united nations
educational, scientific
and cultural
organization

international atomic
energy agency

the
abdus salam
international centre for theoretical physics

ICTP 40th Anniversary

SMR.1555 - 34

Workshop on
Nuclear Reaction Data and Nuclear Reactors:
Physics, Design and Safety

16 February - 12 March 2004

Introduction to Nuclear Data

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AUSTRIA

Nuclear Reaction Data for Nuclear Reactors – Physics, Design & Safety

Part-2:

- Data evaluation
- File assembly
- Processing
- Verification & validation

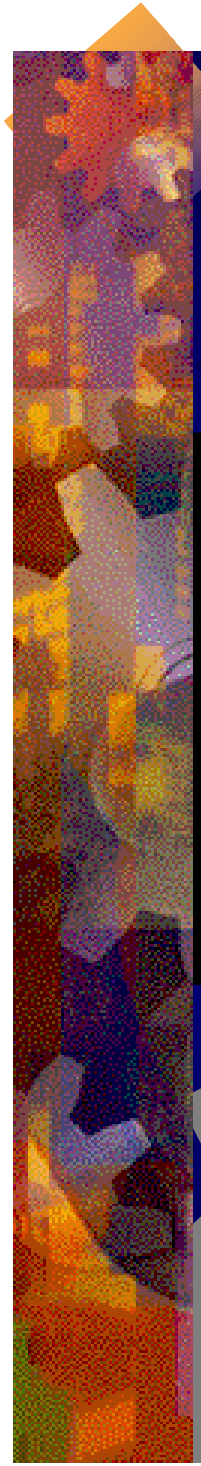
Director:

- Andrej Trkov

Lecturers:

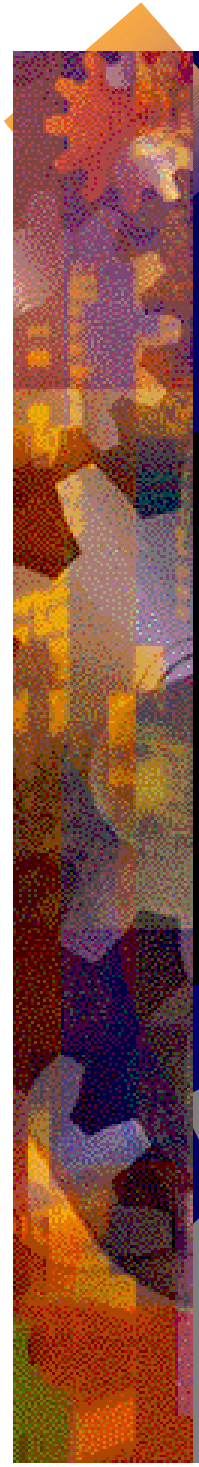
- Otto Schwerer
- Andrej Trkov
- Les Hutton
- Ivo Kodeli

ICTP Trieste, 16 February – 12 March 2004



Overview of Part-2

- **Purpose:** Describe the processes:
  - Data measurements and calculations
  - Evaluation and file assembly
  - Data processing (definitions)
  - File verification and validation
  - Applications
- **Topics**
  - Services from the IAEA
  - ENDF-6 format
  - Data processing, file assembly and verification
  - Codes: **NJOY**, (PrePro, ENDF Util., etc.)



