AMPX Cross-Section Processing Status

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AMPX Nuclear Data

➢Covariance processing updates

- Updated PUFF-IV to process ENDF/B Compact Covariance Format

- Developed automated computational tool to combine low-energy (< 5 keV) File 33 low-fidelity covariance data from ORNL with high-energy low-fidelity File 33 covariance data from BNL

  - Combined File 33 data produced for 219 fission products

  - Processed covariance data into COVERX format for testing with SCALE sensitivity/uncertainty analysis tools

- Developed computational tool to convert File 32 resonance parameter covariance matrices (RPCM) to File 33 groupwise covariance matrices (GWCM)

File 32 → File 33 Methodology

- RPCMs (File 32) of some actinides is very large
  - ^{235}U RPCM ≈ 1.7 GB

- "Compression" scheme is needed for ENDF
  - Convert RPCM (File 32) into GWCM (File 33)

- Conversion accomplished in Two-step:
  - ✴ Use PUFF-IV to Convert RPCM (File 32) into a group-averaged COVERX file
  - ✴ Use COVCONV module to convert the COVERX file into File 33

- Test on ^{233}U: use GWCM (File 33) to compute uncertainties on various group structures, and compare with the "exact" uncertainties (based on the RPCM).

| Nuclide	File Size with Full RPCMs
^{233}U	100 MB
^{235}U	1.75 GB
^{238}U	680 MB
^{239}Pu	180 MB

^{235}U Evaluation

➢ ORNL performed retroactive resonance analysis to calculate RPCM using SAMMY R-matrix software

