



# NNDC Progress Report

(NRDC meeting, Sapporo, April. 20-23, 2010)

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# NNDC Staff Changes

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## ● Reaction data

- ★ Sam Hoblit (covariances, ENDF evaluation) joined in April 2010 as a staff member
  - Education: Ph.D. in Physics, University of Illinois
  - Experience: Laser-Electron-Gamma-Source (LEGS) at BNL, polarized photon beams up to 0.4 GeV
  - Responsibilities: Covariances, ENDF valuations, **EXFOR**

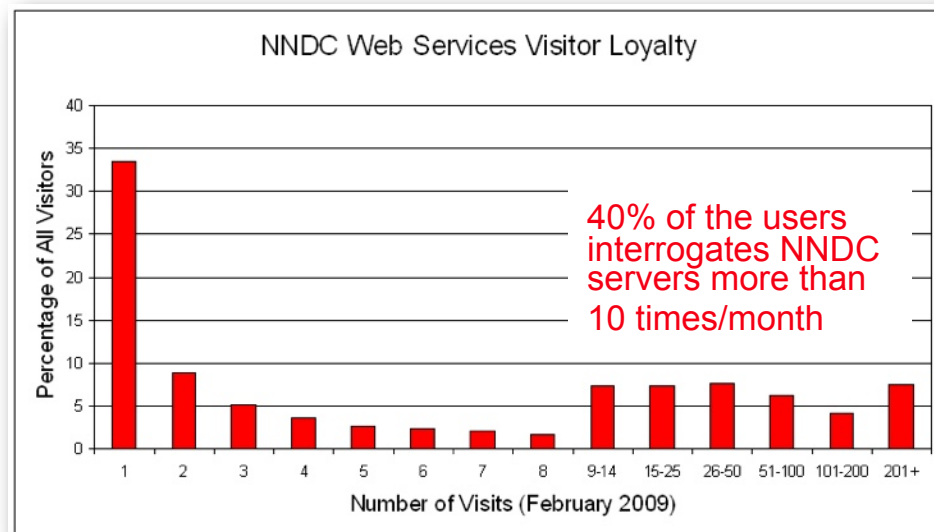
## ● Structure data

- ☒ Manojeeet Bhattacharya (NSR) left NNDC in July 2009
- ★ Sujit Tandel (ENSDF evaluation) joined as a staff member in Feb. 2009
- ☒ Sujit Tandel left NNDC in March 2010
- ★ Chris Ouellet (ENSDF evaluation) joined as Postdoc in March 2009
- ☒ Chris Ouellet (ENSDF evaluation) left in April 2010
- ★ Tim Johnson (ENSDF evaluations, software develop.) joined in April 2010
- ★ New postdoc position (ENSDF evaluation) will be advertised

# Upgrade of NNDC Server System

## Better and faster services to the users

- ◆ Extended possibilities of on-line calculations
  - ◆ integration and arithmetic operations on cross section files
  - ◆ visualization of covariances
  - ◆ advanced interactive plotting of decay schemes and reaction data
- ◆ More users can be served simultaneously
- ◆ Faster access
- ◆ Space for storing and distributing large files such as covariances and preprocessed files



Feature	Current 2004	New 2009
Total # processors/cores	8	32
Total processing power (GHz)	23	107
GFLOPS	111	586
Total RAM (GB)	22	240
Total disk storage (TB)	1.5	11.7
Total purchase cost	\$ 67k	\$ 73k



# SYBASE to migration at NNDC

## Stay away from commercial software!

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- ◆ Sybase relational database used by NNDC since 2001 for all web based services (cost **\$4k/y**)
- ◆ When requested to move license to the new server Sybase decided that NNDC is not properly licensed.
- ◆ New license model:
  - ◆ **~\$80k/y** for the old 2-CPU server
  - ◆ **~\$250k/y** for the new 8-core server
- ◆ Sybase threatened legal action for license noncompliance (**~\$500k**)
- ◆ Eventually, Sybase dropped the case it could not sustain
- ◆ **NNDC abandoned Sybase and migrated all databases to the open source MySQL (\$5k/y maintenance, perpetual license)**

