State of the EMPIRE

M. Herman
National Nuclear Data Center
Brookhaven National Laboratory

Nuclear Data Week, Nov. 14-18, 2011

BROOKHAVEN NATIONAL LABORATORY
a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

EMPIRE developer team

- Developers
  - **M. Herman (BNL, Upton)**
  - **R. Capote (IAEA, Vienna)**
  - **M. Sin (University of Bucharest)**
  - **A. Trkov (JSI, Lubljana)**
  - B. Carlson (ITA, Sao Jose dos Campos)
  - P. Oblozinsky (Bratislava)
  - C. Mattoon (LLNL, Livermore)
  - **G. Nobre (BNL, Upton)**
  - H. Wienke
  - **S. Hoblit (BNL, Upton)**
  - Young-Sik Cho (KAERI, Daejeon)
  - V. Plujko (University of Kiev)
  - V. Zerkin (IAEA, Vienna)
- Contributors
  - **D. Brown** (BNL, Upton)
  - E. Betak (SAS, Bratislava)
  - M. Pigni (ORNL, Oak Ridge)
  - V. Plujko (University of Kiev)
  - S. Mughabghab (BNL, Upton)
  - T. Kawano (LANL, Los Alamos)
  - A. Ventura (ENEA, Bologna)

EMPIRE-3.1 (Rivoli)

Nuclear Reaction Model Code

Neutron Resonances

Coupled Channels

DWBA

Optical Model

Multistep Direct

Multistep Compund

Exciton Model

Hybrid MC Simulation

HRTW

Hauser-Feshbach

Optical Model for Fission

ENDF Formatting

Verification

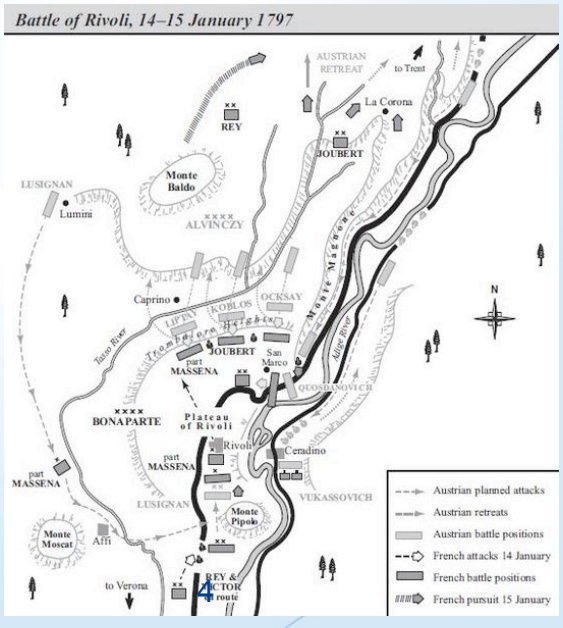
Kalman Filter

Covariances

EMPIRE-3.1 Rivoli

- Released in March 2012
  - Web site updated
  - New installation script
  - Manual updated
  - New test cases
  - Set of benchmarks

In a two-days battle of Rivoli fought in January 14-15, 1797 close to the lake Garda Napoleon Bonaparte defeated final Austrian attempt to relieve siege of Mantua and secured French control of northern Italy. Subsequent French offensive into Austrian Tirol ended the first Italian campaign.



Major new features in EMPIRE-3.1 (Rivoli)

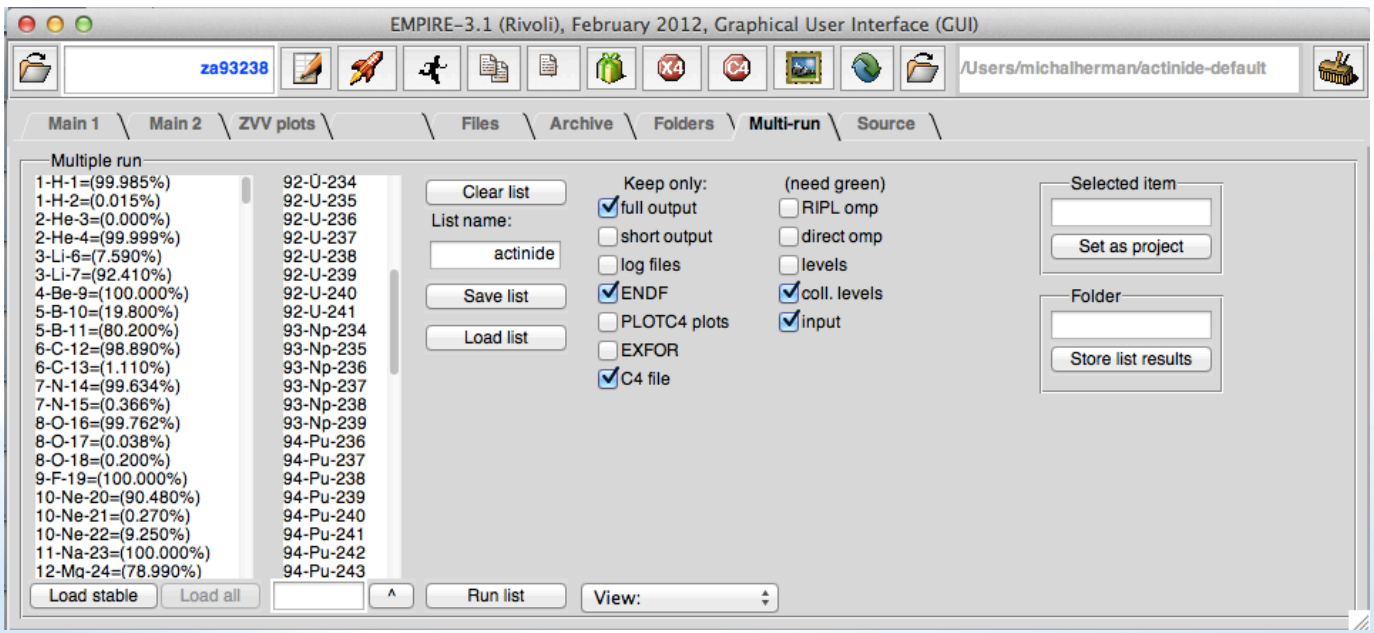
- Covariance capabilities using Kalman filter and Monte Carlo
- Resonance module to produce MF2 and MF32 from the Atlas of Neutron Resonances
- RIPL-3 library of input parameters
- New version of Coupled Channel code ECIS-2006
- Coupled Channel code OPTMAN for soft-rotor calculations
- Improved treatment of fission
- Improved defaults for actinides (further improvement underway)
- Parity dependent level densities
- New parametrization of EGSM level densities
- Input controlled adjustment of the level density shift
- Three additional ejectiles (d, t, ^{3}He)
- Platform independent retrieval of EXFOR data
- Fully operational on Mac OS X

Major post-Rivoli changes (1038 Svn commits since Nov. 2, 2011)

- Improved makefiles
- New IO subroutines for ENDF-6
- PFNS implemented, Los Alamos and Kornilov (1st chance fission)
- Covariances for PFNS, mu-bars, and nu-bars
- Plotting of PFNS, mu-bars, and nu-bars
- Angular distributions for compound elastic and inelastics
- Simulation of the Engelbrecht-Weidenmueller transformation (scaling compound inelastic)

Default calculations with EMPIRE-3.1
fission on actinides in ENDF/B-VII.1

- 72 materials from ^{227}Ac through ^{255}Fm
- the same input for all materials
- no parameter adjustment except choice of the options
- 30 cases out of 72 went through (lack of fission barriers, misidentified 2+ state in MSD - 6 crashed)



Default input 1/3

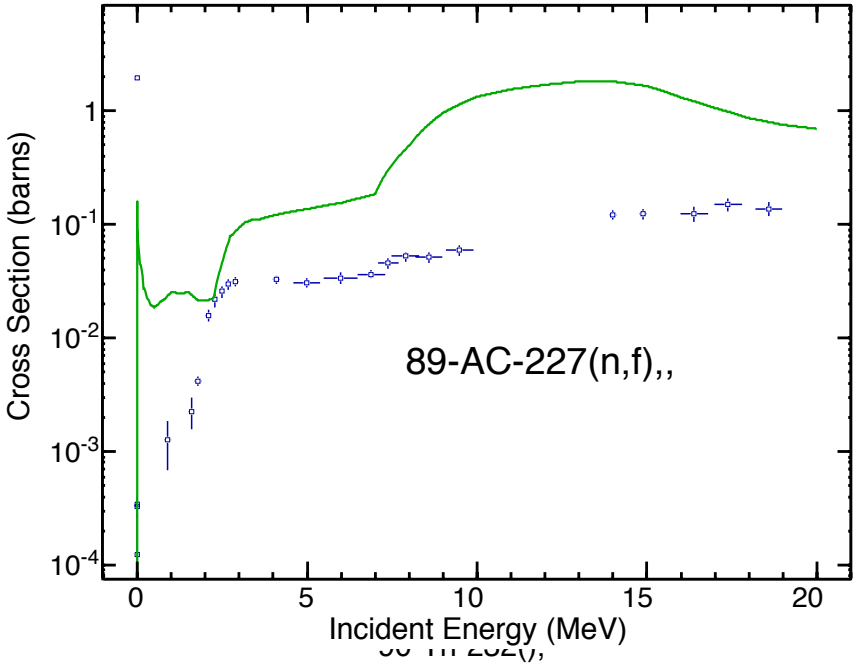
```
0.001                ;INCIDENT ENERGY (IN LAB)
241.0  95.0          ;TARGET A, Z
  1.    0.           ;PROJECTILE A, Z
2                    ;NUMBER OF NEUTRONS  TO BE EMITTED
0                    ;NUMBER OF PROTONS   TO BE EMITTED
0                    ;NUMBER OF ALPHAS    TO BE EMITTED
0                    ;NUMBER OF DEUTERONS TO BE EMITTED
0                    ;NUMBER OF TRITONS   TO BE EMITTED
0                    ;NUMBER OF He-3      TO BE EMITTED
0  0. 0.             ; reserved
@Default calculations of actinides
IOUT       3.
NEX      080.                    Number of points in the outgoing energy grid
ENDF       0.                    No ENDF formatting by default (much faster runs)
RECOIL     0.                    No recoils are calculated.
```

