ENDF/B-VII.1beta5 Phase 1 Testing

Data Verification

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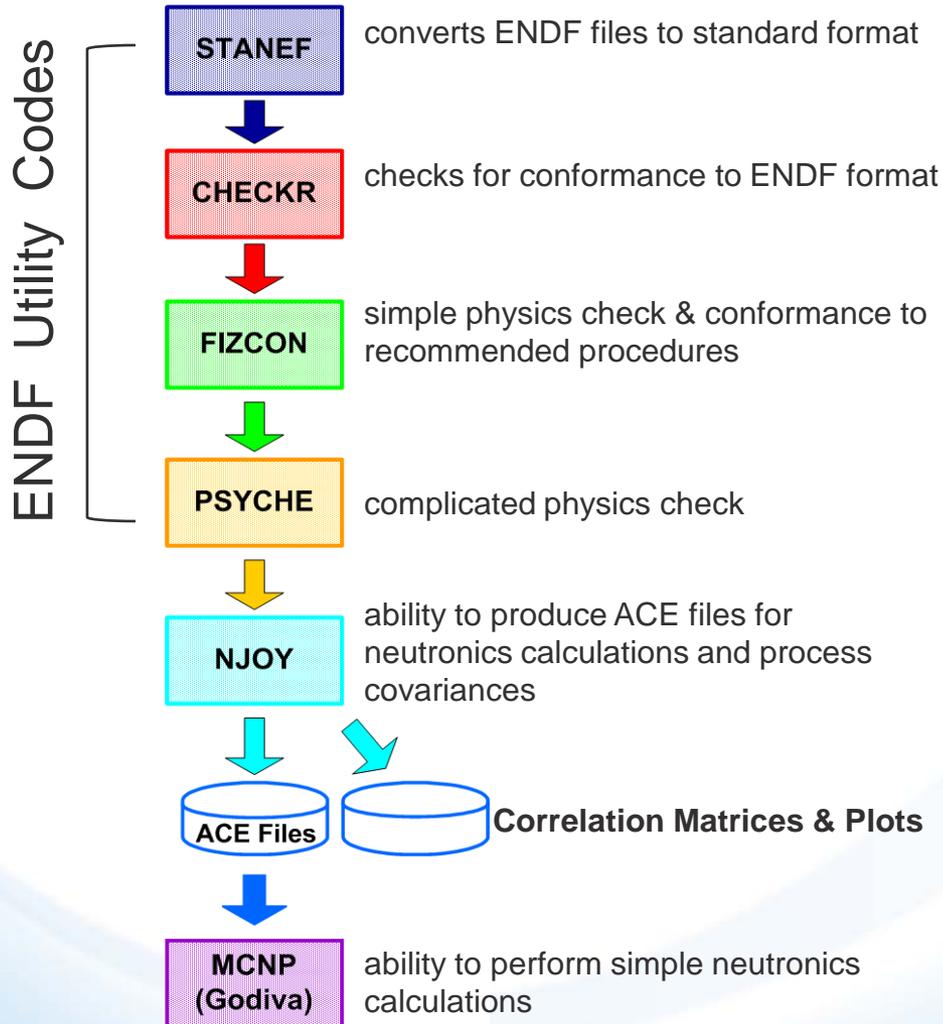Brookhaven National Laboratory

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Outline

- **Data verification process flow**
- **CHECKR results**
- **FIZCON results**
- **NJOY results**
- **MCNP5 results**
- **Online data verification system**
- **Conclusion and outlook**

Data Verification Process Flow

ENDF Utility Codes

STANEF — converts ENDF files to standard format

CHECKR — checks for conformance to ENDF format

FIZCON — simple physics check & conformance to recommended procedures

PSYCHE — complicated physics check

NJOY — ability to produce ACE files for neutronics calculations and process covariances

ACE Files | **Correlation Matrices & Plots**

MCNP (Godiva) — ability to perform simple neutronics calculations

Platform: NNDC Linux Cluster

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CHECKR Results

- **Be-7**

ERROR(S) FOUND IN MAT= 419, MF= 1, MT=451
EMAX = 8.10E+06 OUT OF RANGE 2.00E+07 - 5.00E+08

A partial evaluation! Need to extend the upper limit of the energy range to at least 20 MeV.

FIZCON Results (continued)

- **Nb-93, Ge-76, Pu-240** and **Np-237**

ERROR(S) FOUND IN MAT=*xxx*, MF= x, MT= xx

SECTION DOES NOT SPAN THE SAME ENERGY RANGE

   AS FILE 3, MT= xx

A section in a File must cover the same incident energy range as was used for the same section in File 3.