➢ Existing ENDF/B File 2 resonance parameters did not change

➢ Reich-Moore evaluation:
  – Resolved region: 1×10^{-5} eV to 2250 eV
  – 3193 resonances with 5 parameters per resonance—127,467,753 elements in upper triangular RPCM
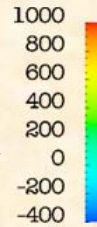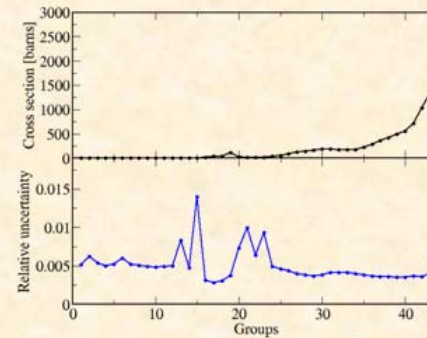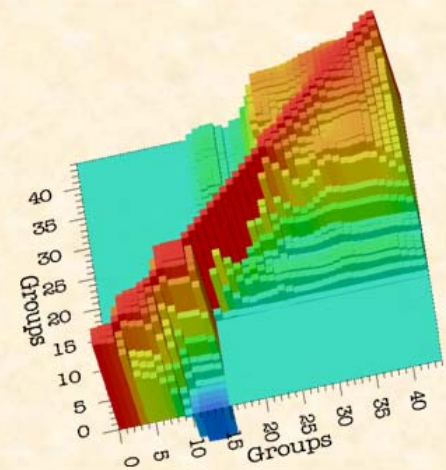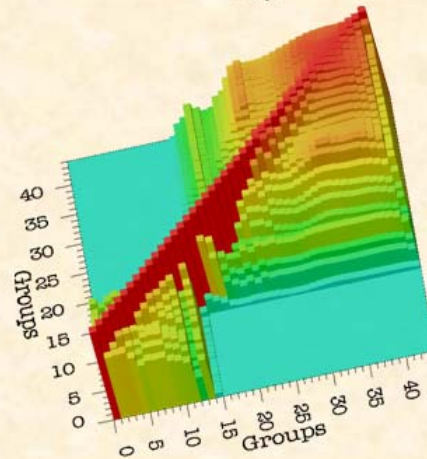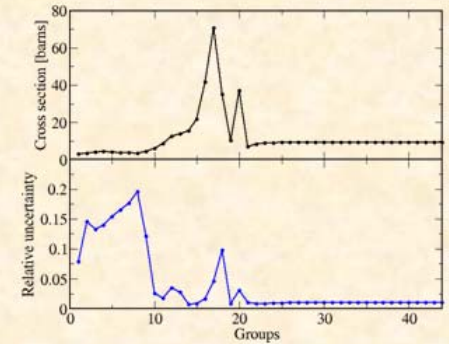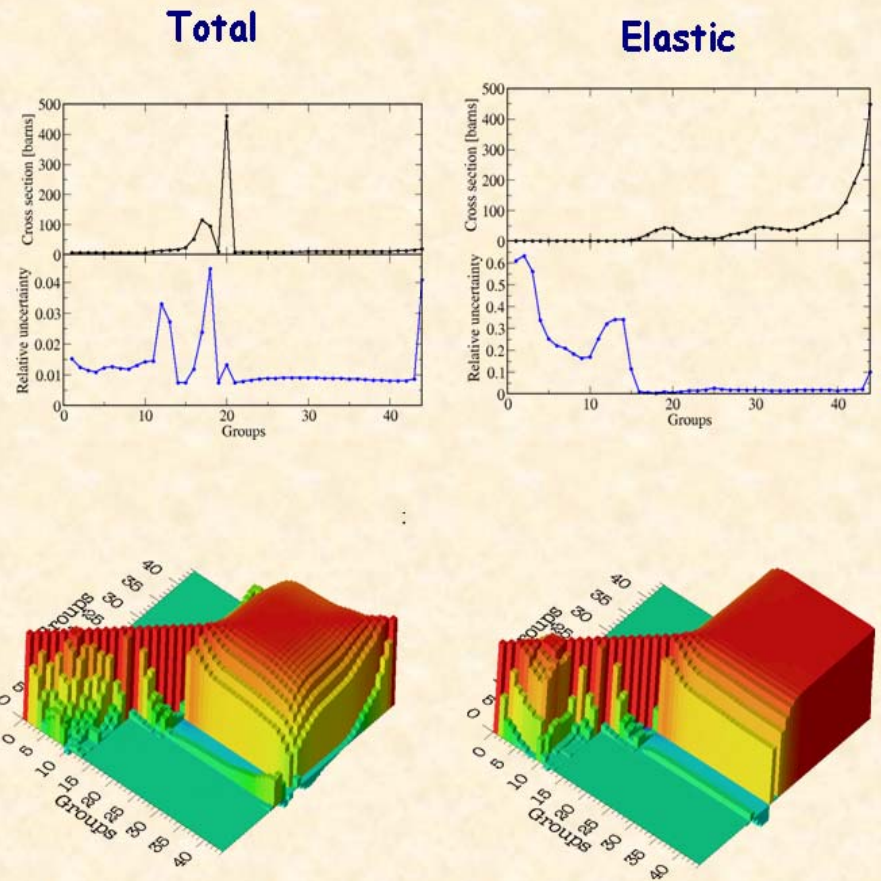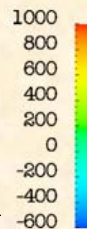
²³⁸U Evaluation