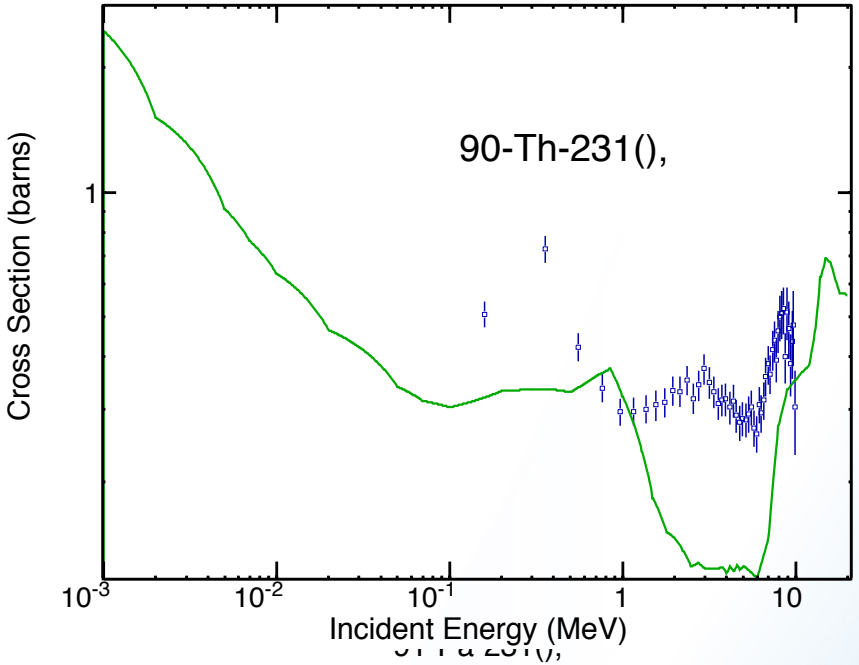
Default input 2/3

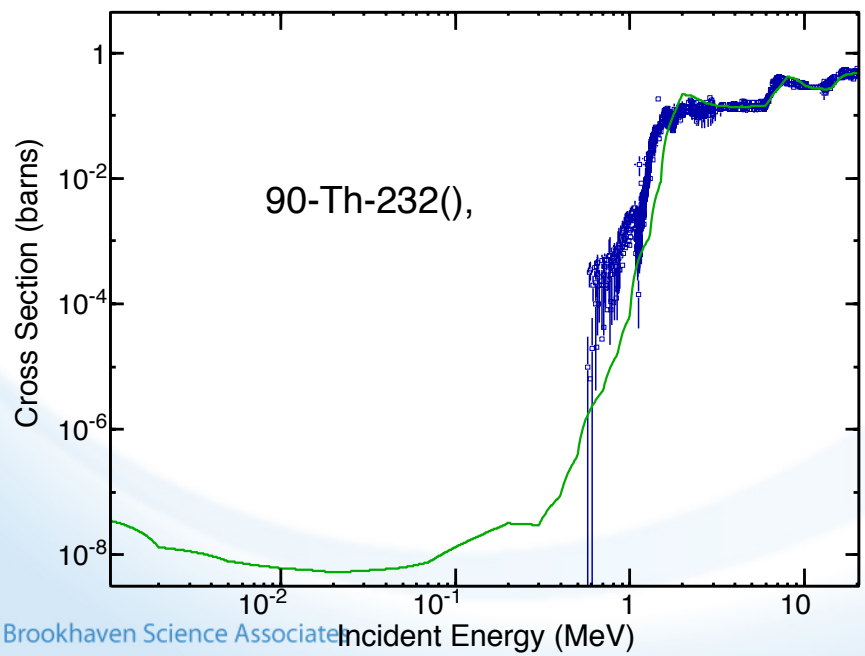
```
**********************
* HAUSER-FESHBACH INPUT
**********************
LEVDEN      0.                  EGSM level densities above ground state
HRTW        3.                  Width fluctuations considered up to 3 MeV
GSTRFN      1.                  Gamma ray strength function (PLujko MLO RIPL-2)
**********************
* OPTICAL MODEL INPUT
**********************
DIRECT      1.                  CC TLs for the incident channel + DWBA
**********************
* Prequilibrium models
**********************
MSD         1.                  ! Quantum statistical Multi-Step-Direct model
MSDMIN      0.1                 ! MSD starts at 0.1 MeV
MSC         1.                  ! Quantum statistical Multi-Step-Compound
```

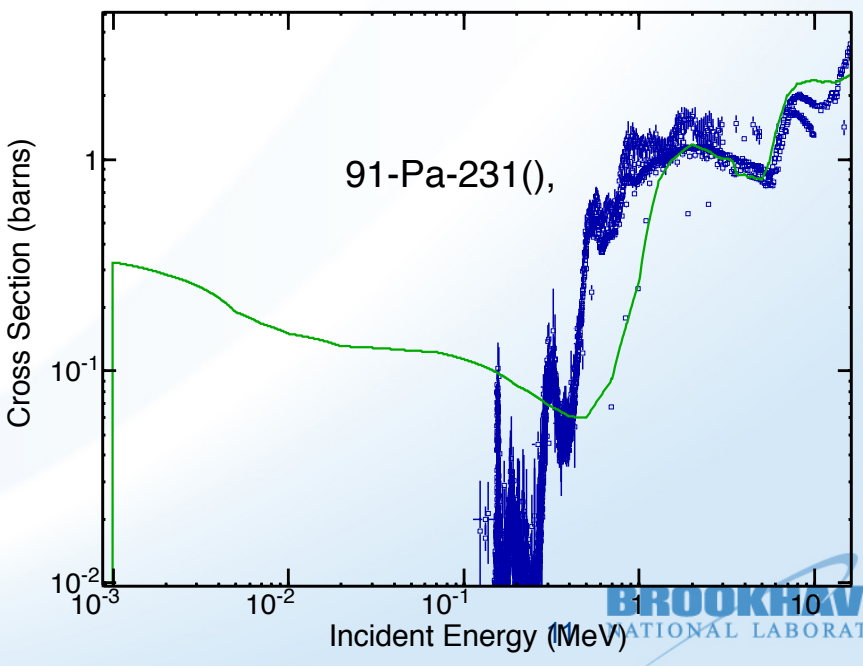
Default input 3/3

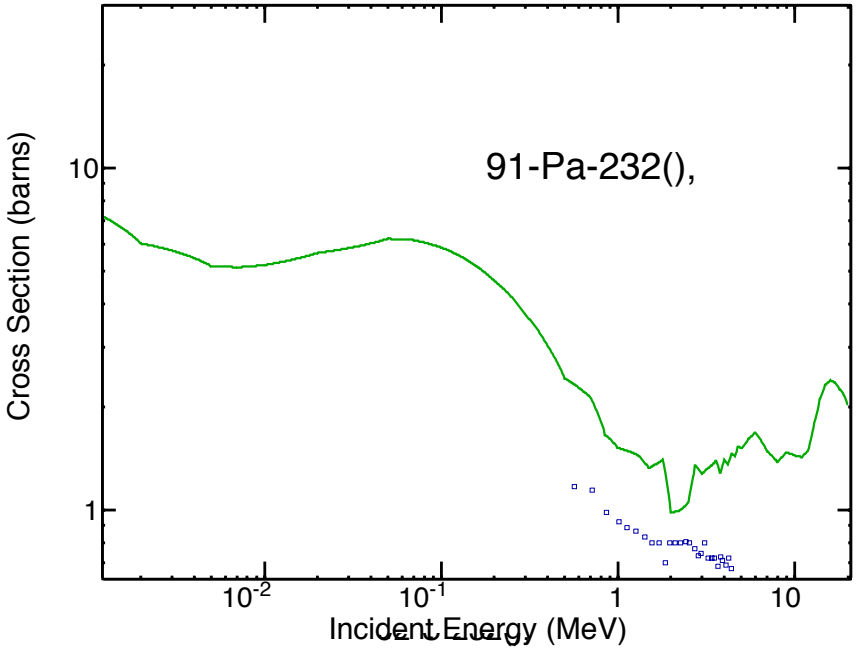
```
**********************
* FISSION
**********************
FISMOD     0.          ! Single-mode fission (default), Multimodal fission (1-2)
FISOPT     1.          ! Optical model for fission (partial damping with absorption)
FISBAR     1.          ! RIPL experimental fission barriers
FISDIS     1.          ! RIPL fission discrete states above the barrier
FISDEN     0.          ! EGSM level densities at saddle points
FISSHI     0.          ! Fission of light projectiles  (default for A>220)
GO
0.002                  ! Incident energies ...
0.005
0.007
0.01
…
20.0
```