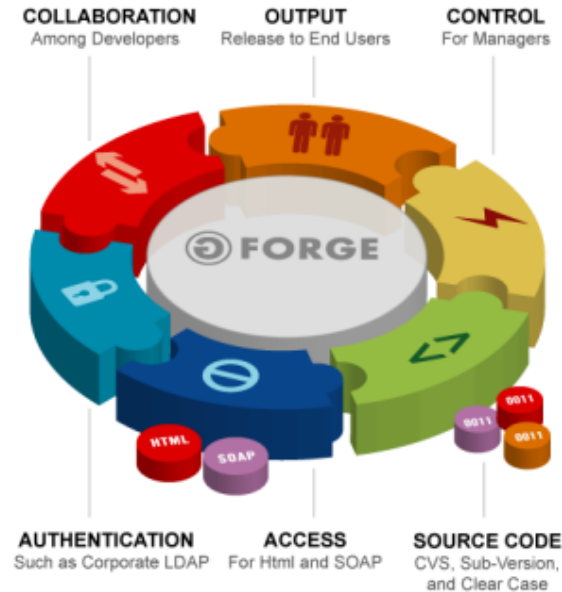


(<https://ndclx4.bnl.gov/gf/>)

# Collaborative environment for nuclear data development.

## Features:

- Apache web server
- Manage file releases
- Document management
- News announcements
- Surveys for users and admins
- Issue (bug) tracking
- Task management
- Subversion (SVN) versioning system
- File uploading/downloading
- Mailing lists



(c) 2004, GForge Group, L.L.C.

## Current projects:

- ENDF/B-VII
- ENDF-6 manual
- EMPIRE code





# ENDF/B-VII.0 → ENDF/B-VII.1



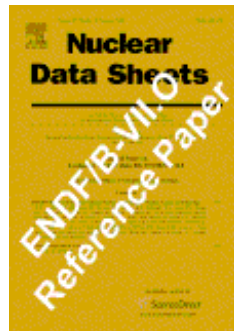
Released December 2006  
(16 years after ENDF/B-VI)



CSEWG 2006

## Major contributors

- LANL (actinides, light nuclei, thermal neutron scattering)
- BNL (fission products resonances & fast, decay data)
- ORNL (resonances)



206 citations  
(SCOPUS)

Release December 2011  
5 years after ENDF/B-VII.0

## Major improvements:

- structural materials
- minor actinides
- covariances (110 materials for AFCI)
- eliminating some deficiencies
- fixing errors

## Roadmap:

- beta0 version December 2010
- beta1 version June 2011
- beta2 version September 2011?
- release & paper December 2011



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NRDC

Sapporo, April 20-23, 2010



# ENDF/B-VII.1 Status

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**New evaluations:** 9Be, 19F, 27Al, 35Cl, 37Cl, 39K, 41K, 46Ti, 47Ti, 49Ti, 50Ti, 52Cr, 53Cr, 55Mn, 58Ni, 60Ni, 74As, 75As, 78Kr, 90Zr, 123Xe, 124Xe, 180W, 182W, 183W, 184W, 186W, 185Re, 187Re, 237U, 239U, 240Pu, 240Am

IAEA

**New covariances:** 235U, 238U, 239Pu

**Corrected for ACE library:** 1H, 45Sc, 89Y, 96Zr, 97Mo, 242Am, 242m1Am

**Simple fixes:** 3H, 22Na, 87Rb, 113Cd, 233U, 236U, 241Am

**Taken from other libraries:** 63Cu, 65Cu, 174Hf, 176 Hf, 177Hf, 178Hf, 179Hf, 180Hf

**JENDL Actinoid files:** 225Ac, 226Ac, 227Ac, 227Th, 228Th, 229Th, 230Th, 231Th, 233Th, 234Th, 229Pa, 230Pa, 231Pa, 232Pa, 230U, 231U, 232U, 234Np, 235Np, 236Np, 238Np, 239 Np, 236Pu, 237Pu, 238Pu, 241Pu, 242Pu, 244Pu, 246Pu, 240Cm, 241Cm, 242Cm, 243Cm, 244Cm, 245Cm, 246Cm, 247Cm, 248Cm, 249Cm, 250Cm, 245Bk, 246Bk, 247Bk, 248Bk, 249Bk, 250Bk, 246Cf, 248Cf, 249Cf, 250Cf, 251Cf, 252Cf, 253Cf, 254Cf, 251Es, 252Es, 253Es, 254Es, 254m1Es, 255Es, 255Fm