From Basic Nuclear Data to Applications

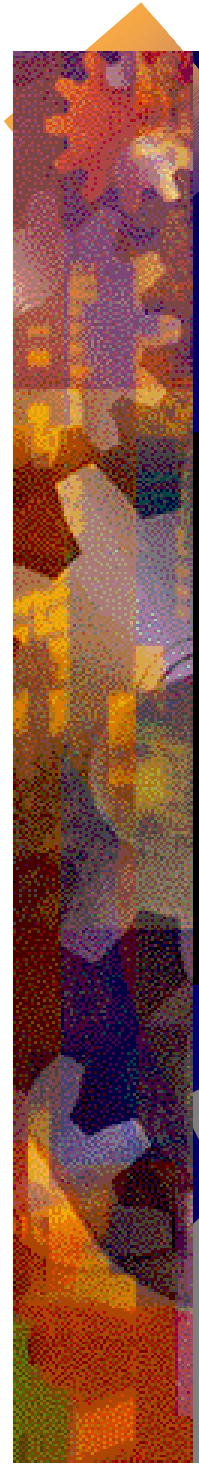
Andrej Trkov

International Atomic Energy Agency

Nuclear Data Section

Vienna - AUSTRIA

ICTP Trieste, 16 February – 12 March 2004



Introduction

- **Activities**
  - Basic nuclear data production
  - Evaluation & file assembly
  - Processing, verification & validation
  - Applications
- **Nuclear data types**
  - Integral
  - Differential
  - Processed $\Rightarrow$ Data reduction

Nuclear Data Production

Experimental Measurements

- Integral cross sections
- Differential cross sections
- Benchmark experiments
  - Critical lattices
  - Flux/power distributions
  - Reaction rates
  - Spectra

Calculations

- Nuclear model codes

Examples:

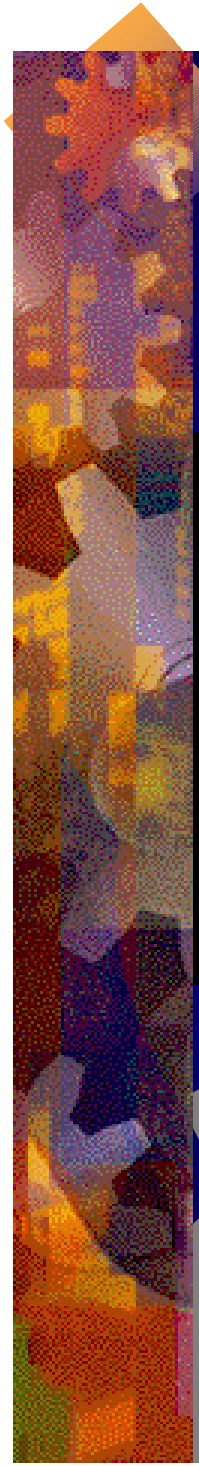
Criticality safety benchmark experiments

SINBAD shielding benchmarks database

Nuclear Data Production

Demand for new data

- Non-existence of data - New applications (medical, astrophysics, ADS, etc.)
- Discrepancies in measurements
- Deficiencies revealed in integral tests
- Large uncertainties - Availability of improved apparatus or experimental techniques



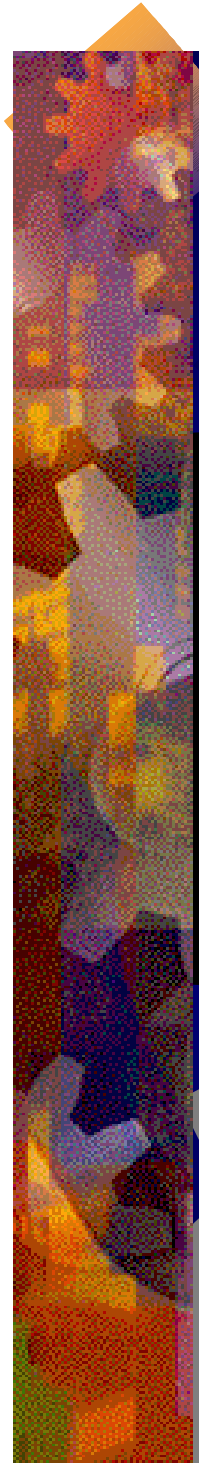
Nuclear Data Production

Nuclear Data Centres

- **NNDC** USA and Canada (Brookhaven)
- **CJD** Russia and former USSR (Obninsk)
- **NEA** West Europe & Japan (Paris)
- **IAEA** Other (Vienna)

Database Formats

- **CINDA** Index of references
- **EXFOR** Experimental data



Nuclear Data Evaluation

Procedures

- Data selection
- Statistical averaging of experimental data
- Fitting of parameters (resonance range)
- Use of theoretical models
- Formatting