- ➤ ORNL performed new resonance evaluation for ENDF/B-VII.0

- ➤ RPCM prepared using retroactive resonance analysis

- ➤ Existing ENDF/B File 2 resonance parameters did not change

- ➤ Reich-Moore evaluation:
  - – Resolved region: 1×10^{-5} eV to 2000 eV
  - – 3343 resonances with 3 parameters per resonance— no correlations for fission width
 - – 127,467,753 elements in upper triangular RPCM
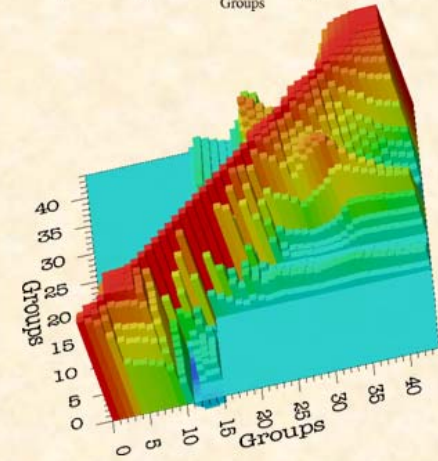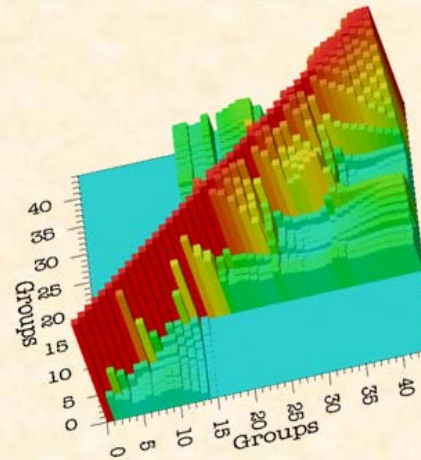
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²³⁹Pu Evaluation

➤ ORNL performed new evaluation of resolved resonance region using SAMMY R-matrix software

➤ RPCMs prepared as part of resonance analysis

➤ Reich-Moore evaluation:

– Resolved region: 1x10-5 eV to 2500 eV

– 1045 resonances with 5 parameters per resonance—13,659,195 elements in upper triangular RPCM
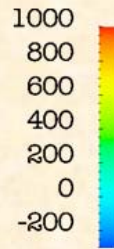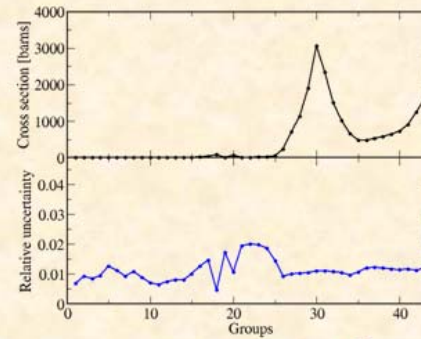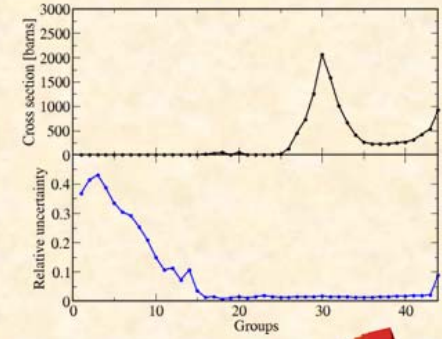
Methodology to Convert File 32 to File 33

ENDF File Structure

File 1: General information

File 2: Resonance parameters

File 3: Point-wise reaction cross sections

File 31: Data covariance for nu(bar)

File 32: Covariance data for resonance parameters

File 33: Data covariance for reaction cross sections

File 32 and File 33 affected in this work

STEP 1.

File 32 to File 33 conversion using PUFF-IV:
   a) Process File 32 only; ignore File 33
   b) Super Grid not collapsed to User Grid!

Output: Group-wise covariance matrix (coverx format) on a super grid

File 2 header: ^{233}U

LRU=1, [1e-5eV, 600eV]

LRU=2, [600eV, 40keV]

File 32 header: ^{233}U

LRU=1, [1e-5 eV, 600eV]

LRU=2, [600eV, 40keV]