# Covariances for ENDF/B-VII.1

## Recent and ongoing project/activities

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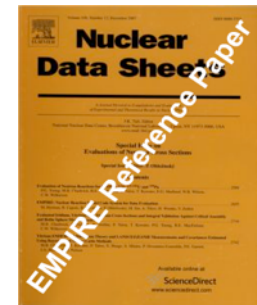
- **AFCI/GNEP** project (BNL, LANL) will provide 110 covariances, which will serve as a reference for constructing ENDF-6 formatted covariance files for ENDF/B-VII.1.
  - AFCI-1.2 library, August 2009
  - AFCI-1.3 library, April 2010
  - AFCI-2.0 library, August 2010
- **Evaluation of MF32** (ORNL), **MF33** (LANL) covariances for the individual materials.
- The **low-fidelity** covariance project - a full set of simple estimates for all ENDF/B-VII.0 materials (BNL, LANL, ORNL and ANL).
- Work continues on improvement of covariance evaluation methodology and on validation of the **processing codes PUFF and NJOY**.
- **Workshop** on Neutron Cross Section Covariances was held in Port Jefferson, NY, June 24-27, 2008 attended by 53 participants from 11 countries who presented 39 contributions.
- **Second Workshop** on Covariances was held in Port Jefferson, NY, June 23, 2009





# EMPIRE-3 (Arcola)

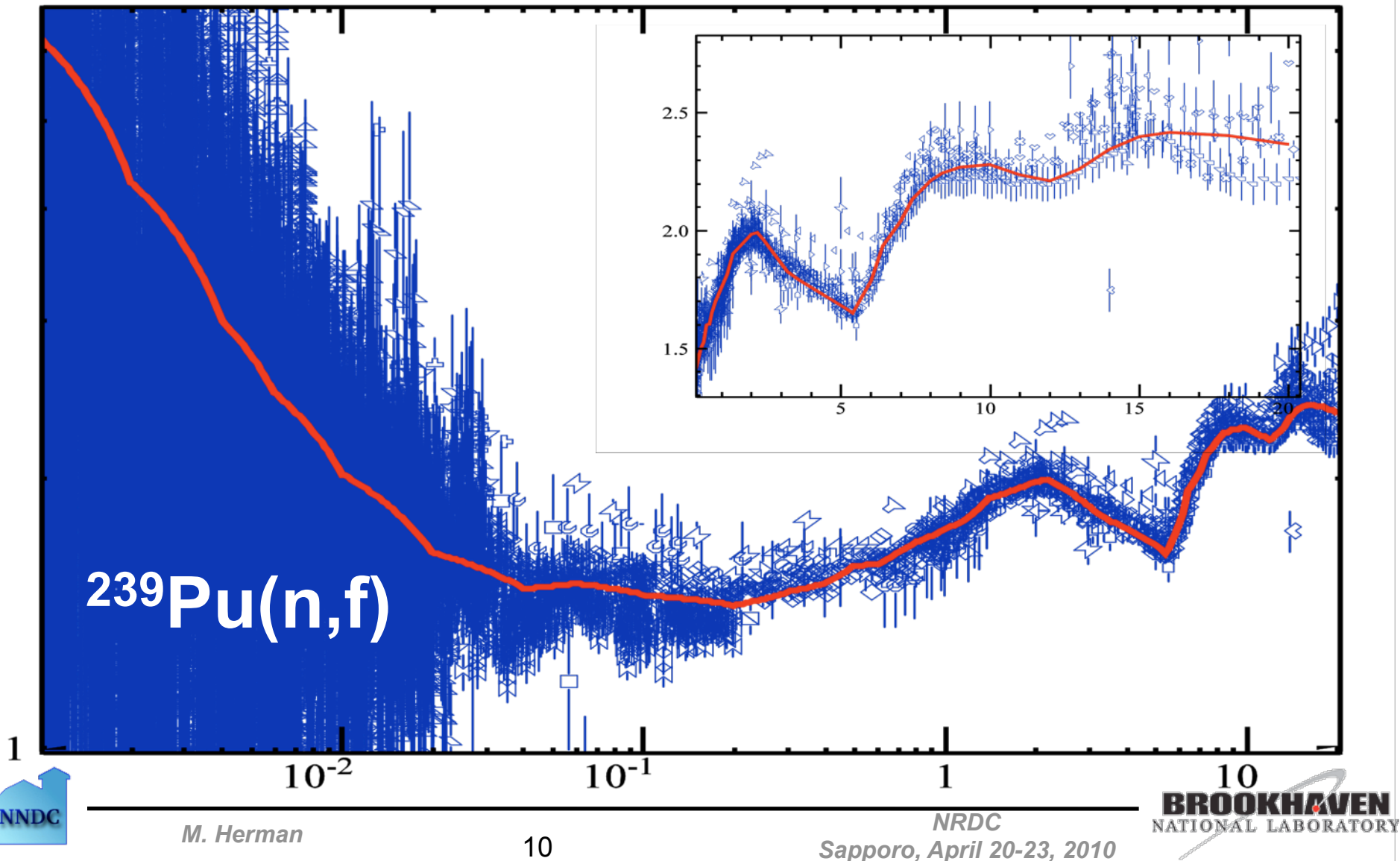
- Resonance module (Cho, Oblozinsky, Mughabghab)
  - covariance data (MF=32)
  - adjustment of resonance parameters to reproduce thermal uncertainties
  - arbitrary correlations among gamma-widths and among neutron-widths
  - new 'kernel method' under development
- Six ejectiles (n, p, alpha, g, d, t,  $^3\text{He}$ ) + light ion; includes ENDF-6 formatting (Capote, Trkov)
- RIPL-3 combinatorial level densities with parity dependence
- Upgrade of ZVView package - 2-D and 3-D plotting of covariance matrices (Zerkin)
- **Parametrization of the fission channel (M. Sin)**
- Working towards EMPIRE-3.0 release (Mattoon) (new Python scripts, covariance handling, 'run nearly everywhere' except Windows)