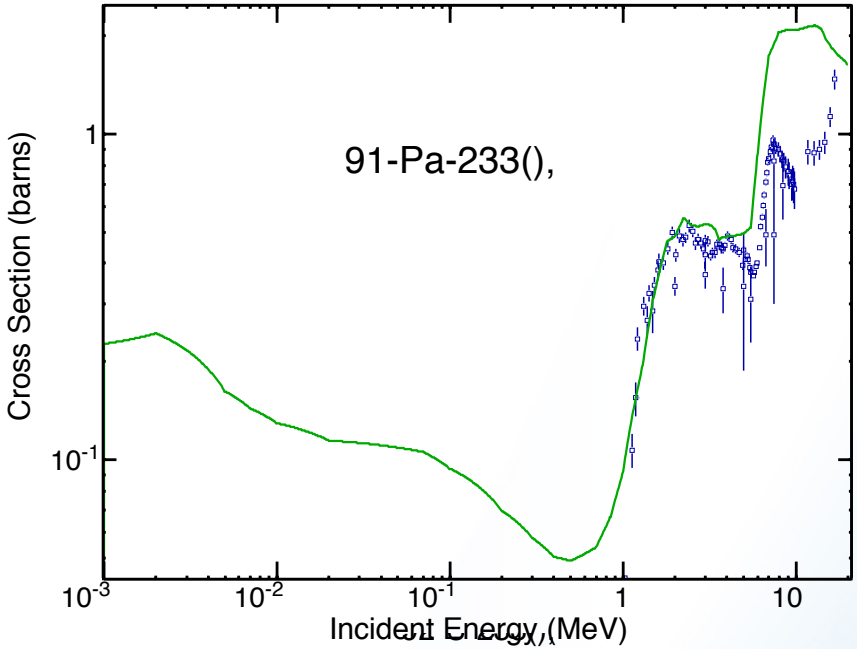


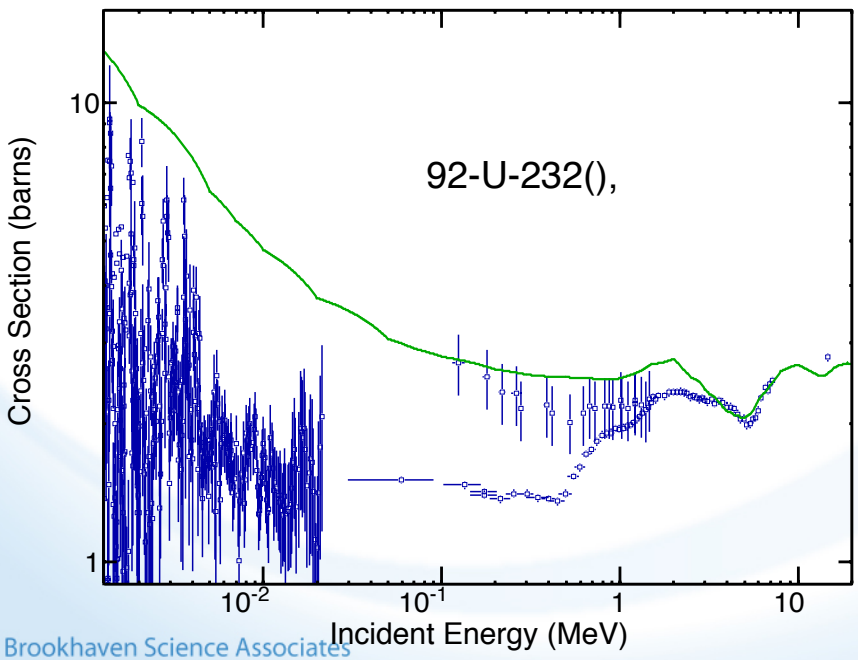


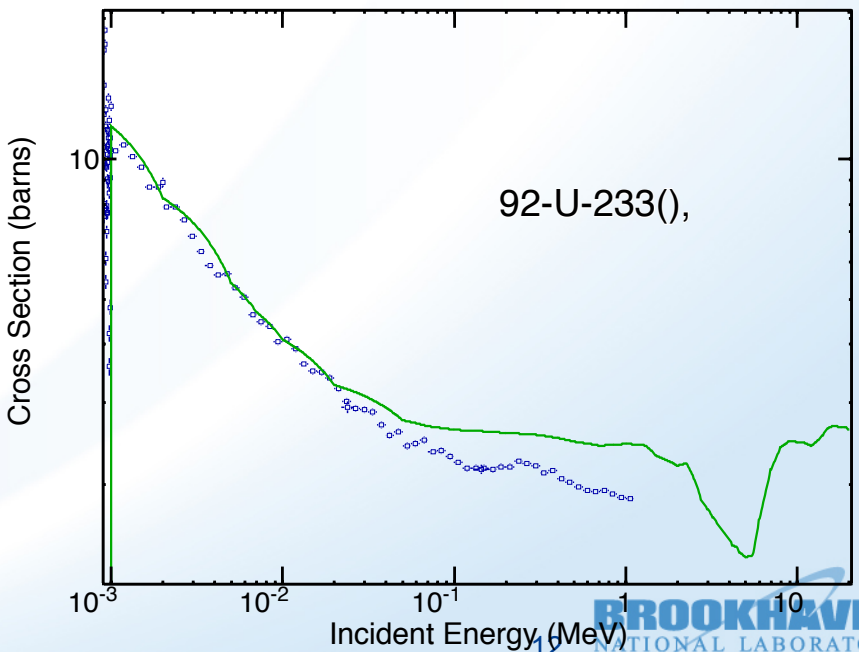


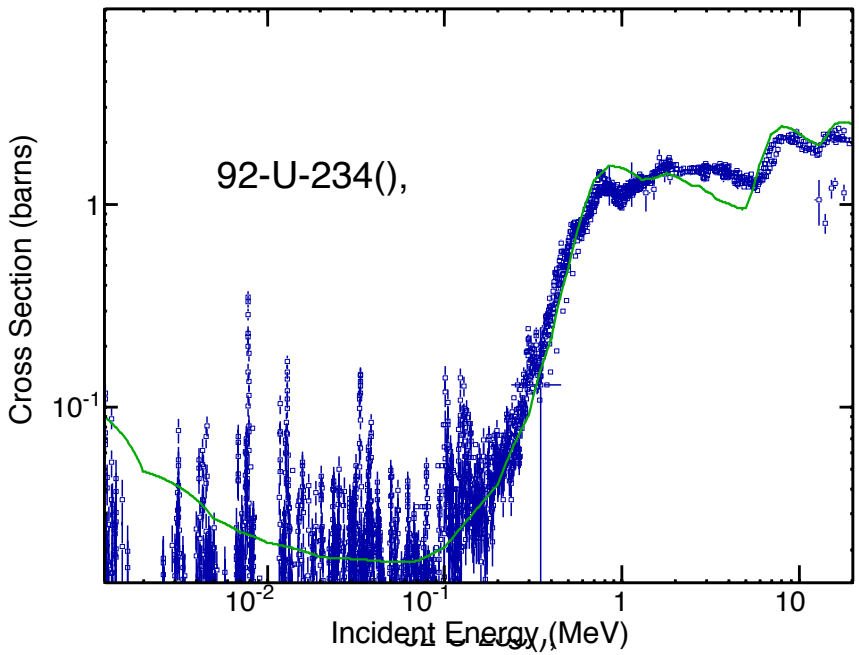


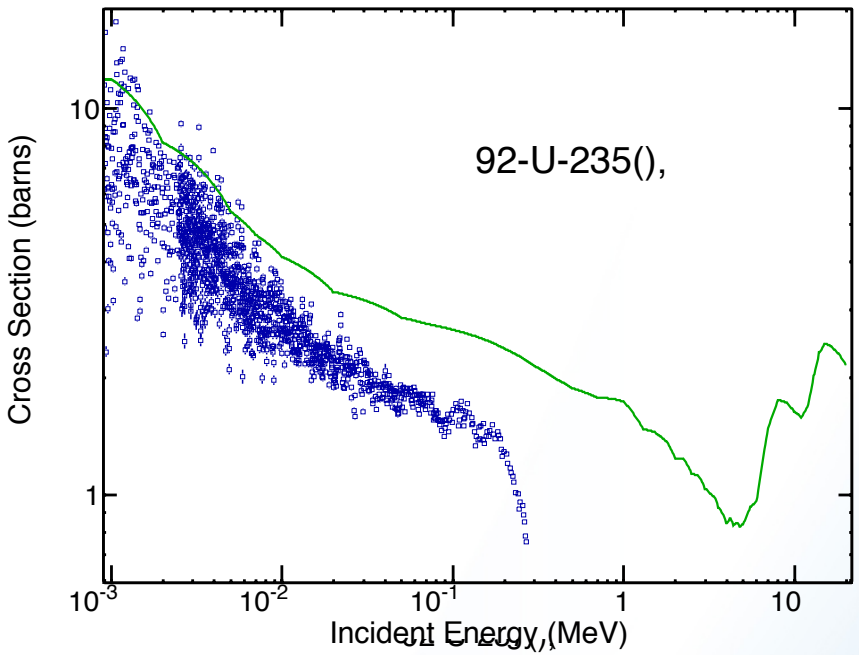

91-Pa-232(),
Cross Section (barns)
Incident Energy (MeV)

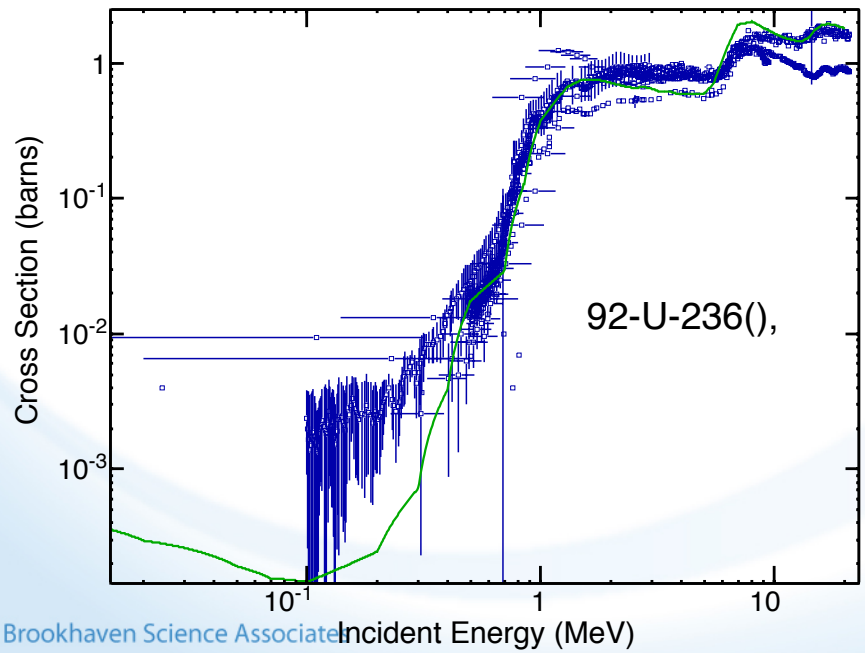

91-Pa-233(),
Cross Section (barns)
Incident Energy (MeV)

