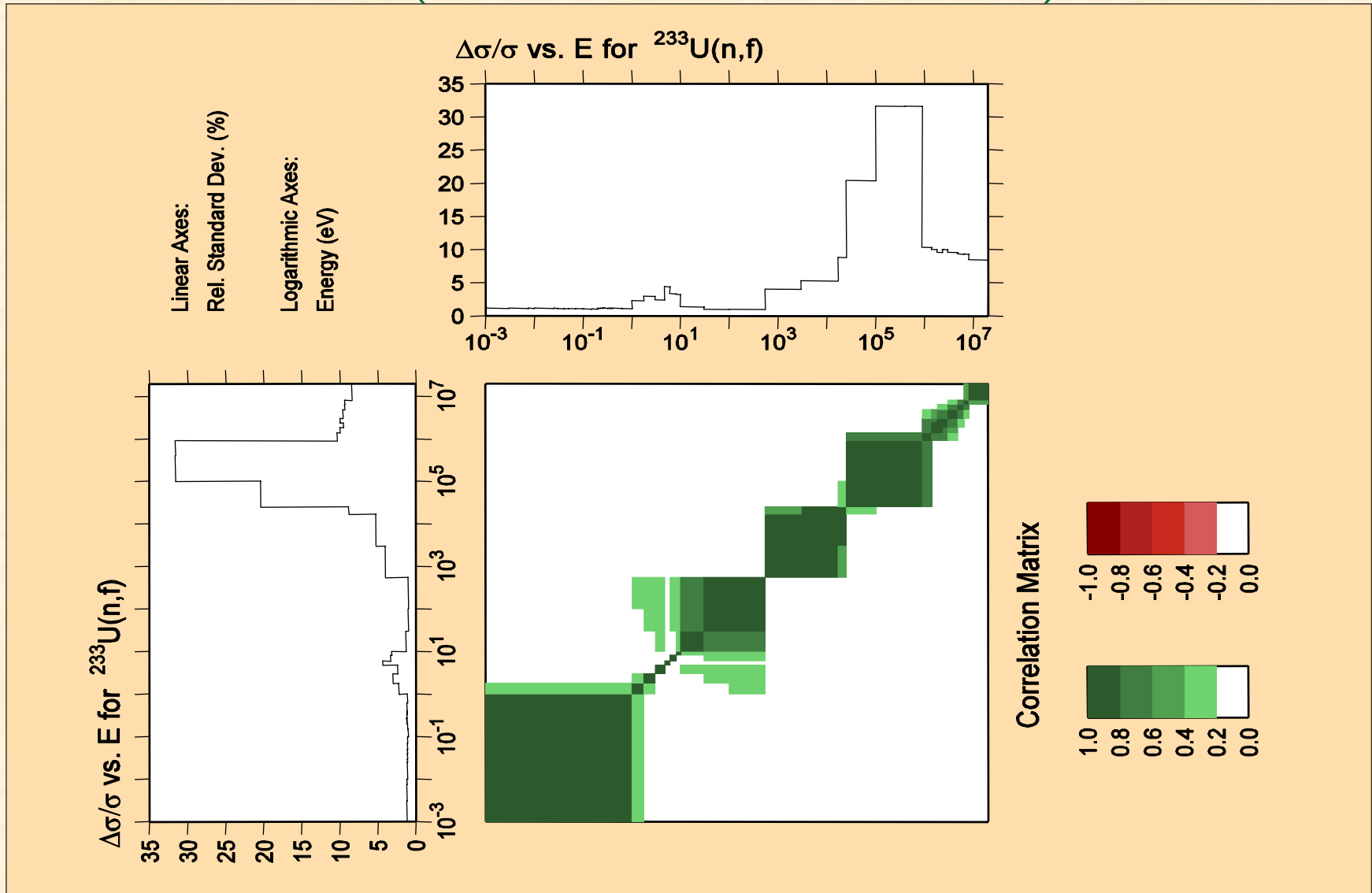
ERRORJ Processed Covariance (Total Cross Section)



ERRORJ Processed Covariance (Capture Cross Section)



ERRORJ Processed Covariance (Fission Cross Section)



²³⁵U Covariance Matrix

Full covariance has been generated in the energy range from 10^{-5} to 2250 eV (RR) and from 600 to 25 keV (UR)