Nuclear Data Evaluation

Formats

- **UKNDL U.K. (obsolete)**
- **KEDAK Germany (obsolete)**
- **ENDF-4 U.S.**
- **ENDF-5 U.S.**
- **ENDF-6 U.S. - generally accepted**
  Also adopted for
  ENDF/B-VII (expected in 2005)

Nuclear Data Evaluation

Format Selection

ENDF-6

- Documented
- Widely used
  - Software support
  - Data Exchange
- Large existing database
  - Freely available

Other

- Not defined or
- Not documented or
- Not generally accepted

Nuclear Data Evaluation

Recently Released Libraries

BROND-2.2	Russia
CENDL-2.1	China
ENDF/B-VI Rev.8	U.S.A.
JEF-3.0	Europe
JENDL-3.3	Japan

Announced:

CENDL-3	China
BROND-3	Russia
ENDF/B-VII (2005)	U.S.A.

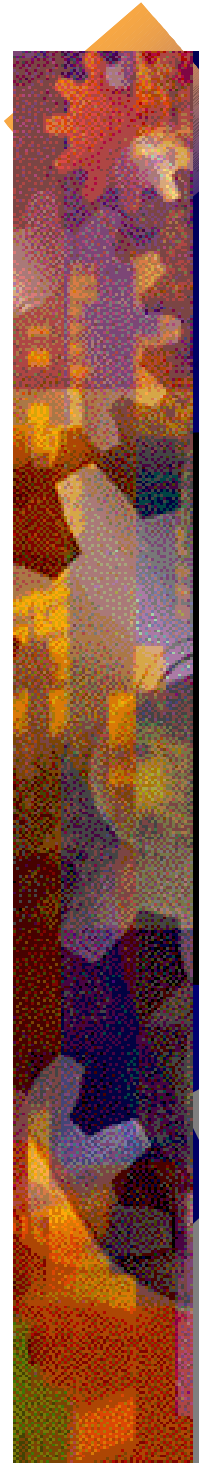
Note: All libraries are in ENDF-6 format

Nuclear Data Processing

Purpose

- **Data verification with respect to**
  - format
  - internal consistency
  - comparison with measured data
- **Validation**
  - Benchmark experiments
- **Applications**
  - Preparation of libraries for applications

Nuclear Data Processing



Data Verification

- Formatting errors
- Internal consistency
- Visual inspection (graphical display)
- Comparison with other evaluations for same material reactions
- Comparison with experimental data
- Comparison with measured integral cross sections (requires partial processing)

Nuclear Data Processing

Data Validation

Modelling of integral benchmark experiments

Benchmark databases (examples):

- **SINBAD (shielding)**
- **ICSBEP (criticality safety)**

Links for further information:

- **http://www-rsicc.ornl.gov/rsicc.html**
- **http://www.nea.fr/**

Processing into test applications libraries

Nuclear Data Processing

Applications

- Multigroup data libraries (energy grid strongly application-dependent)
- Data libraries for continuous-energy Monte-Carlo calculations

Nuclear Data Processing

Data Verification tools

- ENDF Utility Codes
- ENDF Pre-Processing Codes PrePro2000
- ENDF verification support package ENDVER

Data Validation

- Preliminary processing into an application library using production codes NJOY
- Analysis of benchmark experiments
  (Monte Carlo, deterministic, sensitivity analysis…)

Application

- Full library processing
- Rigorous benchmarking

Nuclear Data Processing

Selection of Processing Codes

State-of-the-Art

- (-) Possibly restricted
- (+) Constantly updated
  - Removing bugs
  - Format extensions
  - New features

Other

- Incomplete ?
  - Not all data types processed
- Obsolete ?
  - Not upgraded for ENDF-6 format
- Unverified ?