Schematic User grid

1eV   1000eV   2e+7eV

File 2 grid

1e-5eV   600eV   40keV

File 32 grid

1e-5eV   600eV   40keV

Combine with User grid to form Super grid

Super grid

1eV   600eV   1000eV   40keV   2e+7eV
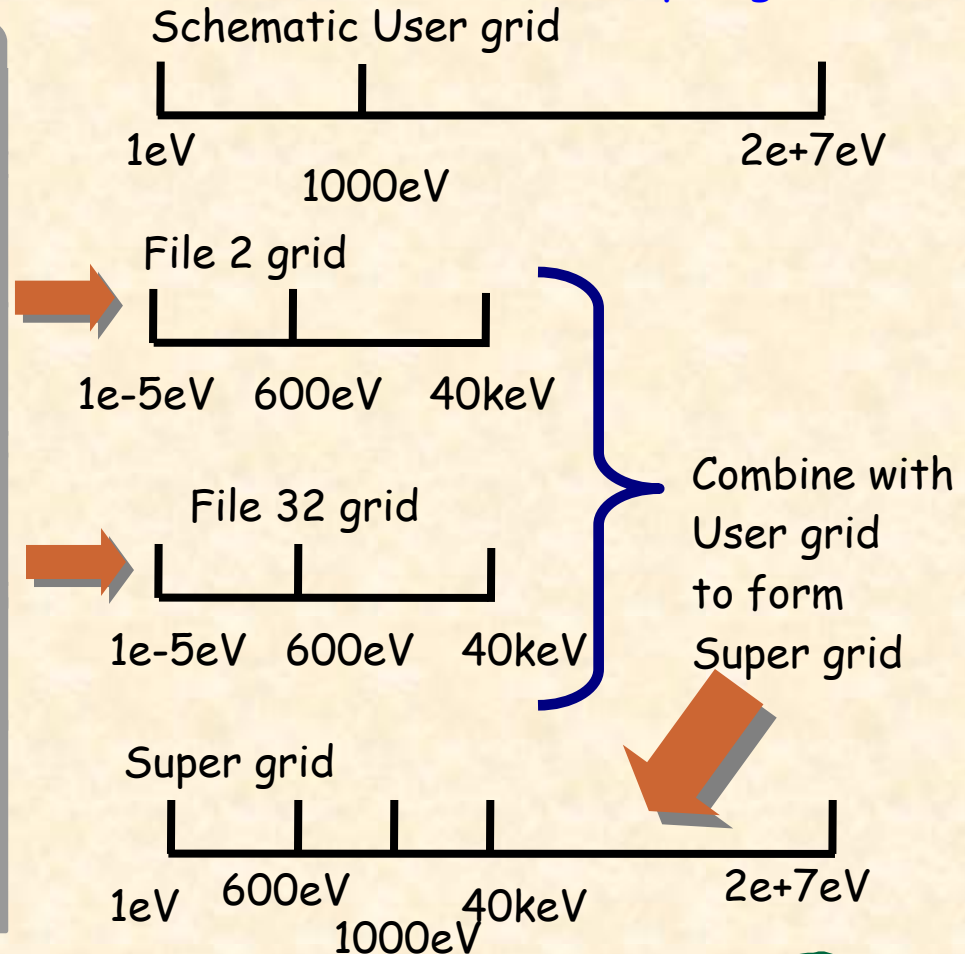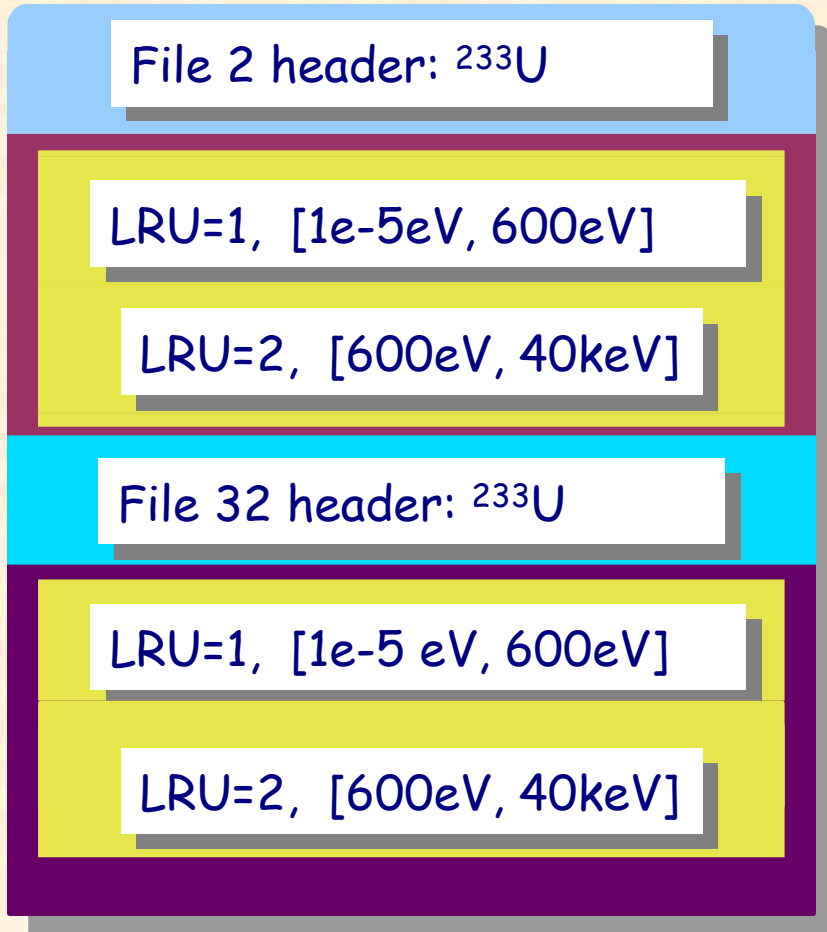
STEP 2.