SAMMY memory size estimation

No. of resonances = 3193

No. of varied parameters per resonance = 5

No. of data points = 80,000

Mem = $(3193 \times 5 \times 80,000) \times 8$

Memory needed = $2 \times \text{Mem} \sim 25$ Gbytes

Resonance Covariance for ^{235}U

Space storage needed for ^{235}U covariance

$$N_{\text{res}}=3193$$

$$N_{\text{par}}=5$$

$$N=N_{\text{res}} \times N_{\text{par}}$$

$$N_s = (N^2/2 + N/2) \times 14$$

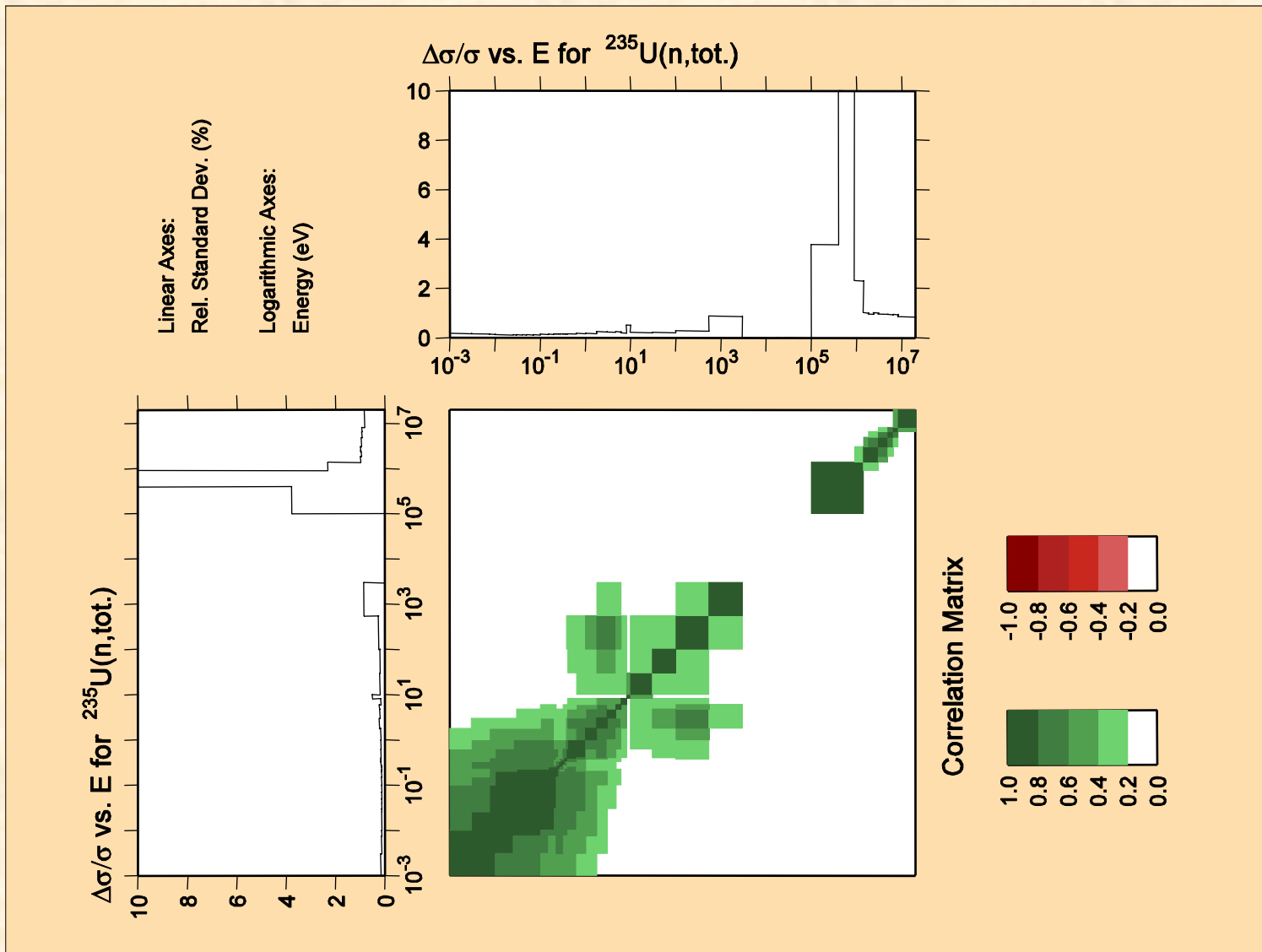
$$N_s \sim 1.8 \text{ Gbytes}$$

Clearly LCOMP=1 is not ideal !!

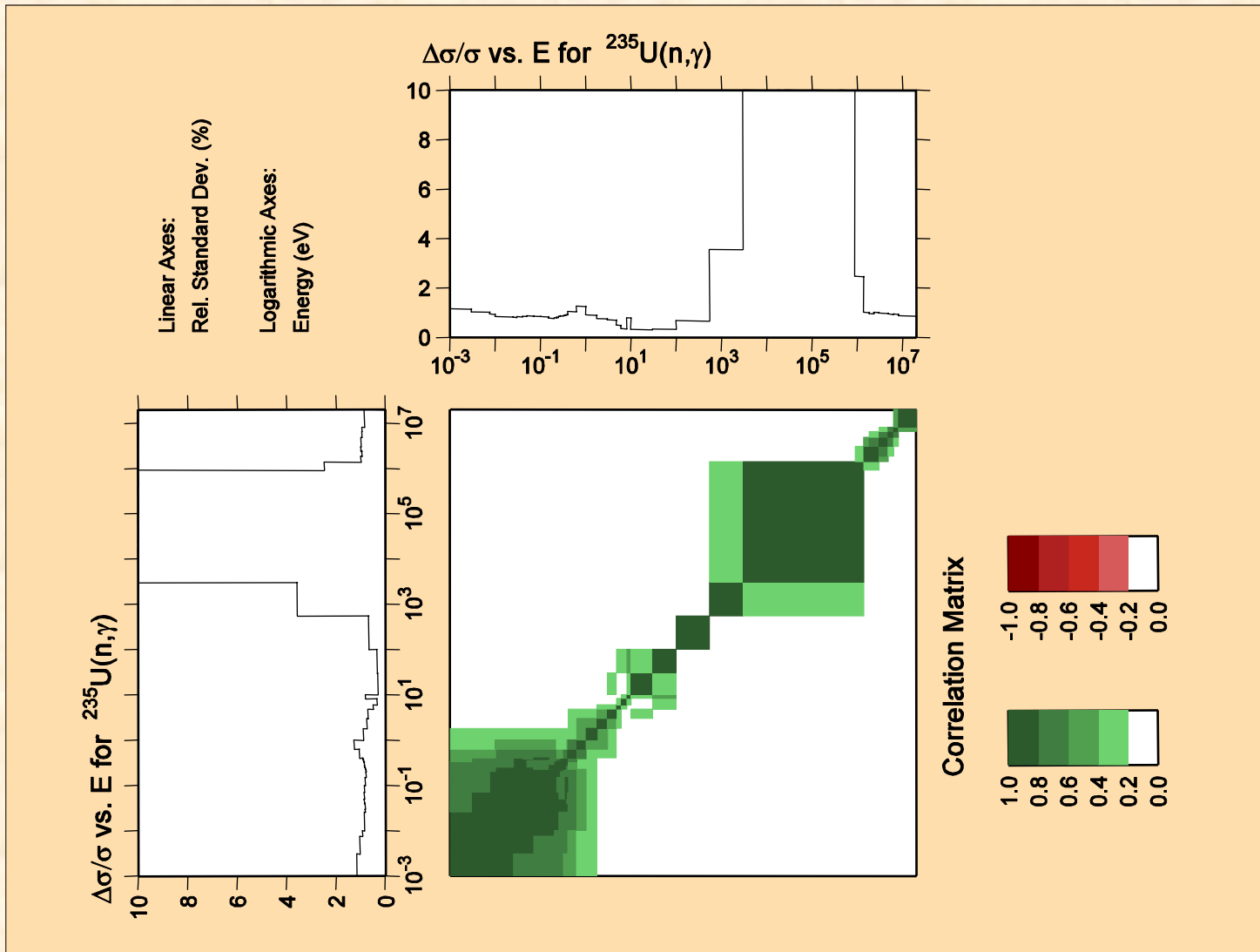
Processing of ^{235}U Covariance with ERRORJ