FIZCON Results (continued)

- **V-50, Ti-49, Zn-65,67,68,70, Nb-93**

ERROR(S) FOUND IN MAT=*xxxx*, MF=*6*, MT= *xxx*
CHECK NORMALIZATION=*x.xxxxxx* AT E=*x.xxxxxE+xx*

<1 or >1

ERROR(S) FOUND IN MAT=*xxx*, MF=*5*, MT= *xx*
NORMALIZATION CHECK INTEGRAL=*x.xxxxxE+xx*

Integral of normalized distribution is not equal to 1. Are they worth fixing? Processing codes usually renormalize distributions anyway.

FIZCON Results (continued)

- **Ar-40, Sn-120, Hf-174,176,177,178,179,180**

ERROR(S) FOUND IN MAT=*xxxx*, MF=*5*, MT=*xxx*

FOR LF=1 EPMAX FOUND TO BE *x.xxxxxE+xx*

Some entries in MF5's table for outgoing neutron energy found too high and:
- Violates $E' \leq E - Q$ by energy conservation law.
- Contributes to energy balance problems.

NJOY Results

- All 423 materials successfully processed using a combination of NJOY-99.369 and NJOY-2010 (for F-19 and Cl-35)

- ACE libraries generated at 300K and 1500K (for COMARRA), and correlation matrices/plots produced for (n,tot), (n,el), (n,inel), (n,2n) and (n,g).

- NJOY's ACER module flagged problems in energy distribution of alpha production in 43 materials:

  C-nat, N-14, O-16, F-19, Al-27, Si-28,29,30, P-31, Ca-40,43,46, 48, Cr-50,52,53,54, Fe-54,56,57, Ni-58,60,61,62,64, Cu-63,65, Nb-93, Mo-97, Eu-153, Ta-180, Hg-198,199,200,201,202,204, Pb-204,206,207,208, Bi-209, Am-243

MCNP5 Results

- All 423 materials successfully processed using GODIVA at 50 million histories
  - 10,000 neutrons
  - 5025 cycles
  - discard first 25 cycles

ADVANCE: Online Data Verification System
(Automated Data Verification and Assurance for Nuclear Calculations Enhancement)

- **The Problem:**
  - Nobody seems to remember to run the checking codes

    "Every evaluation needs to be checked and we humans can't seem to do it right" – D. Brown

- **A Solution:** "continuous integration", a common practice in software development. Every commit or every hour (you pick), retest any evaluation that changed.

- **To Implement:**
  - Control by cronjob or by subversion directly
  - Run all checking and processing codes automatically
  - Automatically parse all messages in log files
  - Generate summary report of verification process

ADVANCE: Online Data Verification System (continued)

ENDF/B-VII.1/neutrons/Ta

status	isotope	abundance	svn log	ENDF (orig. file)	STANEF (log)	STANEF (output diff)	CHECKR (log)	FIZCON (log)	PSYCHE (log)	fudge (warnings log)	reactionSuite (gnd file)	covarianceSuite (gnd file)	NJOY (log)	AMPX (log)
😡	^{180}Ta	0.012 +/- 0.002 %	🔗			Files identical			😡 CORE	No file	⭐	No file	No file	No file
✓	^{181}Ta	99.988 +/- 0.002 %	🔗			Files identical			(28 URR dens. (a))	(1 skip total, 1 redun URR (a)) ⭐		No file	No file	No file
✓	^{182}Ta	0.0 %	🔗			Files identical			(1 iffy Q)	(2 xtra interp, 1 skip total, 1 redun URR (a)) ⭐		No file	No file	No file

What do the messages mean?

1. **fudge** info "redun URR (a)": Redundant data in URR
2. **fudge** info "xtra interp": Multple interpolation regions in a file where there didn't need to be that many.
3. **fudge** unimplimented "skip total": Fudge currently ignores the total cross section.
4. **psyche** unknown "URR dens. (a)": Level density in URR not in agreement with PSYCHE's, possibly misguided, expectations
5. **psyche** unknown "iffy Q": Non-threshold reaction with Q value differing from PSYCHE's, possibly misguided, expectations

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Conclusion and Outlook

- ENDF/B-VII.1beta5 423 materials successfully processed with ENDF Utility Codes, NJOY and MCNP.

- Capabilities of ENDF Utility Codes, especially FIZCON, need upgrade for more reliable results (too many non-errors or "false positives")

- Online data verification system under development (code named ADVANCE) to be released sometime in 2012