Nucl. Data Sheets  
Vol. 108 (2007) ↑  
44 citations↑

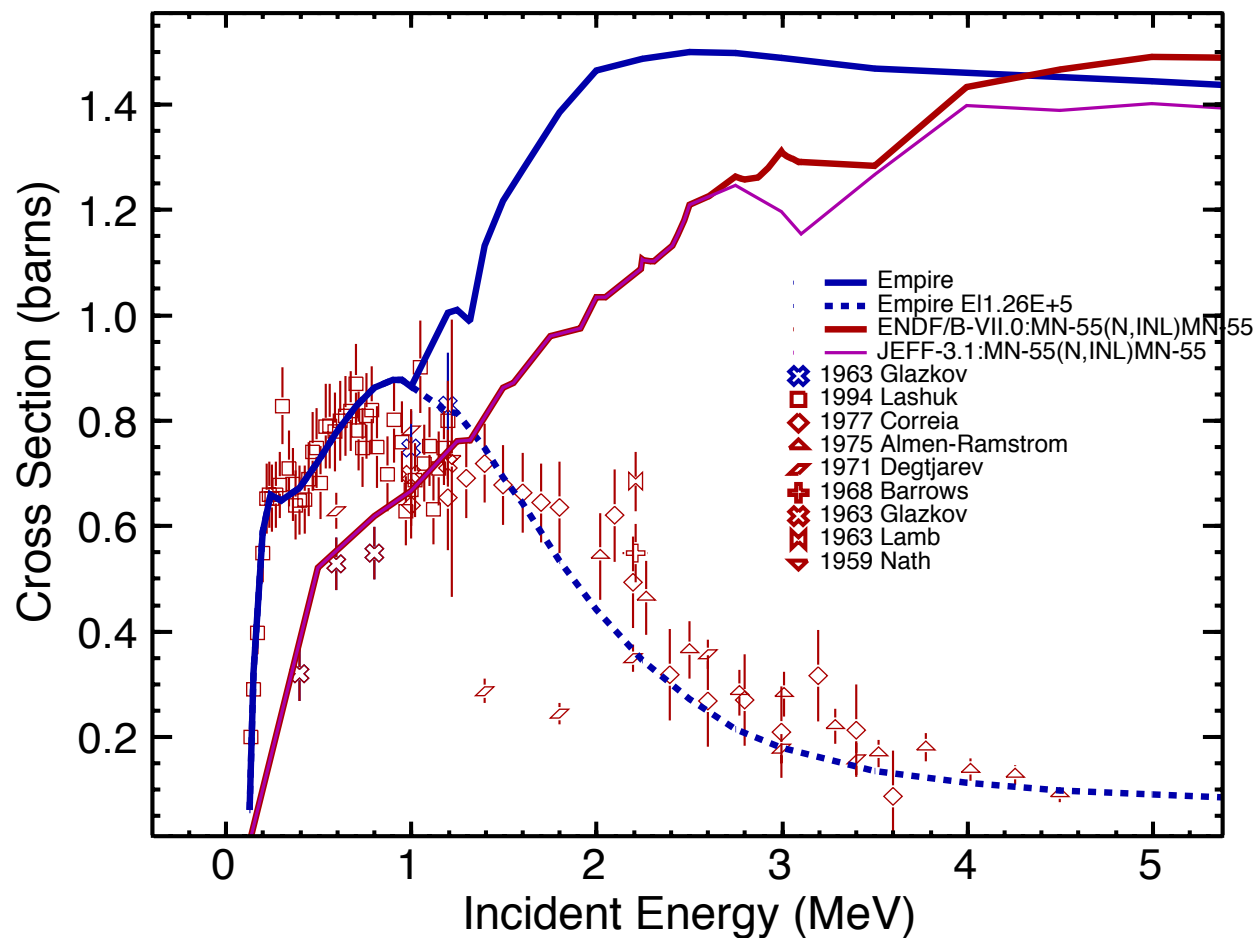
# New fission parametrization