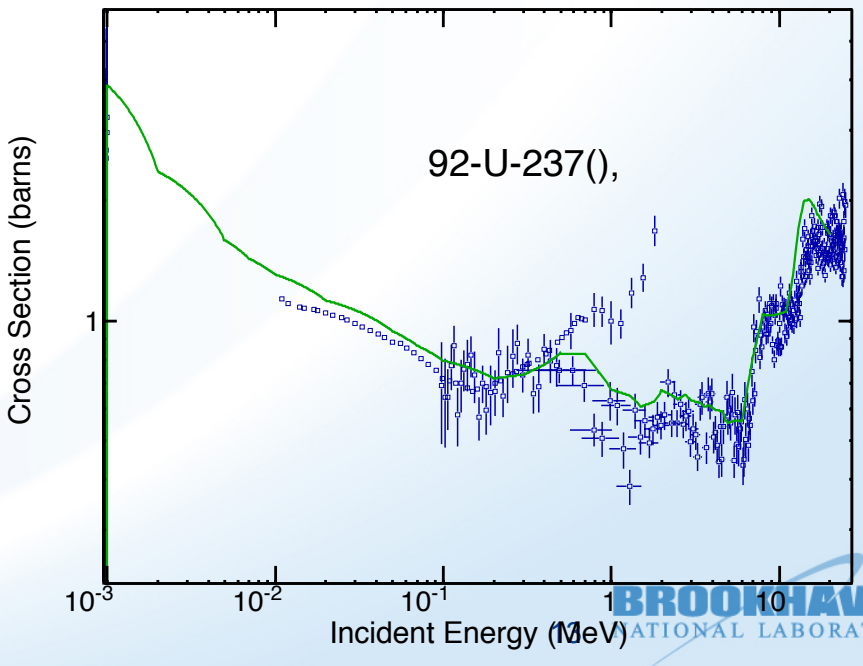

92-U-232(),
Cross Section (barns)
Incident Energy (MeV)

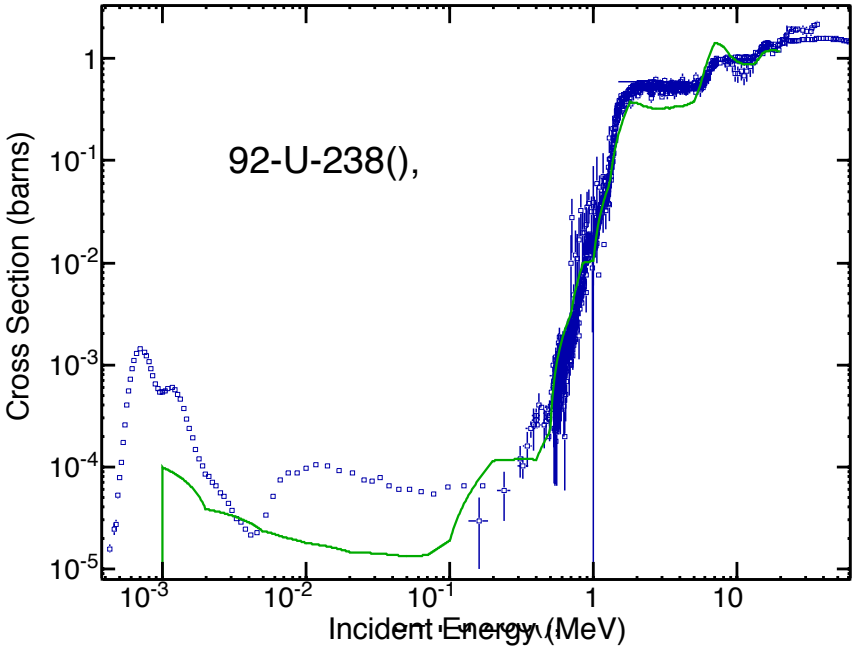

92-U-233(),
Cross Section (barns)
Incident Energy (MeV)

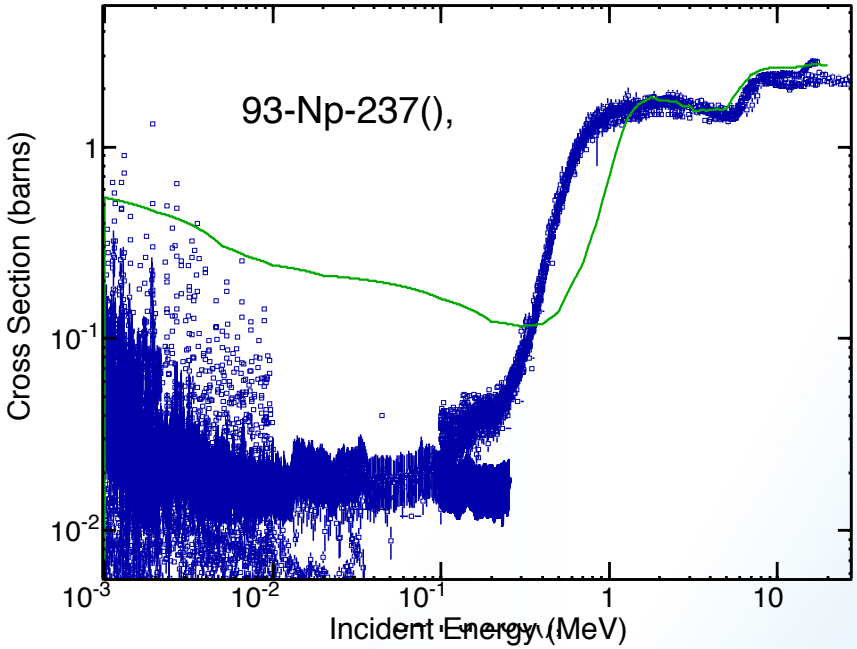

92-U-234(),
Cross Section (barns)
Incident Energy (MeV)

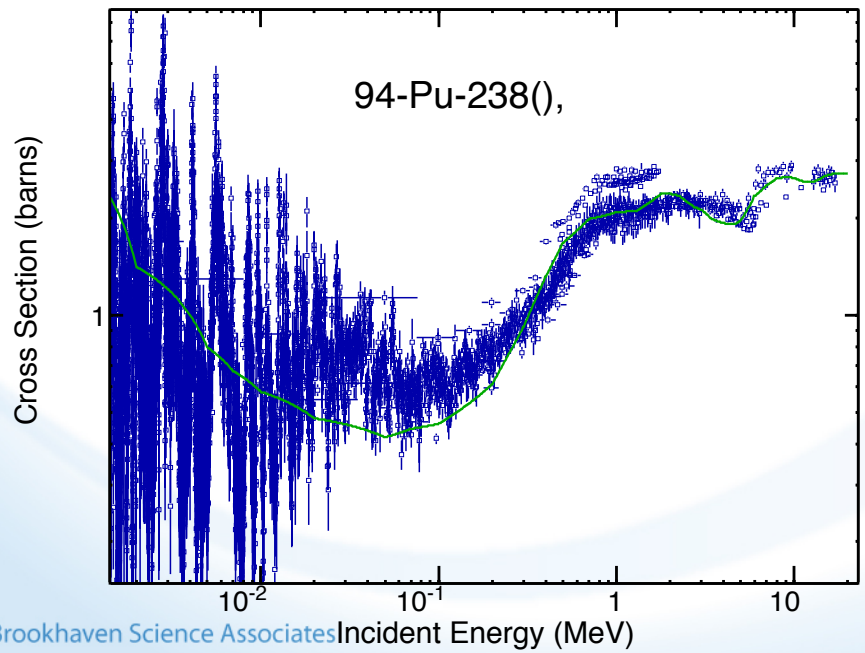

92-U-235(),
Cross Section (barns)
Incident Energy (MeV)

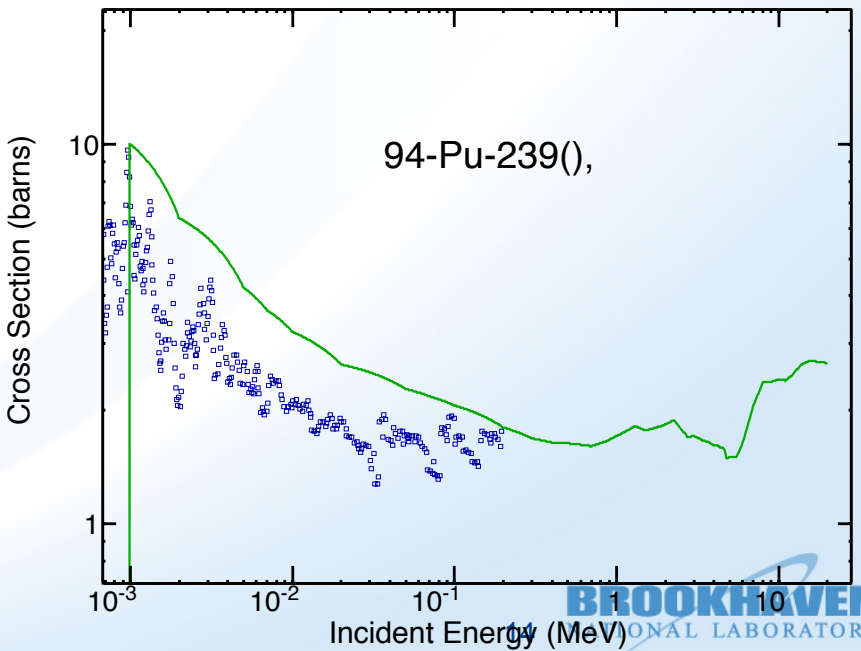

92-U-236(),
Cross Section (barns)
Incident Energy (MeV)