- The dimension needed for ERRORJ to process ^{235}U covariance is equivalent to 15 Gbytes memory
- CPU time ~ 2.5 days

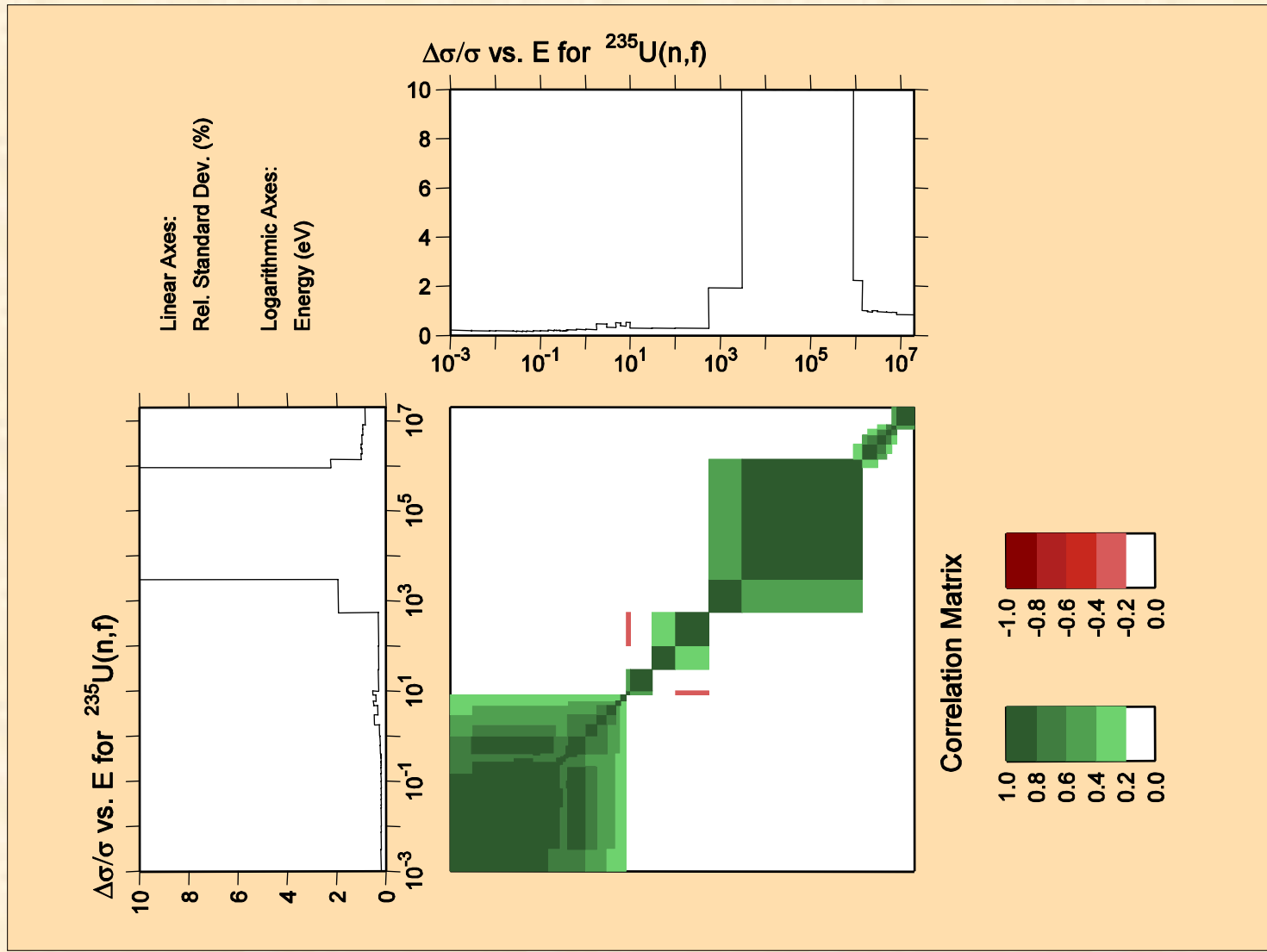
ERRORJ Processed Covariance (Total Cross Section)



ERRORJ Processed Covariance (Capture Cross Section)



ERRORJ Processed Covariance (Fission Cross Section)



²³⁸U Covariance Matrix

Full covariance has been generated in the energy range from 10^{-5} eV to 20 keV (RR)