in EMPIRE

(Mihaela Sin)



# $^{55}\text{Mn}(n,n')$

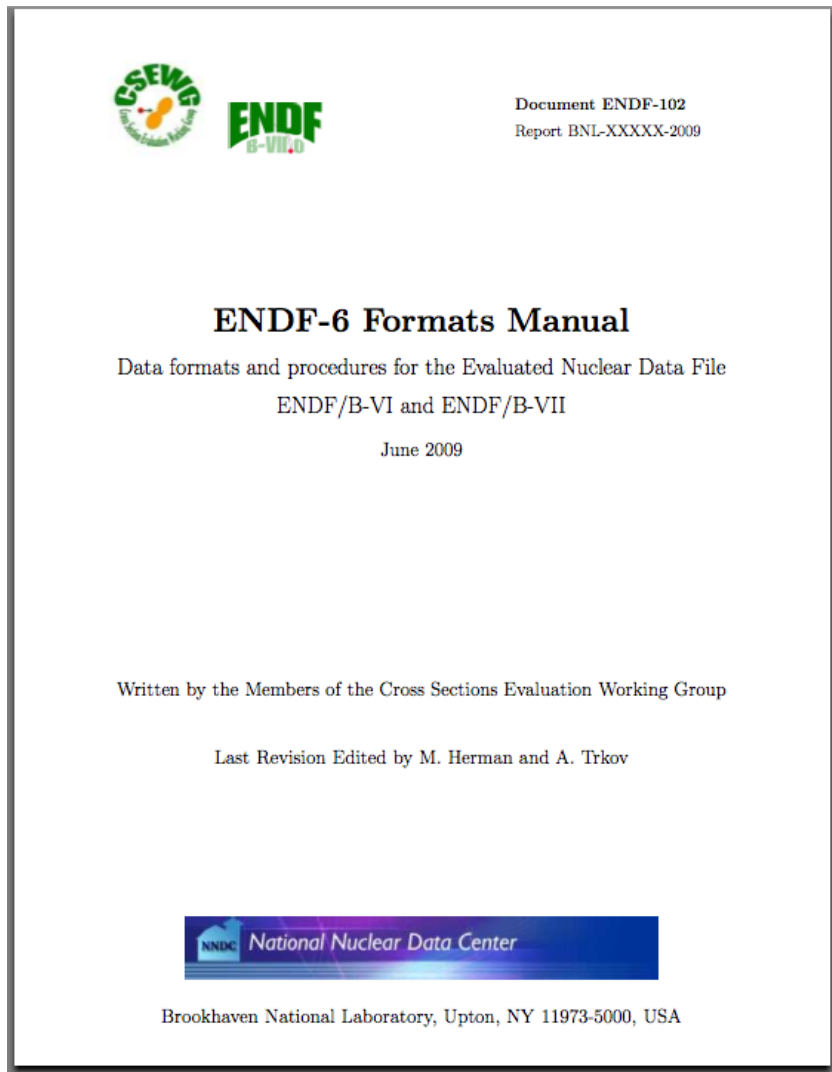
(Capote; in EMPIRE we trust!)