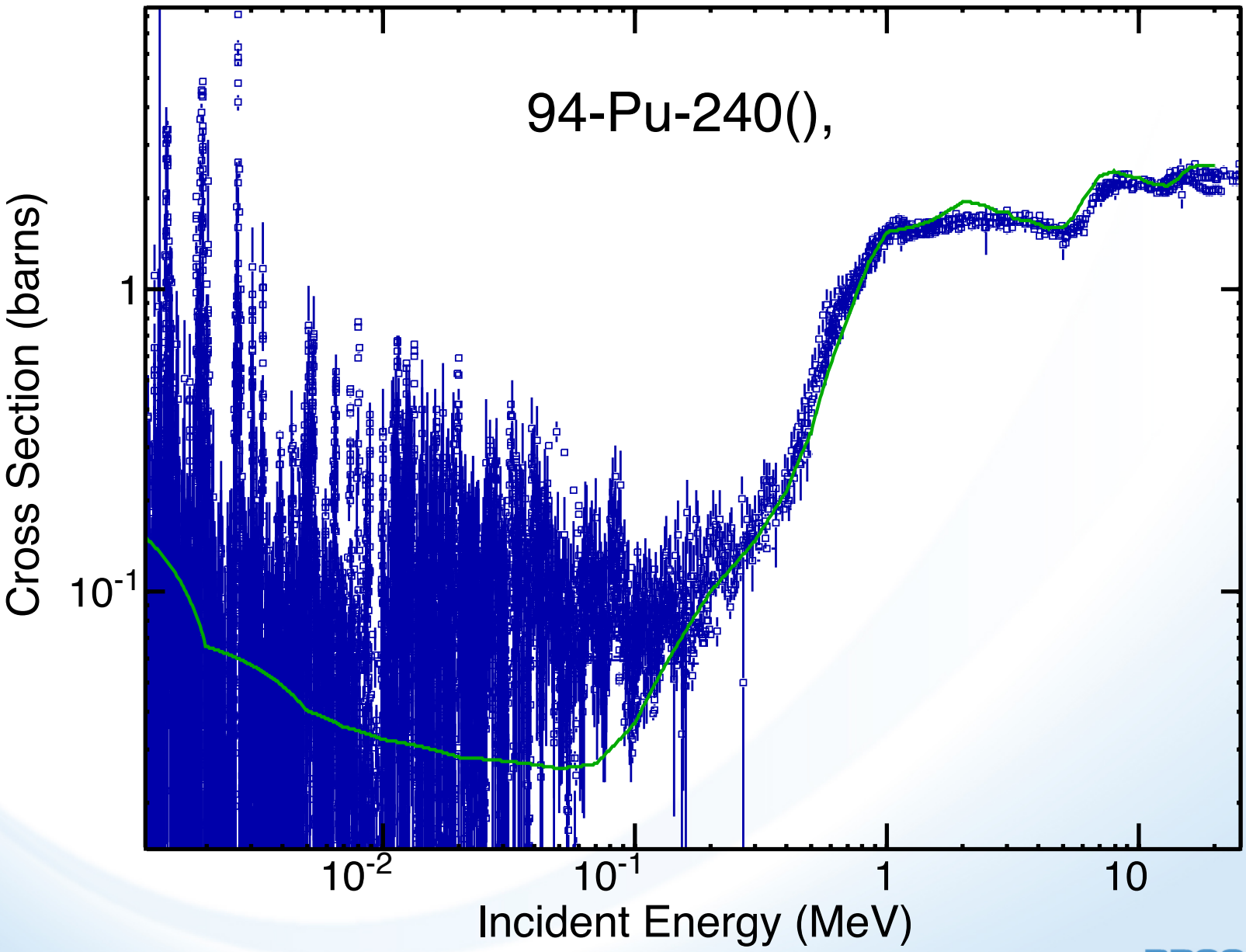

92-U-237(),
Cross Section (barns)
Incident Energy (MeV)

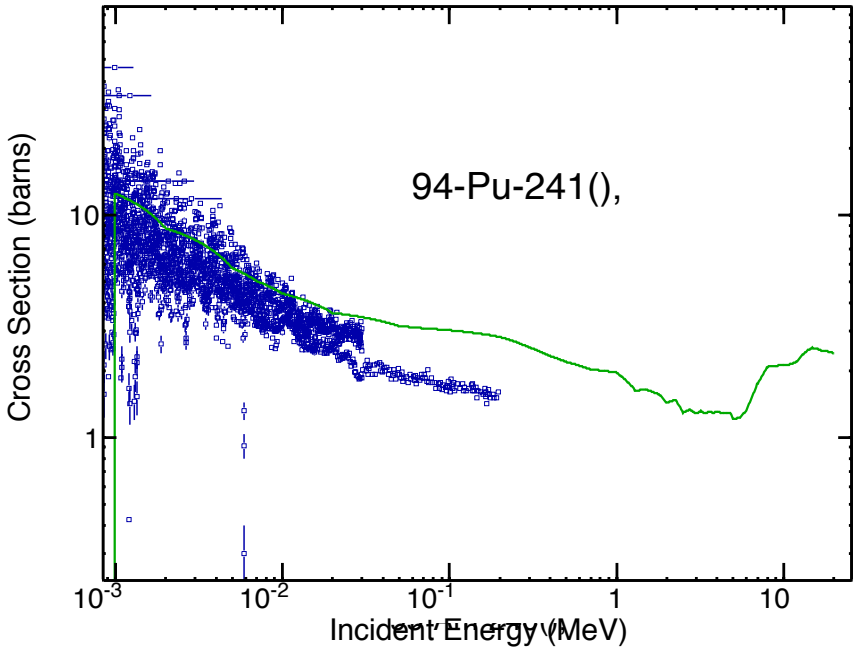

92-U-238(),
Cross Section (barns)
Incident Energy (MeV)

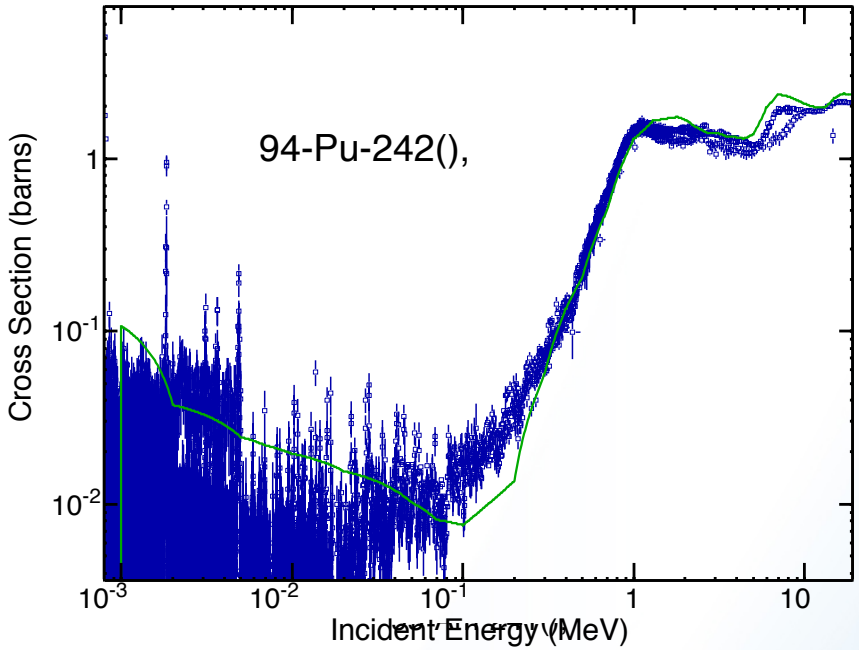

93-Np-237(),
Cross Section (barns)
Incident Energy (MeV)

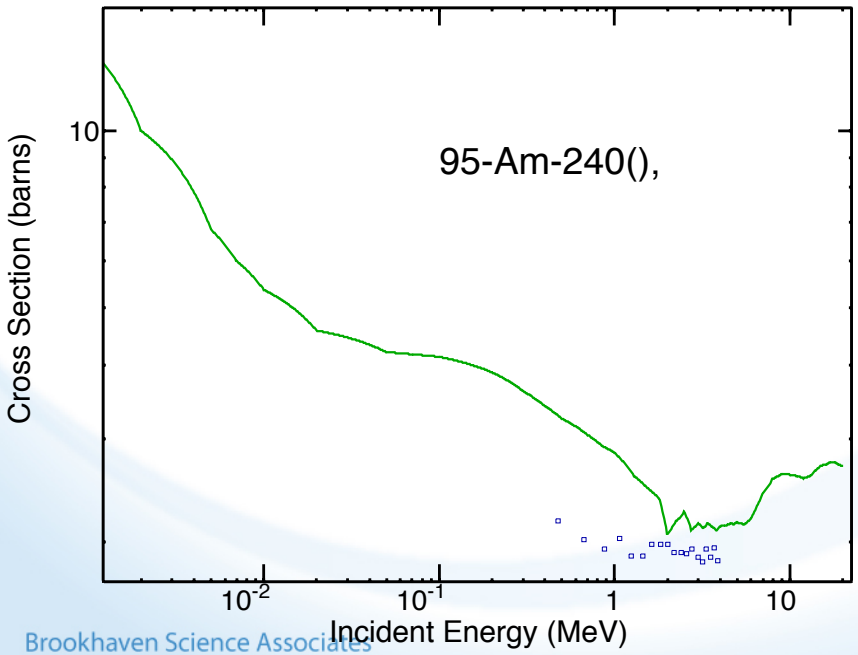

94-Pu-238(),
Cross Section (barns)
Incident Energy (MeV)