SAMMY memory size estimation

No. of resonances = 3343

No. of varied parameters per resonance = 3

No. of data points = 20,000

Mem = $(3343 \times 3 \times 20,000) \times 8$

Memory needed = $2 \times \text{Mem} \sim 5$ Gbytes

Resonance Covariance for ^{238}U

Space storage needed for ^{238}U covariance

$$N_{\text{res}}=3343$$

$$N_{\text{par}}=3$$

$$N=N_{\text{res}} \times N_{\text{par}}$$

$$N_s = (N^2/2 + N/2) \times 14$$

$$N_s \sim 700 \text{ Mbytes}$$

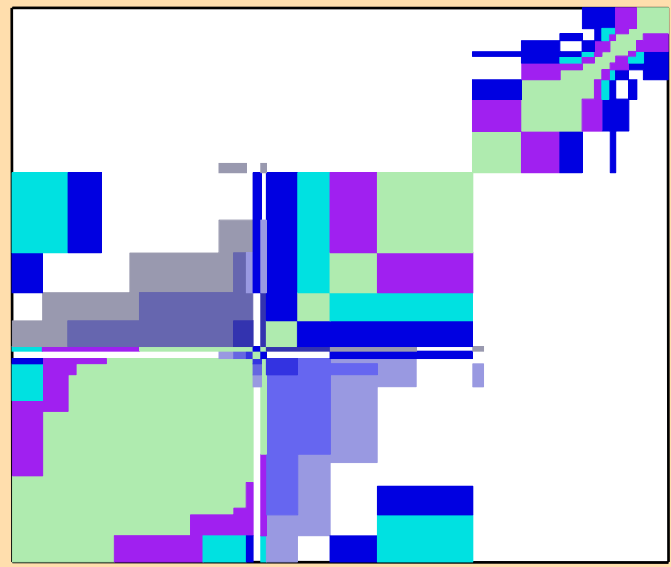
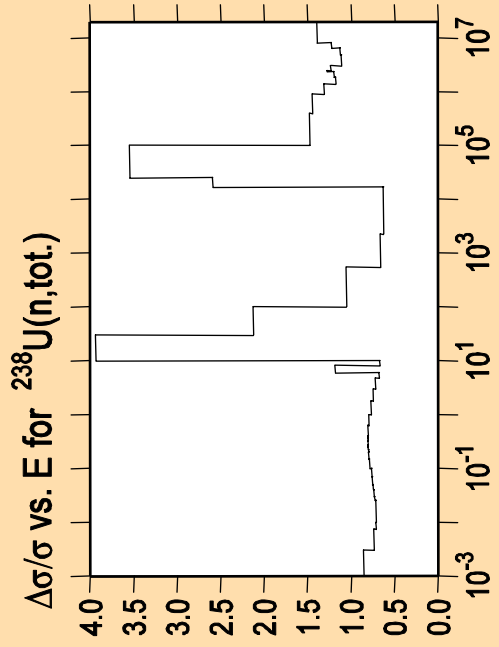
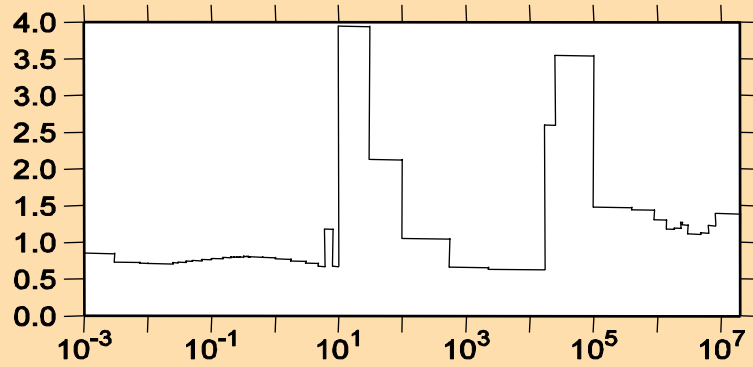
Clearly LCOMP=1 is not a ideal !!

ERRORJ Processed Covariance (Total Cross Section)

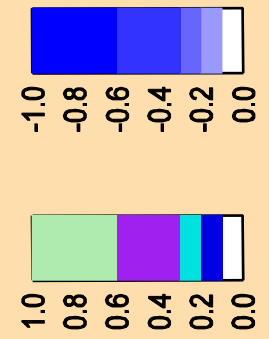
Linear Axes:
Rel. Standard Dev. (%)

Logarithmic Axes:
Energy (eV)

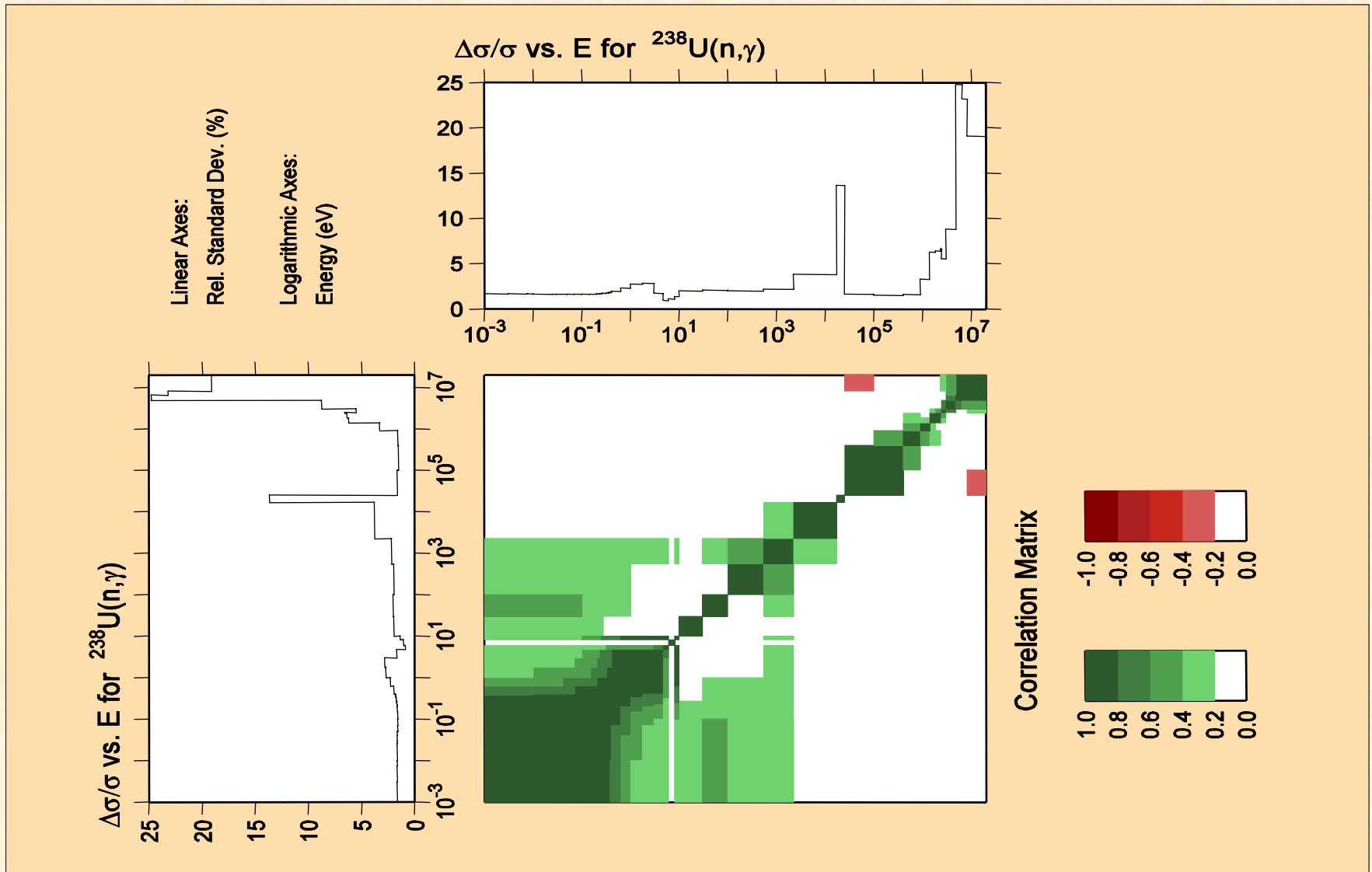
$\Delta\sigma/\sigma$ vs. E for $^{238}\text{U}(n,\text{tot.})$