Convert Coverx file obtained in STEP 1 into File 33 format (COVCONV):

   a) For each matrix in Coverx file, the COVCONV module
       - converts it to File 33 format (LB=5 full matrix)
       - appends it to the prior High-Energy File 33

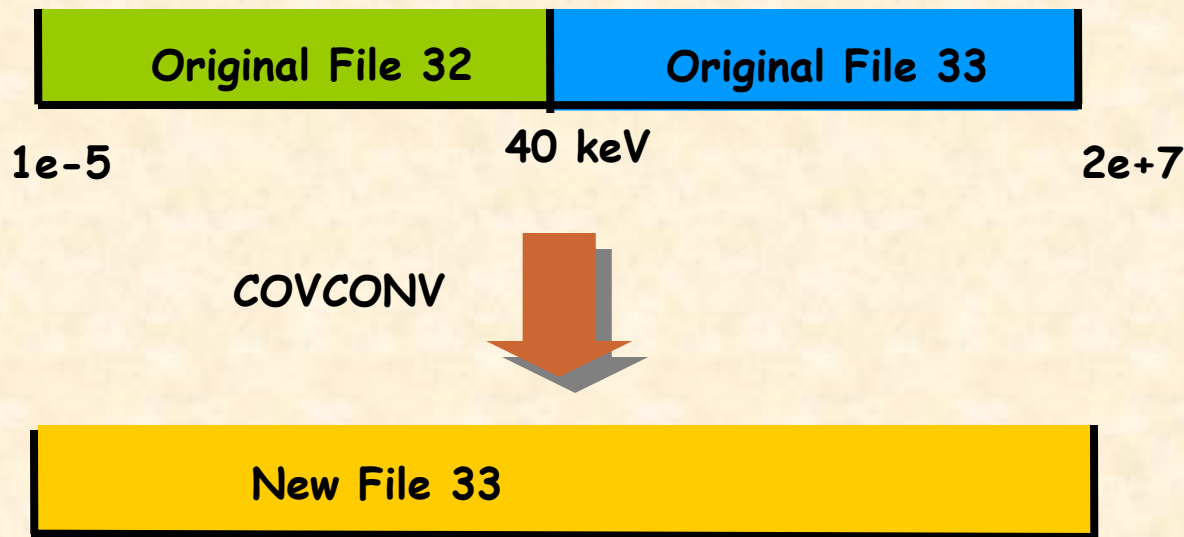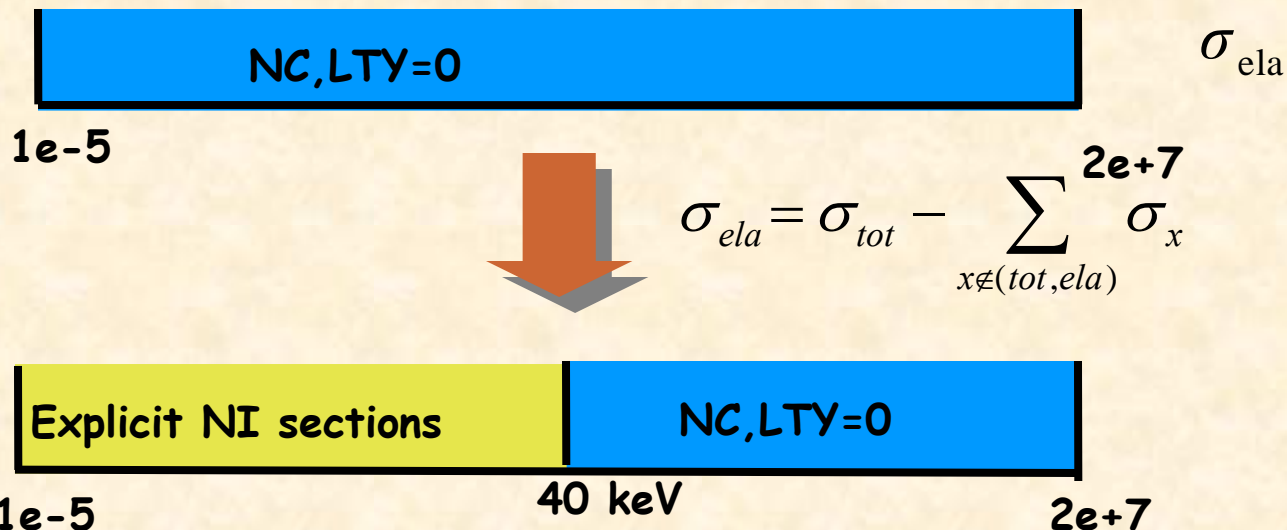Finally, manually delete File 32 and replace the original File 33
    with the one above