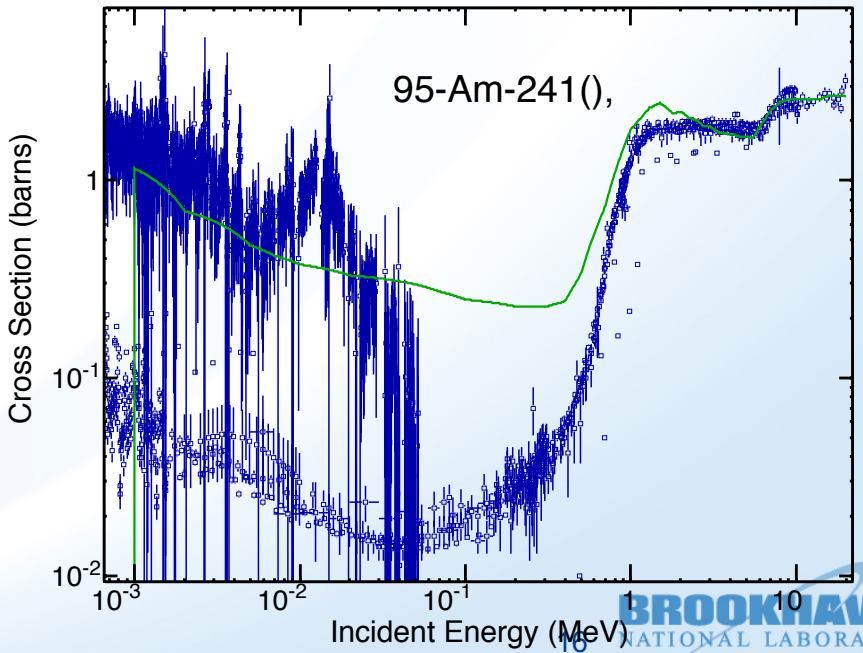

94-Pu-239(),
Cross Section (barns)
Incident Energy (MeV)

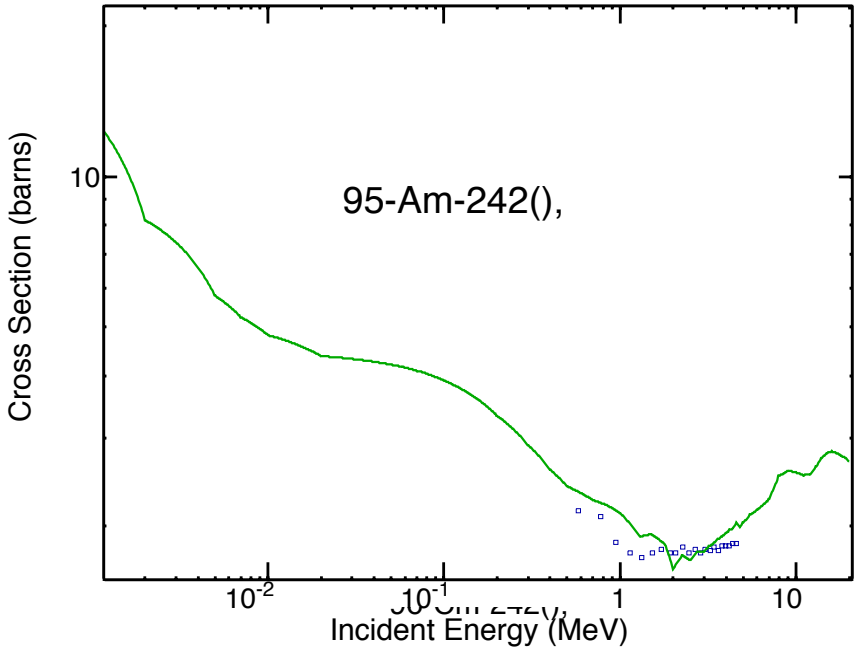

94-Pu-240(),
Cross Section (barns)
1
10^{-1}
10^{-2}
10^{-1}
1
10
Incident Energy (MeV)

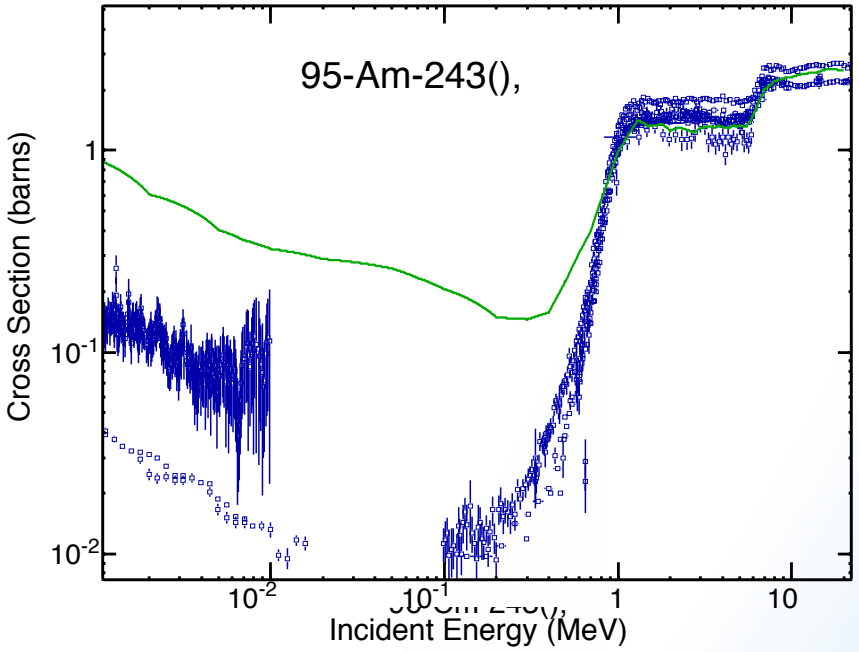

94-Pu-241(),
Cross Section (barns)
Incident Energy (MeV)

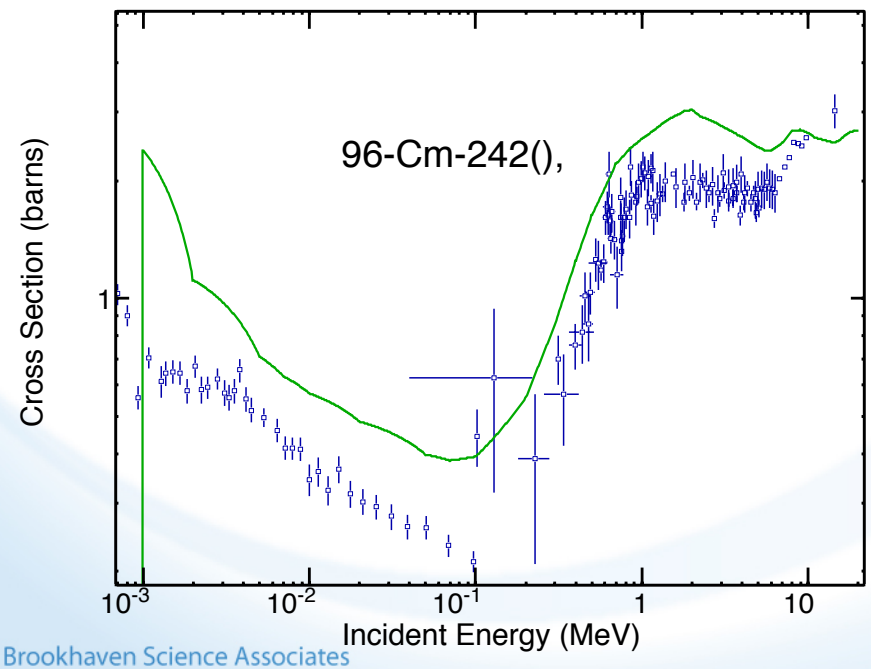

94-Pu-242(),
Cross Section (barns)
Incident Energy (MeV)

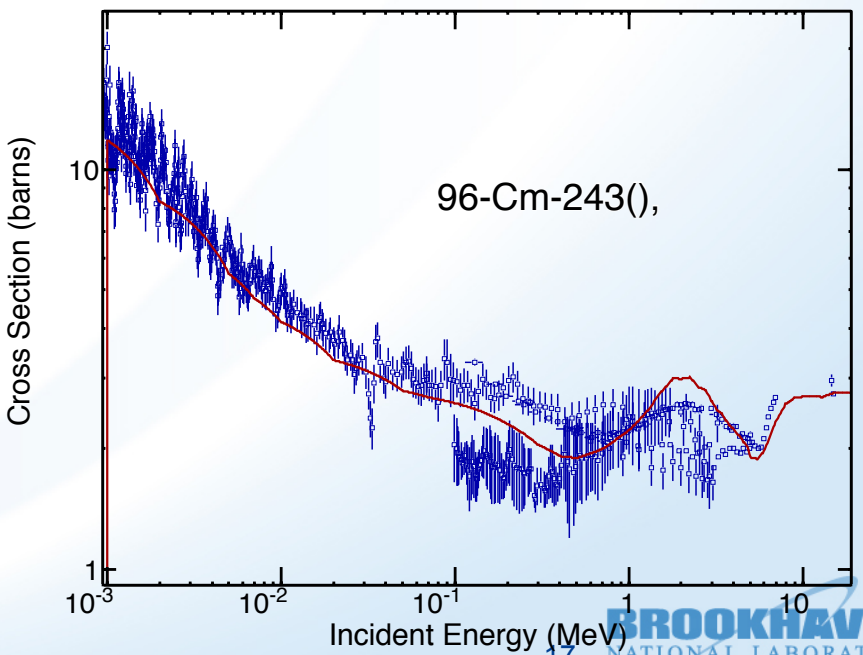

95-Am-240(),
Cross Section (barns)
Incident Energy (MeV)

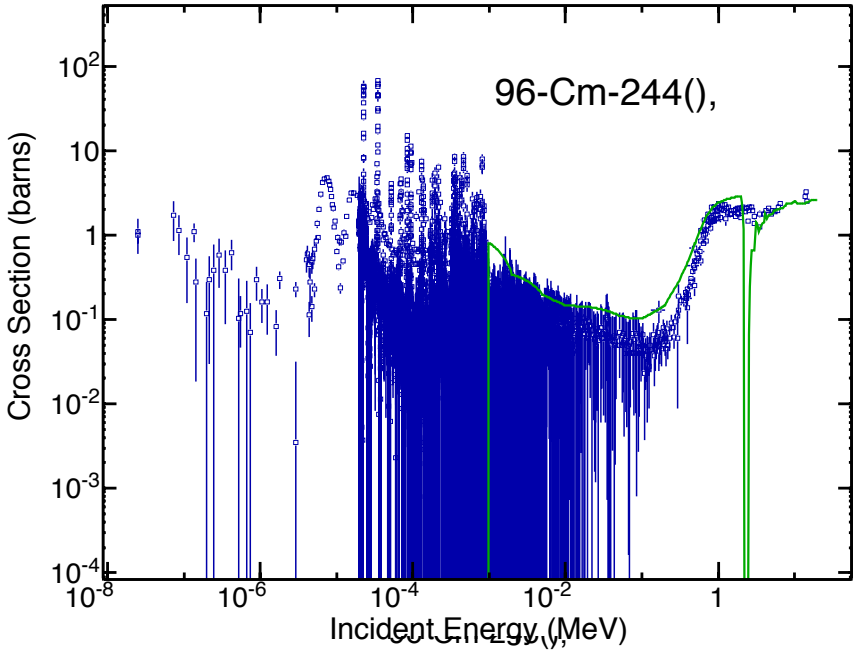

95-Am-241(),
Cross Section (barns)
Incident Energy (MeV)