Correlation Matrix



ERRORJ Processed Covariance (Capture Cross Section)



^{239}Pu Covariance Matrix

Full covariance has been generated in the energy range from 10^{-5} eV to 2.5 keV (RR)

SAMMY memory size estimation

No. of resonances = 1045

No. of varied parameters per resonance = 5

No. of data points = 20,000

Mem = $(1045 \times 5 \times 20,000) \times 8$

Memory needed = $2 \times \text{Mem} \sim 1.7$ Gbytes

Resonance Covariance for ^{239}Pu

Space storage needed for ^{239}Pu covariance

$$N_{\text{res}} = 1045$$

$$N_{\text{par}} = 5$$

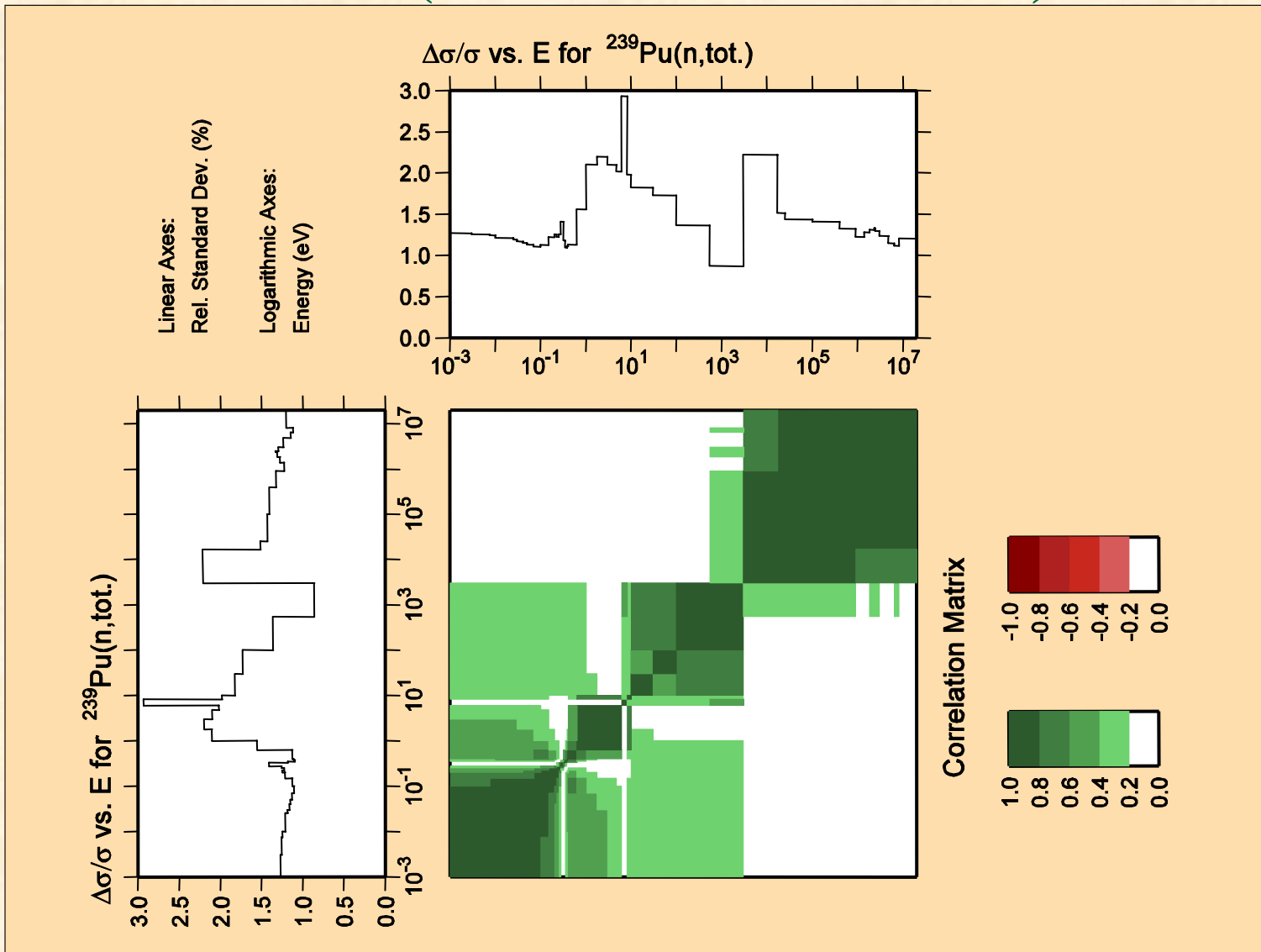
$$N = N_{\text{res}} \times N_{\text{par}}$$