^{233}U has an NC File 33 Section with LTY=0 for elastic c.s.

- Loss of precision, due to a single precision ENDF and Coverx format, caused errors in computation of GWCM for the implicit (LTY=0) File 33 MT=2 section (elastic)

- Hence, MT=2 LTY=0 energy range was limited to high energy only, above 40 keV, and covariance matrix computed directly from ENDF parameters below 40 keV.

$$\sigma_{ela} = \sigma_{tot} - \sum_{x \notin (tot, ela)} \sigma_x$$

| NC,LTY=0 | σ_{ela} |

1e-5

$$\sigma_{ela} = \sigma_{tot} - \sum_{x \notin (tot, ela)}^{2e+7} \sigma_x$$

| Explicit NI sections | NC,LTY=0 |

1e-5   40 keV   2e+7

AMPX Nuclear Data for SCALE

- ## Cross-Section Processing Updates
  - POLIDENT module that generates CE cross-sections from resonance parameters was updated to Fortran 90.
  - Updated POLIDENT to handle LRF=7—testing showed excellent agreement with SAMMY results

- ## Library generation and testing activities
  - Continuous-energy ENDF/B-VI.7, VI.8, and VII.0 neutron libraries for CE-KENO in SCALE 6—testing in progress
  - Coupled neutron-gamma shielding library (200n-44g) based on ENDF/B-VI.8
    - MONACO: New Monte Carlo shielding code in SCALE 6
    - Initiated library testing
  - Comprehensive recommended covariance data library prepared for SCALE 5.1 and SCALE 6
    - Use evaluated covariance data where possible—includes new ^{235}U, ^{238}U, and ^{239}Pu covariance data
    - ORNL low-energy low-fidelity covariance data
  - PUFF-IV used to prepare 15-group ^{235}U, ^{238}U, and ^{239}Pu covariance data for WPEC SG26

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CE-KENO Library Development & Testing

➢ CE-KENO cross sections for all ENDF/B-VII.0 nuclides have been generated using AMPX

➢ CE-KENO V.a and CE-KENO-VI as well as the AMPX-generated continuous energy cross sections are being tested extensively with benchmark problems

➢ Integration of CE and MG transport into single KENO code package along with improved computational efficiency improvements

