Proposed format modifications in the resonance region

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Topics to be covered

- **File 32, LRU = 1, LCOMP = 1, LRF = 7**

- **File 32, LRU = 1, LCOMP = 2, number of digits**

- **Ambiguity with respect to File 32**

- **Documentation**

- **SAMMY manual**

File 32 LRU=1 LCOMP=1 LRF=7

- **Translation**
  - **File 32 ➜ Resonance parameter covariance matrix**
  - **LRU = 1 ➜ resolved resonance region**
  - **LCOMP = 1 ➜ the "usual" covariance format, printing individual matrix elements**
  - **LRF = 7 ➜ "R matrix limited" format**

- **Why now?**
  - **Oversight on my part: This format should have been included in ~~last year's~~ proposal for LRF = 7 for File 2**

    2004's

File 32 LCOMP=1 LRF=7, continued

- **Details are contained in draft pages for ENDF-102**
  - **Necessarily different from LRF = 3, because spin groups may have different numbers of channels**

- **Implemented in SAMMY and in PUFF/AMPX**
  - **Needed also in ERRORJ/NJOY**

File 32 LRU=1 LCOMP=2

- **Translation**
  - **File 32 ➜ Resonance parameter covariance matrix**
  - **LRU = 1 ➜ resolved resonance region**
  - **LCOMP = 2 ➜ compact format**
    - **Uncertainties plus 2-digit signed integer correlation coefficients**

- **Proposed modification**
  - **N-digit, where N = 2, 3, 4, 5, 6**
    - **N = 2 is default**

File 32 LRU=1 LCOMP=2, continued

Table on next slide illustrates the savings

- **Why needed**

  - **The compact format is a relatively crude approximation that saves significant file space**

  - **Sometimes, 2 digits are not enough to accurately characterize a covariance matrix**

    - **Use of more digits still saves file space but also provides greater accuracy**

- **Implementation requires only simple coding modifications**

  - **Documented in draft pages for ENDF-102**

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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

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File 32 ambiguity in ENDF-102

- **Convention is not specified in the manual**
  - **Covariance matrices are defined with respect to the exact parameter whose value is given in File 2, not with respect to the related physical parameter**

- **This is relevant for a partial width whose sign is negative …**

Ambiguity, continued

- **Convention for partial widths:** This convention *is* specified in ENDF-102

  - **Suppose γ is negative**

  - $\boldsymbol{\Gamma = 2P\, \gamma^2}$ **is positive**

  - **G = AΓ is written in File 2, where A = sign[γ]**

- **The covariance matrix is to be written with respect to G, not Γ**

  - **This convention is used in ERRORJ, PUFF, SAMMY, SAMRML, …**

  - **Modifications have been drafted for ENDF-102**

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A document in preparation

- **ORNL version of ENDF-102**

  - **Contains the pieces of ENDF-102 pertaining to the resolved resonance region**

    - **In particular, the pieces used in SAMMY & PUFF**

      - **Editorial comments relevant to SAMMY & PUFF are inserted in color**

    - **Eventually, may include unresolved region**

  - **Also contains examples for the various options**

- **Intended primarily for ORNL use, but will be made available on the web**

Document, continued

- **Why is this document needed?**
  - **SAMMY and PUFF users need current and correct versions of the formats**
    - **Mistakes will be corrected**
      - **We cannot guarantee that mistakes do not exist**
      - **We can guarantee that mistakes will be corrected when they are found**
  - **Examples will make the verbal descriptions easier to comprehend**

A document newly completed

- **The 7th revision of the SAMMY manual is now available** without export controls!
  - **Latest version of the code will soon be available from RSICC**

- **Download the manual from http://www.ornl.gov/sci/nuclear_science_technology/nuclear_data/sammy/**