$$N_s = (N^2/2 + N/2) \times 14$$

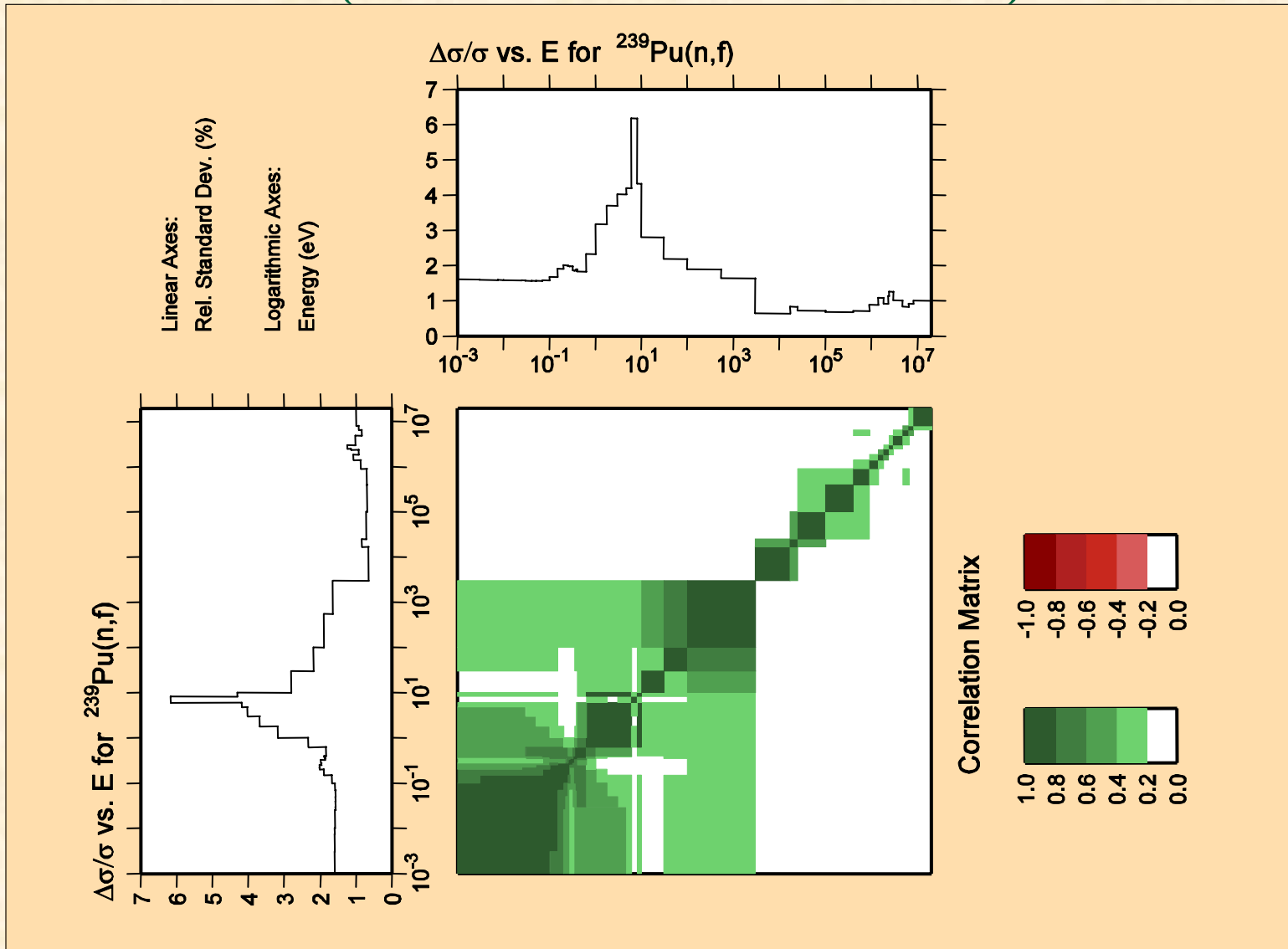
$$N_s \sim 190 \text{ Mbytes}$$

Clearly LCOMP=1 is not ideal !!