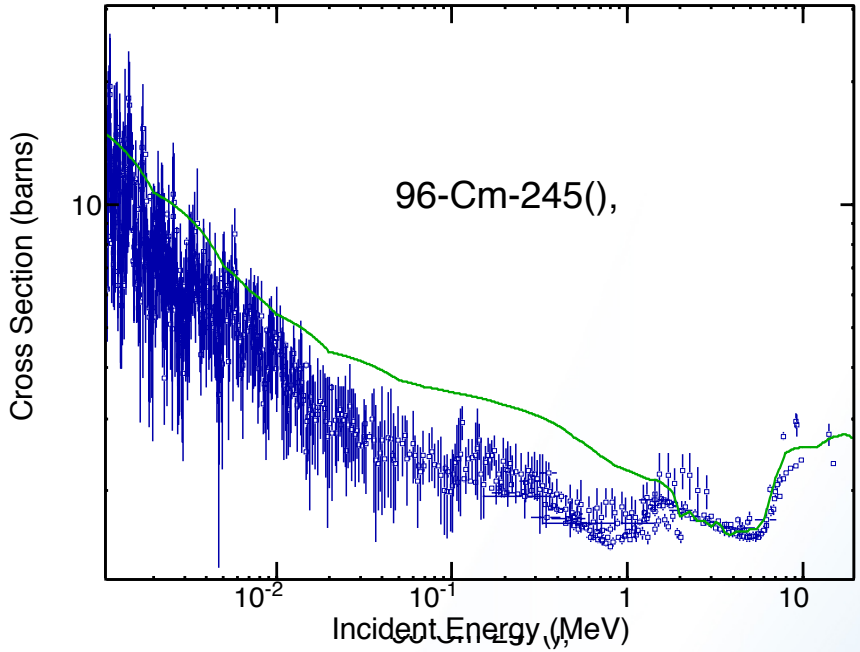

95-Am-242(),
Cross Section (barns)
Incident Energy (MeV)

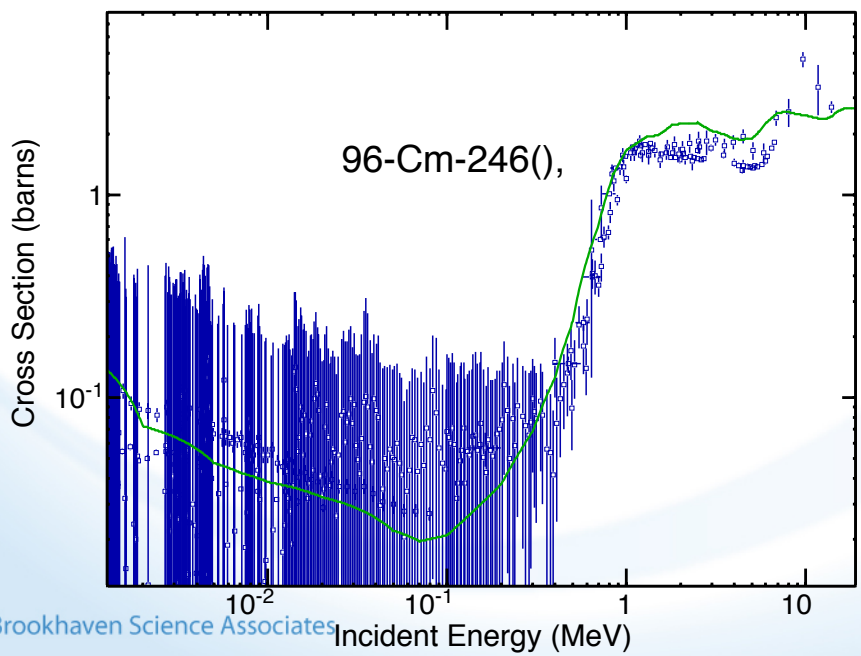

95-Am-243(),
Cross Section (barns)
Incident Energy (MeV)

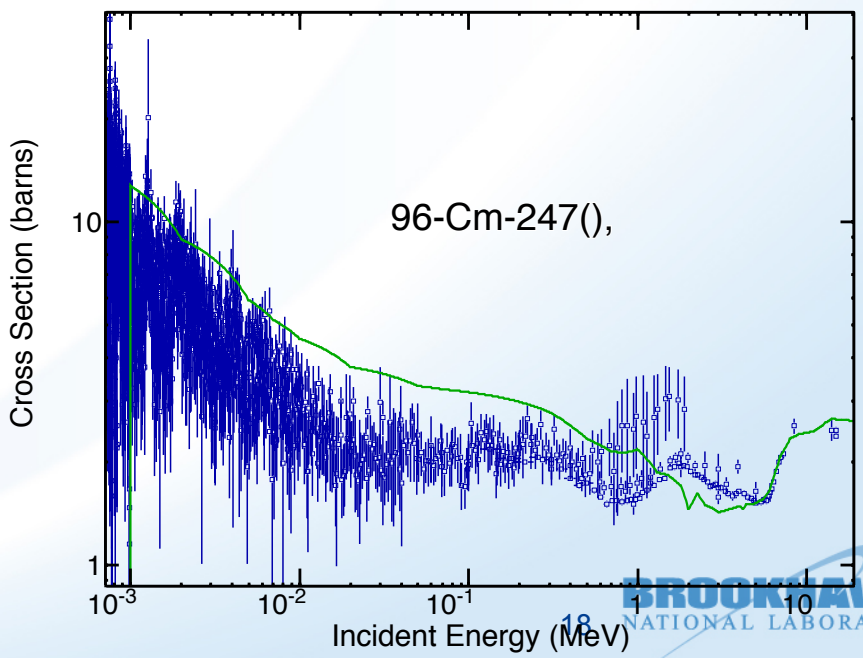

96-Cm-242(),
Cross Section (barns)
Incident Energy (MeV)

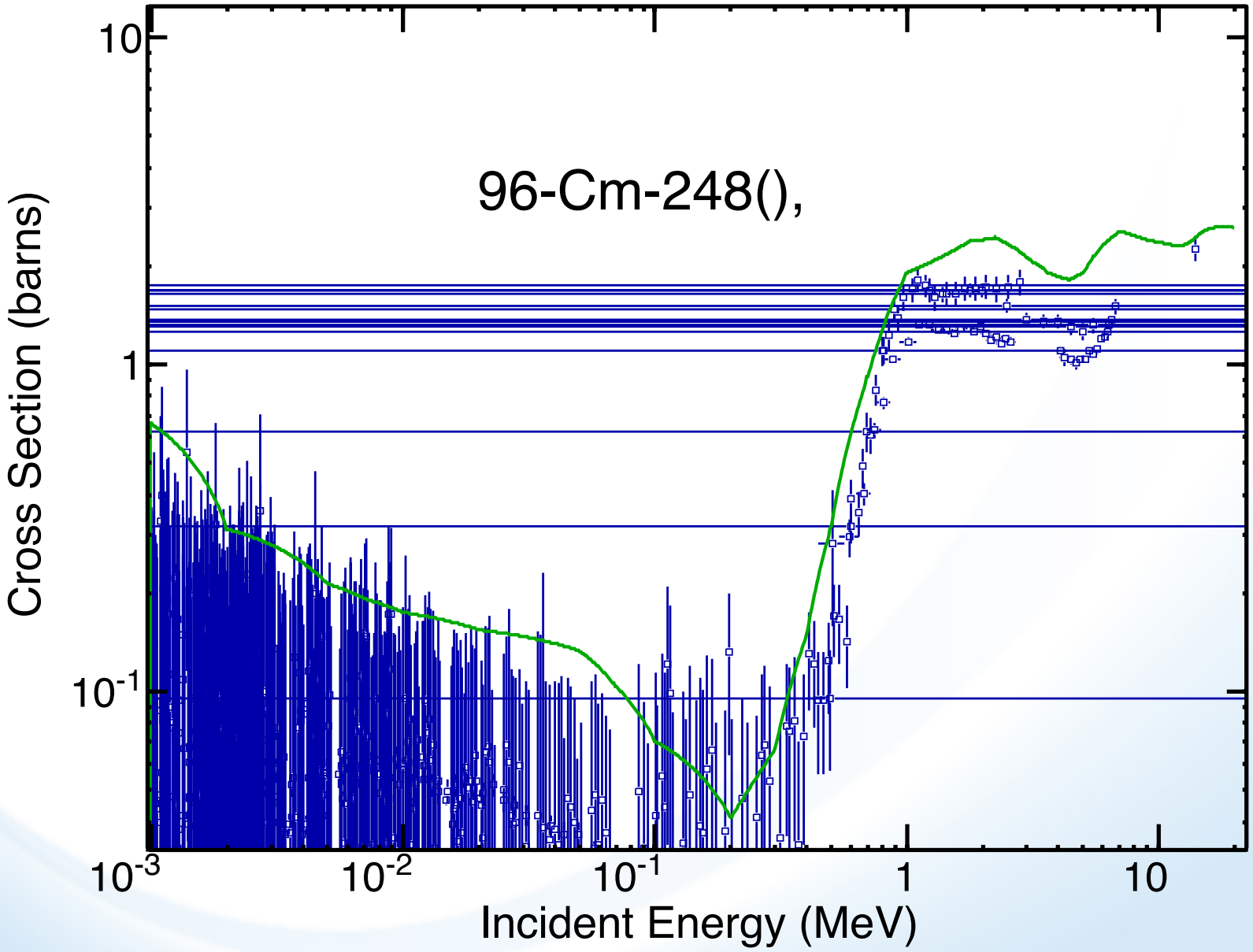

96-Cm-243(),
Cross Section (barns)
Incident Energy (MeV)