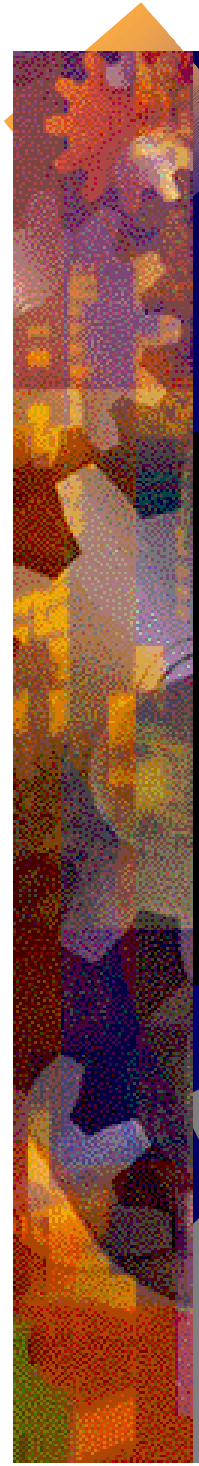
Nuclear Data Classification

- **Basic nuclear data**
- **Evaluated nuclear data files**
- **Processed nuclear data**
  - **Change of data representation**
  - **Reformatting**
  - **Group averaging (preparation of multigroup constants)**
    - ⇒ **Data Reduction**

Nuclear Data Classification

Group averaged nuclear data

- **Problem independent group constants (> 600 groups)**
- **Multigroup constants (26-400 groups)**
- **Problem dependent few-group constants (1 to 18 groups, macroscopic, spatially averaged)**



Group averaged nuclear data

Data Reduction Techniques:

- Averaging w.r.t. energy
- Averaging w.r.t. space

Applying the principle of

reaction rate conservation

Group averaged data – Definitions

Reaction Rates

$$s_g j_g = \int_g s(E).j(E)dE$$

Average Cross Sections

$$j_g = \int_g j(E)dE$$

$$s_g = \frac{\int_g s(E)j(E)dE}{\int_g j(E)dE}$$

Scattering Matrices

$$s_{(l)g\to h} = \frac{\int_{-1}^{1} dm \int_g dE.j(E) \int_h dE'.s\left(E \to E', m\right).P_l(m)}{\int_g j(E).dE}$$

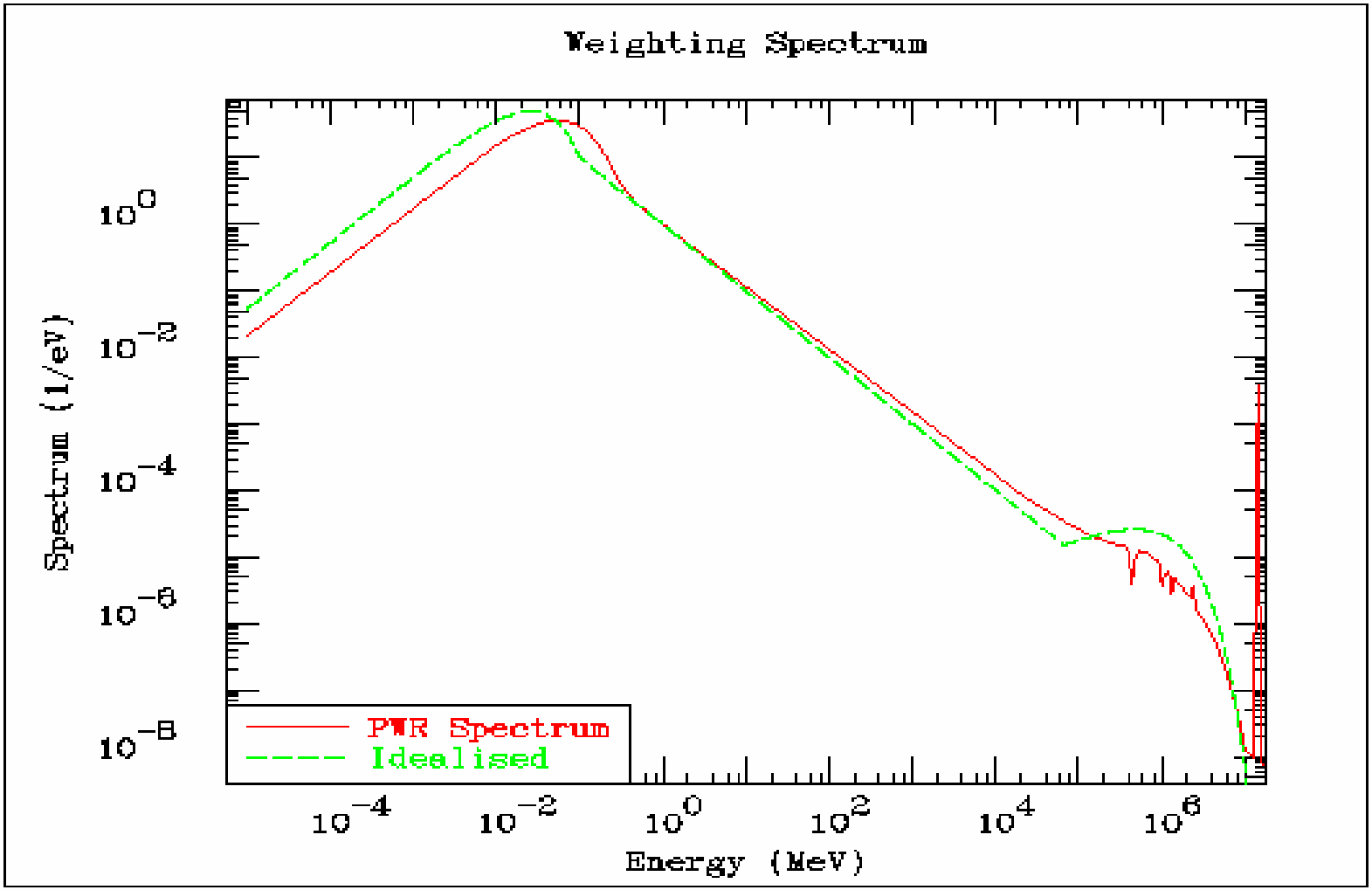
Group averaged nuclear data - Definitions