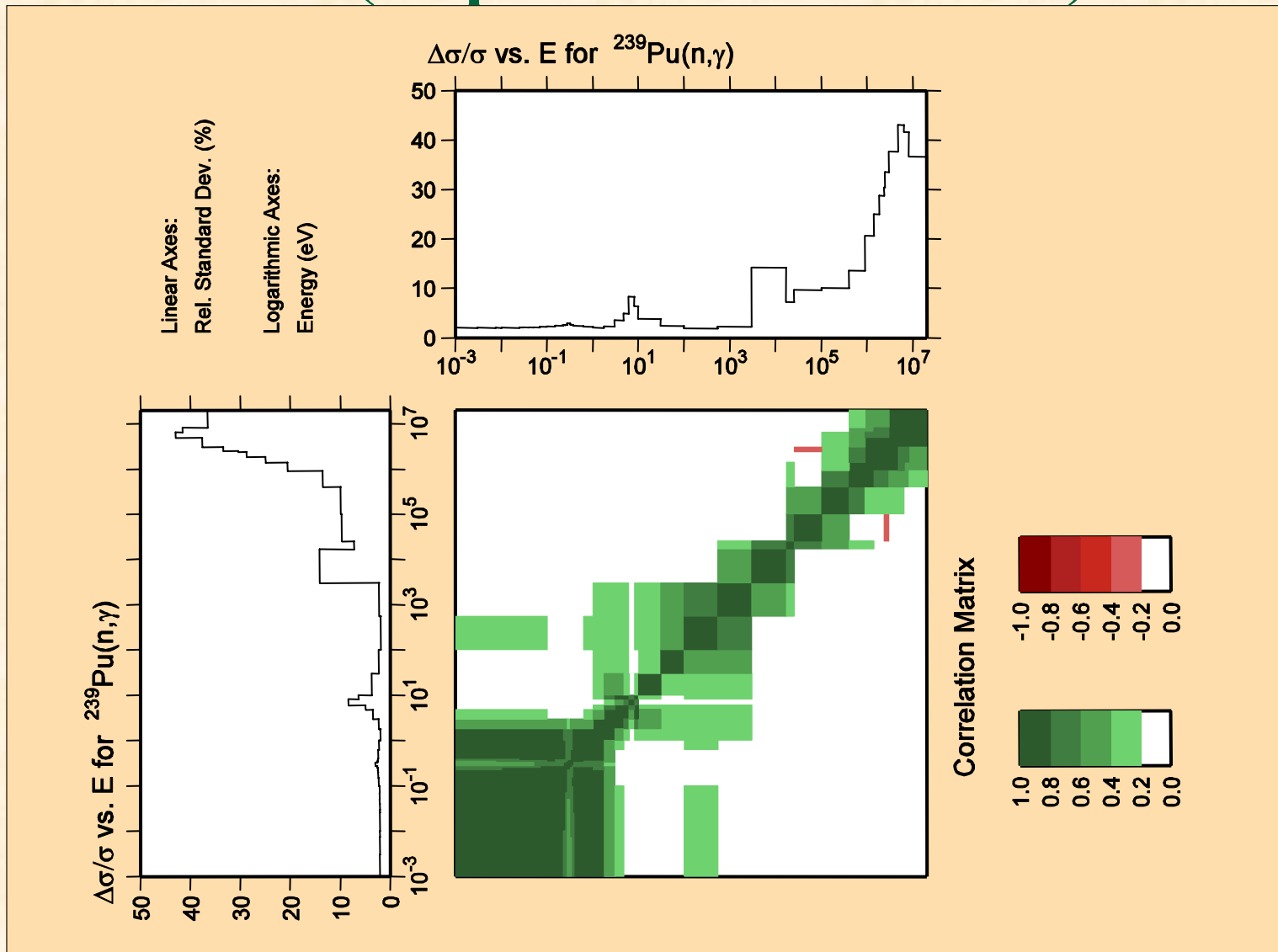
ERRORJ Processed Covariance (Total Cross Section)



ERRORJ Processed Covariance (Fission Cross Section)



ERRORJ Processed Covariance (Capture Cross Section)



^{232}Th Covariance Matrix Evaluation done under IAEA/CRP

Full covariance has been generated in the energy range from 10^{-5} eV to 4 keV (RR)

Unresolved Evaluation Done at GEEL !!

SAMMY memory size estimation

No. of resonances = 927

No. of varied parameters per resonance = 3

No. of data points = 20,000

Mem= $(927 \times 3 \times 20,000) \times 8$

Memory needed = $2 \times \text{Mem} \sim 900$ Mbytes

Resonance Covariance for ^{232}Th

Space storage needed for ^{232}Th covariance

$$N_{\text{res}}=927$$

$$N_{\text{par}}=3$$

$$N=N_{\text{res}} \times N_{\text{par}}$$

$$N_s = (N^2/2 + N/2) \times 14$$

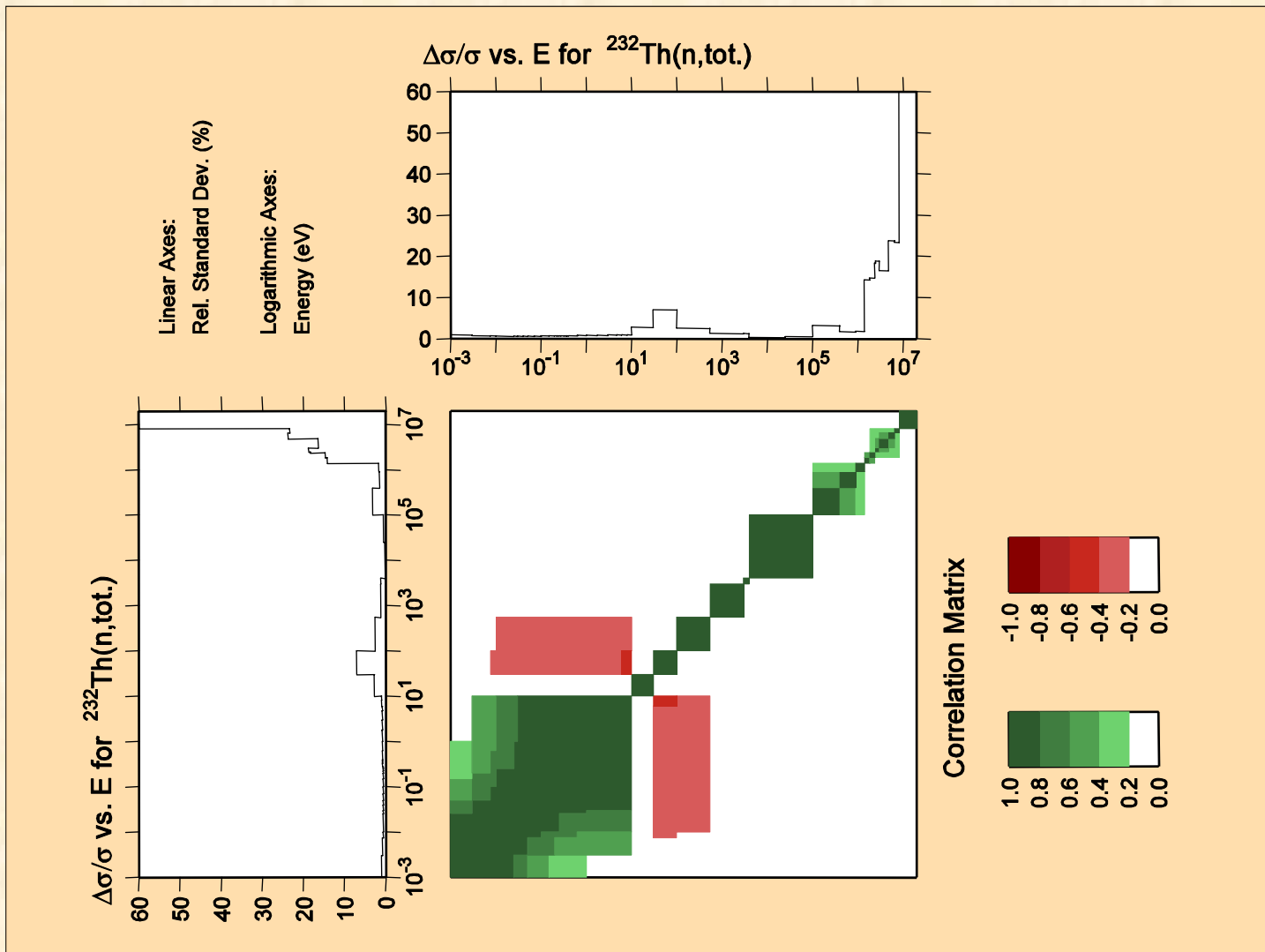
$$N_s \sim 55 \text{ Mbytes (LCOMP=1)}$$