# ENDF-6 manual

## New LaTeX version available on web

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- Edited by M.H. and A. Trkov
- Includes all CSEWG endorsed updates
- Many corrections improvements and clarifications
- Maintained under GForge
- Thanks to: Toshihiko Kawano, Nancy Larson, Cecil Lubitz, Douglas Muir, Donald Smith, Patrick Talou who reviewed parts of the new manual.

*M. Herman*

# 8th release of ENDF checking & utility codes

## Updated single source, output easier to read

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Search the NNDC:

NNDC Site Index
<b>Documentation</b>
Manual (MS Word)
<b>ENDF Utility Codes</b>
<b>CHECKR 8.01</b> ▶
<b>FIZCON 8.01</b> ▶
<b>INTER 7.01</b> ▶
<b>PSYCHE 8.0</b> ▶
<b>STANEF 8.01</b> ▶
<b>Previous versions</b>
ENDF Utility Codes 7.02
ENDF Utility Codes 7.0
ENDF Utility Codes 6.13

## **ENDF Checking & Utility Codes**

The ENDF Checking & Utility Codes correct all bugs reported to NNDC as of February 1, 2009 and supersede all previous releases. A detailed log of changes can be found at the beginning of the respective FORTRAN sources. The suite of ENDF utility codes includes:

- **CHECKR** - Format Checking Code
- **FIZCON** - Procedures & Simple Physics Checking Code
- **PSYCHE** - More complicated physics checking code
- **INTER** - Calculates selected cross sections and integrals
- **STANEF** - Creates directory, adds tape label & converts numeric fields Converts to binary format

Provided are FORTRAN95 sources as well as Linux and MS Windows binaries compiled and statically linked using GFORTRAN in case of Linux and Compaq Visual Fortran 6.1.A in case of Windows. Each code can be run as a command with the ENDF file as an argument or interactively.



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# Sigma: Web retrieval & plotting of ENDF data