96-Cm-244(),
Cross Section (barns)
Incident Energy (MeV)


96-Cm-245(),
Cross Section (barns)
Incident Energy (MeV)


96-Cm-246(),
Cross Section (barns)
Incident Energy (MeV)


96-Cm-247(),
Cross Section (barns)
Incident Energy (MeV)


96-Cm-248(),
Cross Section (barns)
10
1
10-1
10-3
10-2
10-1
1
10
Incident Energy (MeV)

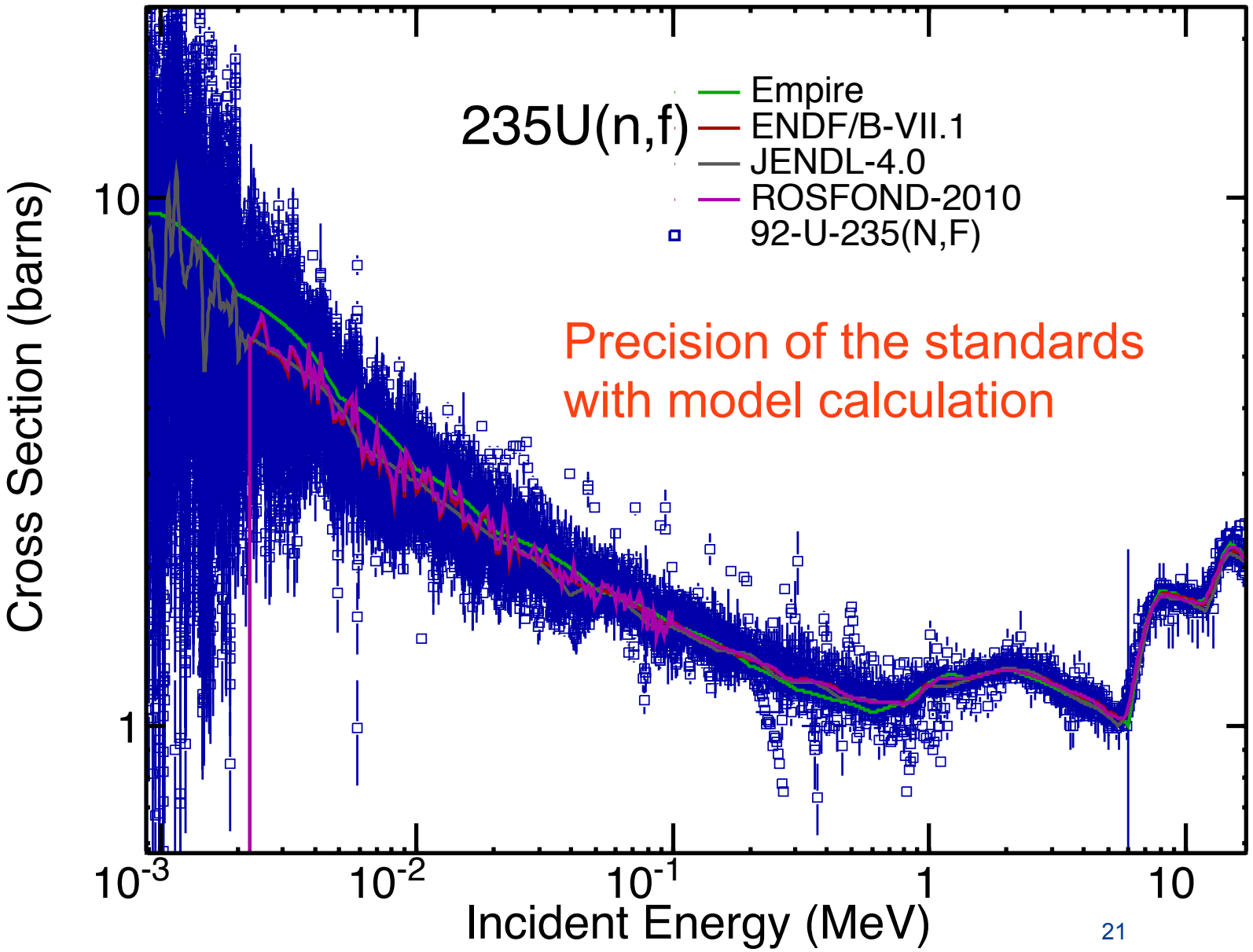
^{235}U
new prior for assimilation (attempt #2) by M. Sin

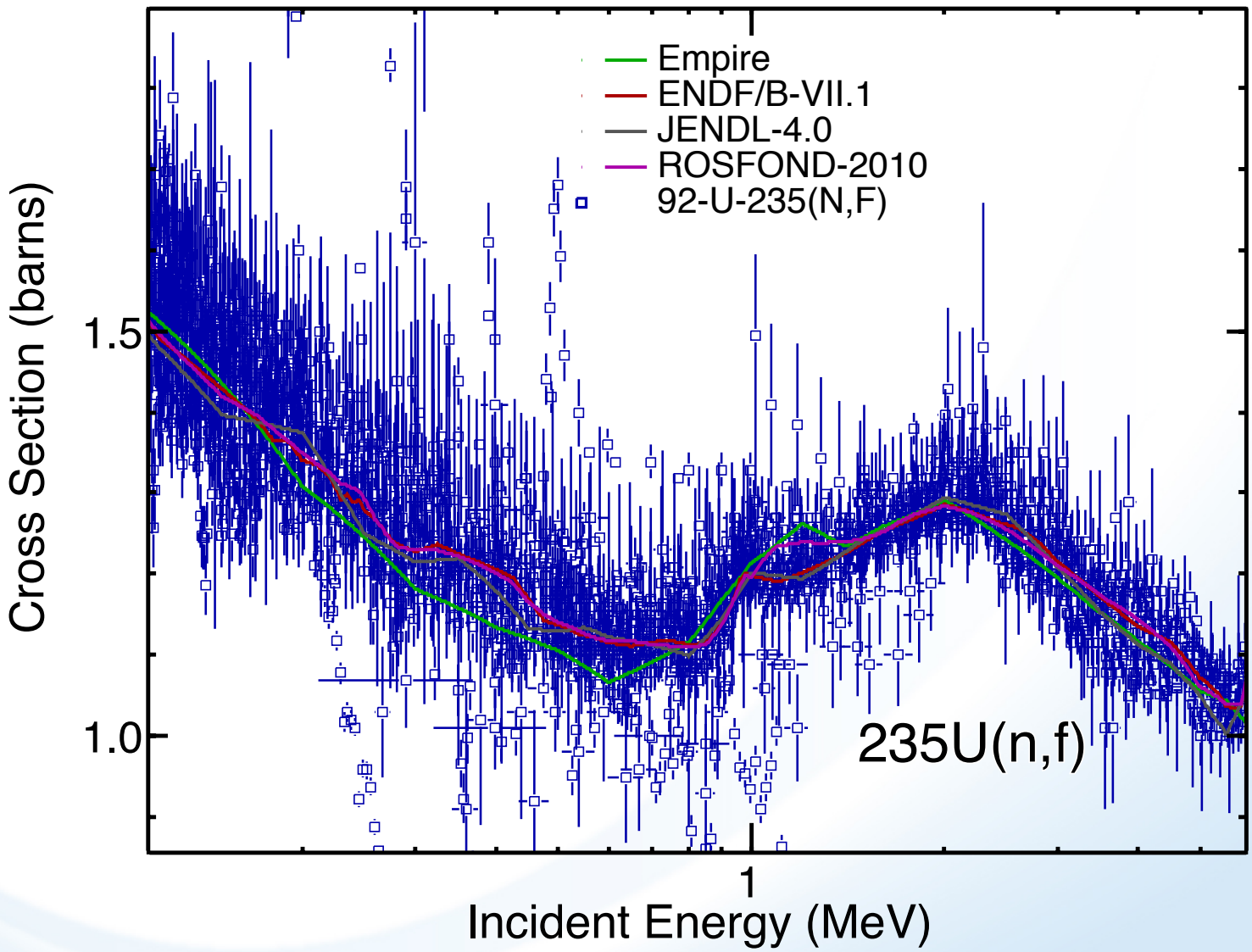
- EMPIRE-3.1
- Adjusted fission input (part of new default)
- Very limited changes in particle channels

EMPIRE INPUT:

```
LEVDEN      0.           ! EGSM level densities
MSD         2.           ! MSD preequilibrium
MSC         1.           ! MSC preequilibrium
EFIT      .730        2  ! adjust MSD contribution
EFIT      .714        3  ! adjust MSD contribution
EFIT     1.414        4  ! adjust MSD contribution
RESNOR   1.25            ! increases MSD
HRTW        2.0          ! HRTW up to 2 MeV
GSTRFN      1.0          ! MLO1 g-strength function
TUNE        2.05 92 236! increase g-str. fun. 236U
DIRECT      1.           ! CC calculations
DIRPOT -2408.            ! Capote OMP
OMPOT  -2408.      1     ! Capote OMP
OMPOT  -5408.      2     ! Capote OMP
FISBAR      1.           ! RIPL fission barriers
FISDEN      0.           ! EGSM level densities
FISDIS      1.           ! discrete levels at saddles
FISOPT      1.           ! optical model for fission
```

Adjusted EMPIRE-3.1 calculations




Empire
ENDF/B-VII.1
JENDL-4.0
ROSFOND-2010
92-U-235(N,F)
Cross Section (barns)
1.5
1.0
235U(n,f)
1
Incident Energy (MeV)

Conclusions

- Current version of EMPIRE is capable of treating actinides
  - improved level densities
  - PFNS calculations with fitting experimental data and covariances
  - improved defaults - reproduce half of the 30 calculated fission cross sections within 20-30%
  - adjusted calculations can reproduce standards within their uncertainties (~2%) without energy dependent tuning

"Give us the tools, and we will do the job."

George Bush, State of the Union 1989