Compact formalism used

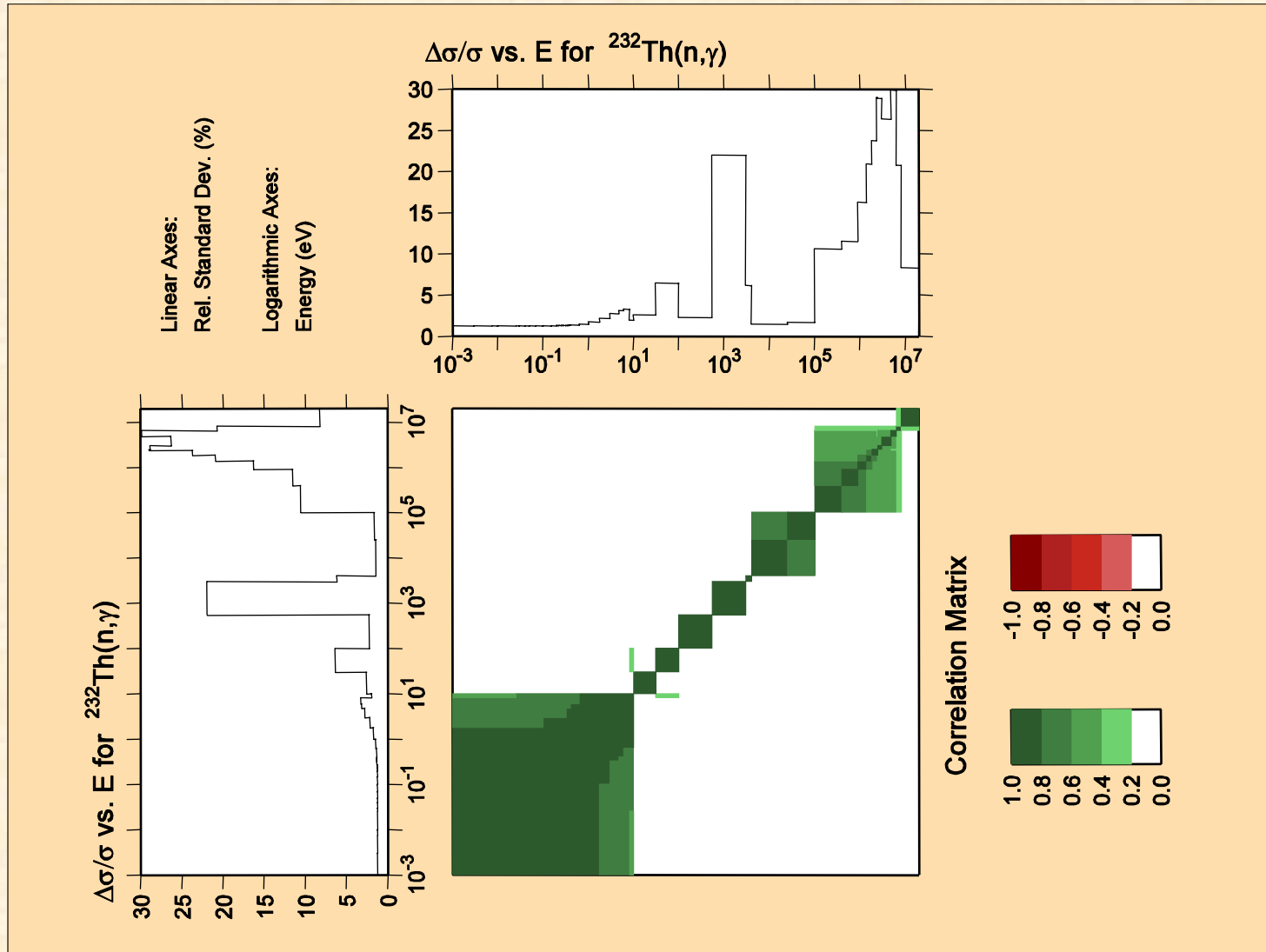
$$N_s \sim 800 \text{ Kbytes}$$

reduction size by a factor of 70 !!

ERRORJ Processed Covariance (Total Cross Section)



ERRORJ Processed Covariance (Capture Cross Section)



Compact format (size reduction estimation)

| Isotope | Lcomp=1 | Lcomp=2 (compact) |
|-------------------------------------|----------------|------------------------------|
| ^{232}Th | 55 MB | 1 MB |
| ^{233}U | 100 MB | 3 MB |
| ^{235}U | 1.8 GB | 60 MB |
| ^{238}U | 700 MB | 8 MB |
| ^{239}Pu | 190 MB | 10 MB |

Concluding Remarks

- **Resonance covariance data were generated for ^{232}Th , ^{233}U , ^{235}U , ^{238}U , and ^{239}Pu using SAMMY**
- **LCOMP=1 option used (clearly not ideal)**
- **Compact formalism used for ^{232}Th (LCOMP=2)**

Note: CPU time for LCOMP=1 and LCOMP=2 ARE THE SAME !!

- **PUFF and ERRORJ code used to process the covariance data**