<http://www.nndc.bnl.gov/sigma>

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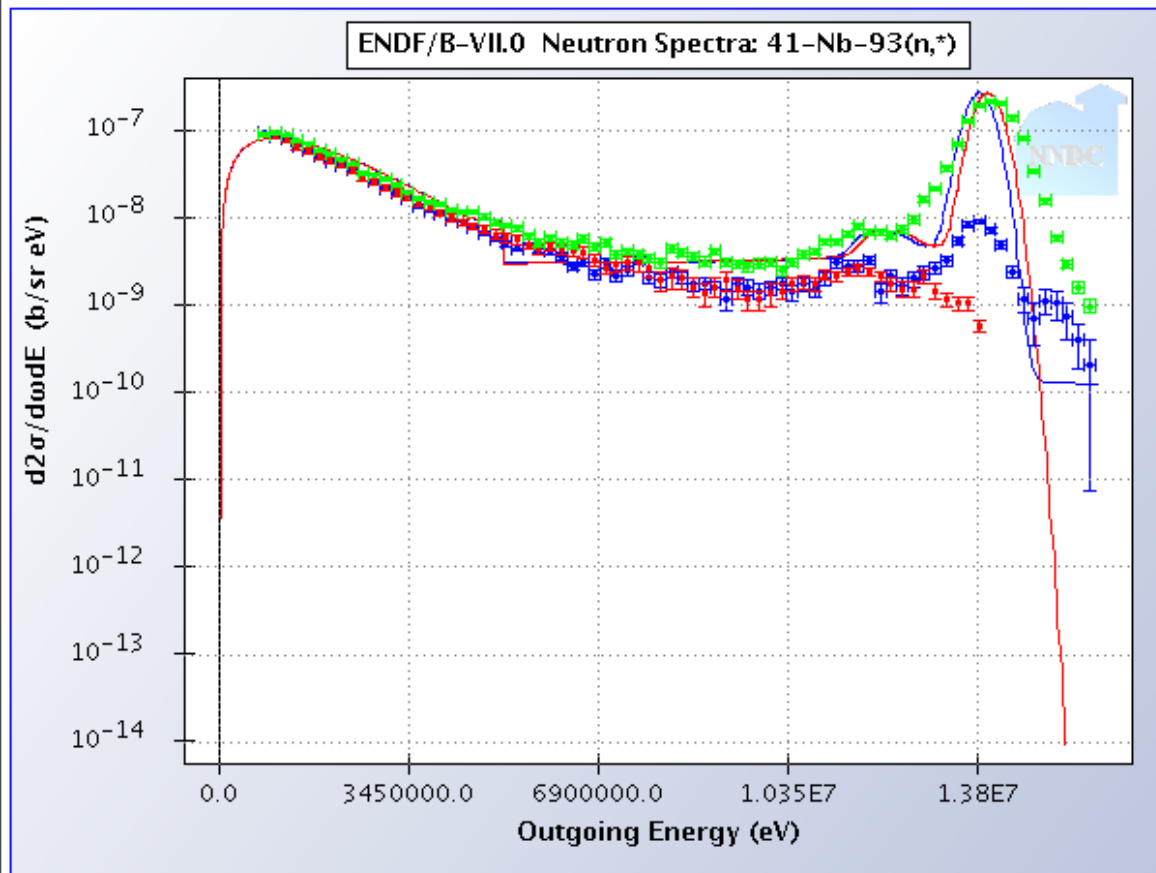
## Sigma-3 released in April 2009 features:

- Plotting energy-angle distributions (MF=6).
- Visualization of covariances (MF=33 with LB=1,5; applies to ~80% of cases).
- Retrieving thermal neutron cross sections & resonance integrals for neutron capture and fission.

These add to the existing capabilities to plot angular distributions (MF4), plot energy spectra (MF5), and mathematical operations on cross sections (MF3) already available in the release 2.