➢ Release with SCALE 6 in 2008

- CE-KENO ENDF/B-VI.7   ▲ CE-KENO ENDF/B-VII.0

Case Number
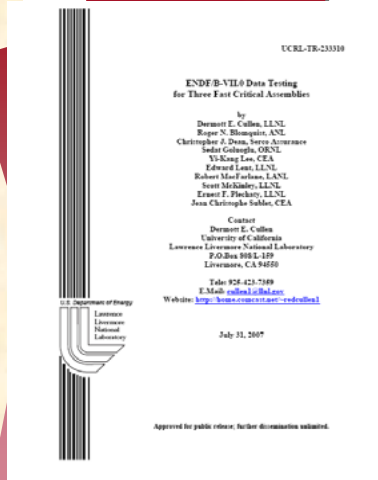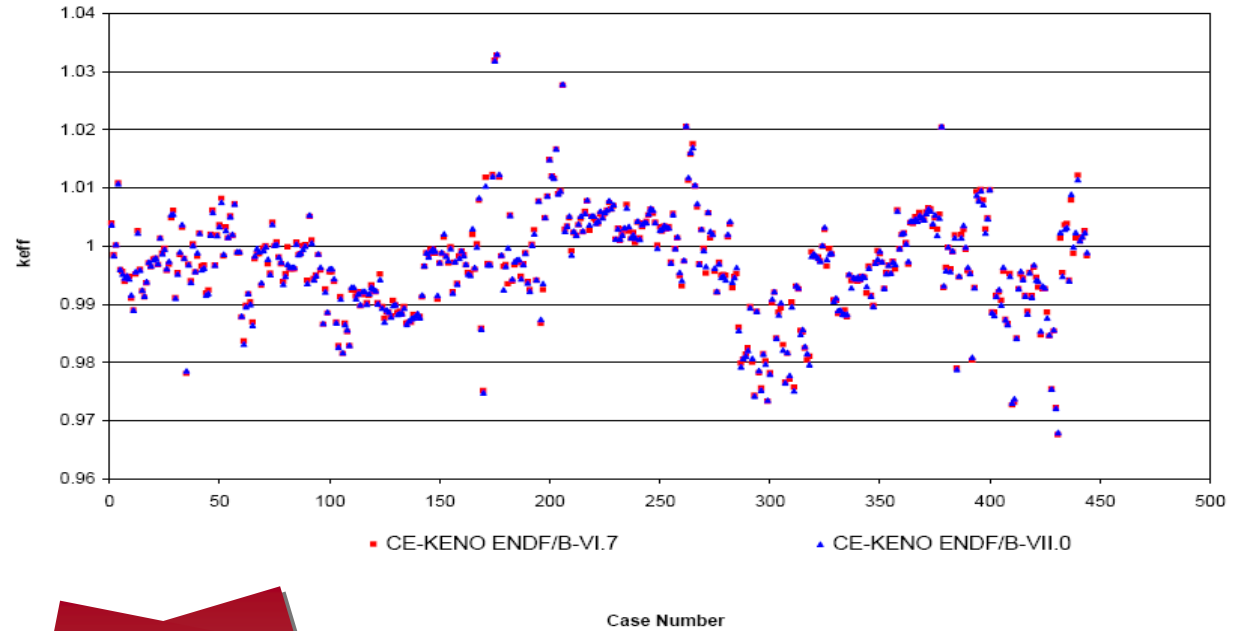
Summary of K-eff Results using ENDF/B-VII.0 data and Many Transport Codes			
	Godiva	Jezebel	Jezebel23
MCNP	0.99985	0.99986	0.99964
TART	1.00019	1.00010	0.99983
COG	1.00057	1.00010	0.99986
TRIPOLI (Sublet)	1.00024	0.99991	0.99979
TRIPOLI (Lee 1)	1.00015	1.00003	0.99978
TRIPOLI (Lee 2)	1.00023	1.00006	0.99981
CE-KENO	0.99971	0.99960	0.99938
VIM	1.00032	1.00011	0.99981
MERCURY	1.00024	1.00071	1.00048
MONK	1.00056	1.00066	1.00086
AMTRAN (Sn)			
ARDRA (Sn)			
MC2000			
MCU			
MVP			
WIMS			