# Sigma-3: MF=6 plotting

## Easy to use



Update Plot
Reset

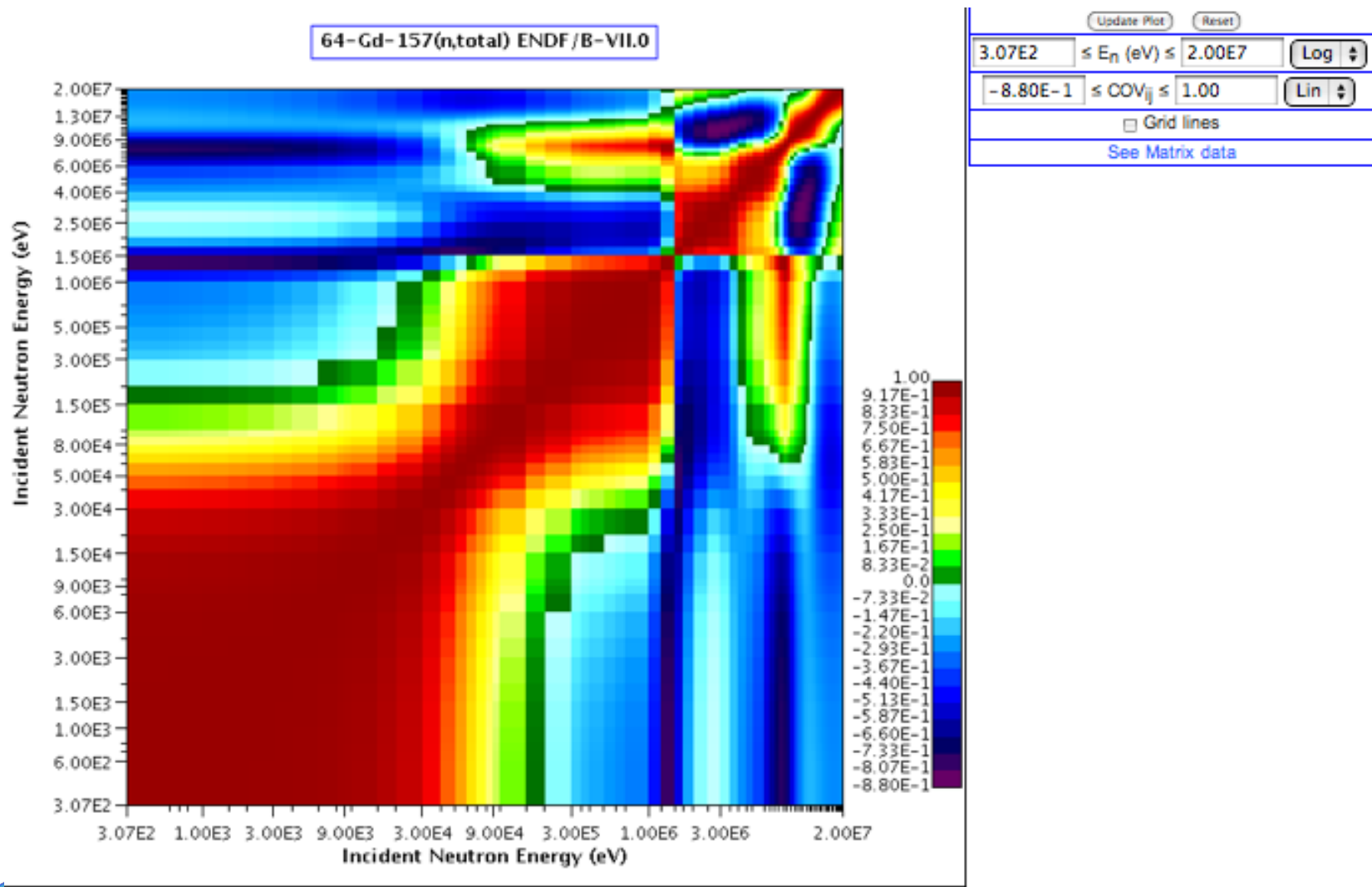
1.0E-5 ≤ X ≤ 2.5E7 Lin

5.69E-15 ≤ Y ≤ 4.01E-7 Log

View evaluated data  
View experimental data

<input type="checkbox"/>	#	Incident Neutron Energy (eV)	Ejectile	Angle (deg)	Reference
<input checked="" type="checkbox"/>	—	1.41E+7	n	90	ENDF/B-VII.0
<input checked="" type="checkbox"/>	—	1.40E+7	n	30	ENDF/B-VII.0
<input checked="" type="checkbox"/>	1	1.41E+7	n	90	Matsuyama 1992
<input checked="" type="checkbox"/>	2	1.41E+7	n	90	Lychagin 1985
<input checked="" type="checkbox"/>	3	1.40E+7	n	30	Matsuyama 1992

# Sigma-3: covariance plotting



# EXFOR compilation at NNDC

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- NNDC EXFOR compiler has not been replaced with a permanent staff member
- Compilation effort continue to be outsourced
  - **Stanislav Hlavac** (Institute of Physics, Slovak Academy of Sciences, Bratislava, Slovakia) compiles EXFOR entries since Nov. 1, 2007
  - **Otto Schwerer**, (retired from NDS, IAEA, Vienna, Austria) reviews new entries since April 1, 2008
- NNDC is planning to continue this arrangement
- In future Sam Hoblit should oversee EXFOR compilation