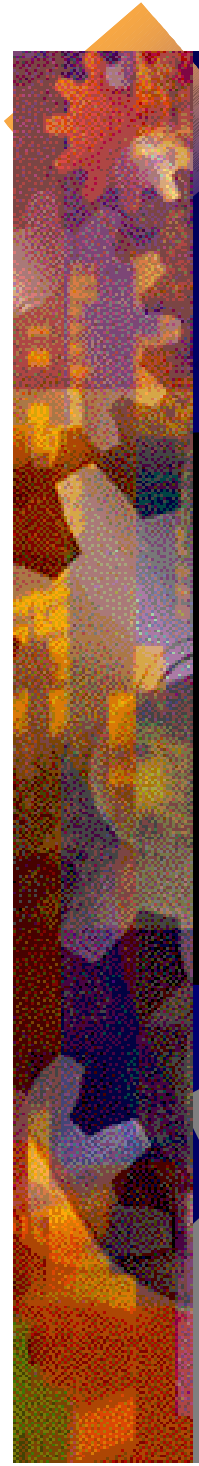
Resonance Range - Neutron Balance

$$S(E) = \Sigma_t(E).j^*(E) \qquad S = \Sigma_m j(E)$$

Intermediate Resonance Approximation

$$j^*(E) = \frac{s_o + l s_p(E)}{s_o + l s_a(E) + s_s(E)} . j(E)$$

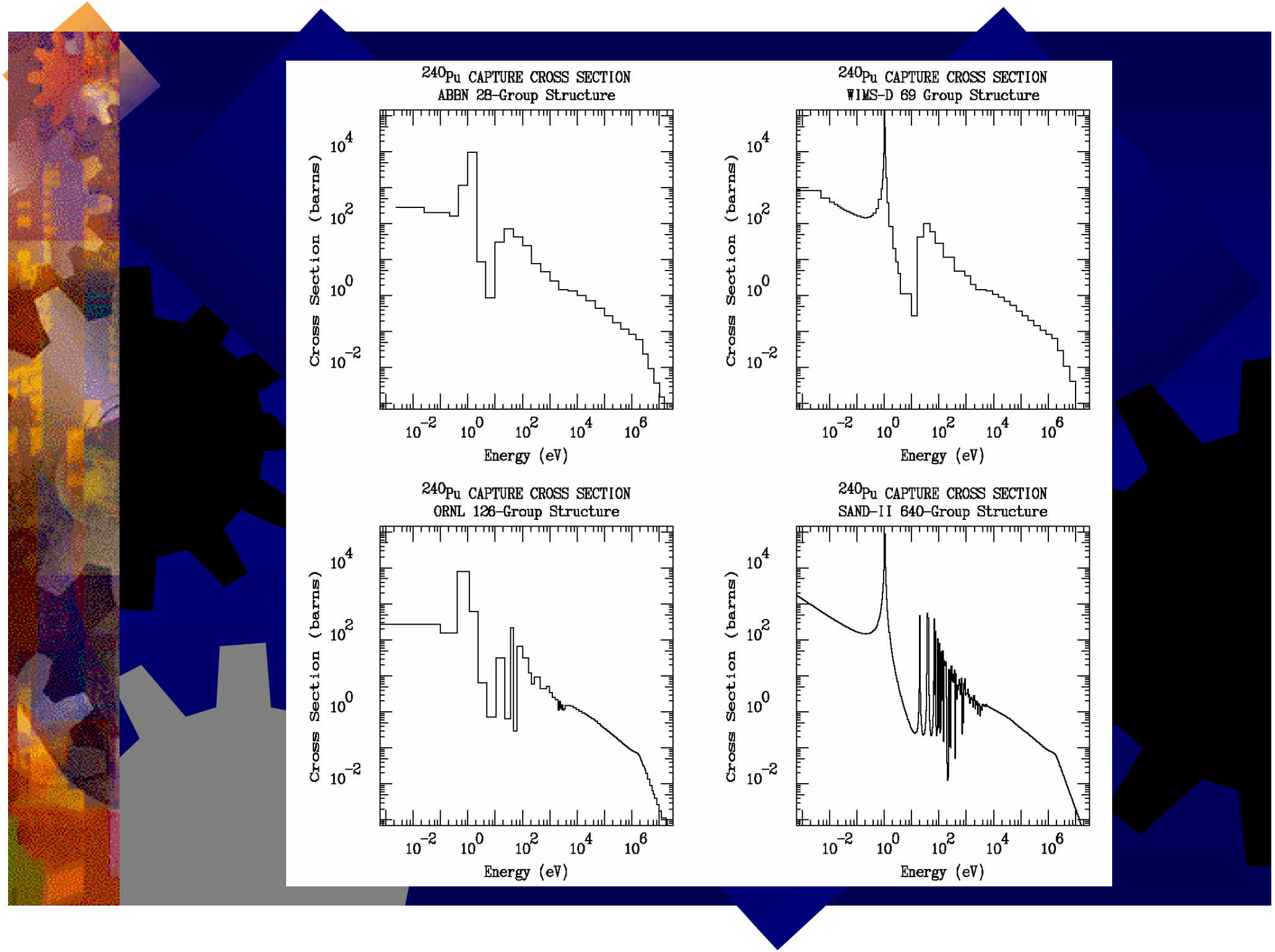

Weighting Spectrum
Spectrum (1/eV)
10^{0}
10^{-2}
10^{-4}
10^{-6}
10^{-8}
PWR Spectrum
Idealised
10^{-4}
10^{-2}
10^{0}
10^{2}
10^{4}
10^{6}
Energy (MeV)



Group averaged nuclear data - Definitions

Multigroup Data – Application dependent

- Thermal reactors
- Fast reactors
- Shielding
- Fusion devices
- Accelerator applications
- etc.


240Pu CAPTURE CROSS SECTION
ABBN 28-Group Structure
Cross Section (barns)
Energy (eV)
240Pu CAPTURE CROSS SECTION
WIMS-D 69 Group Structure
Cross Section (barns)
Energy (eV)
240Pu CAPTURE CROSS SECTION
ORNL 126-Group Structure
Cross Section (barns)
Energy (eV)
240Pu CAPTURE CROSS SECTION
SAND-II 640-Group Structure
Cross Section (barns)
Energy (eV)

Group averaged nuclear data - Definitions

Homogenization (problem dependent)

Reaction Rate

$$\langle \Sigma_g \rangle \langle f_g \rangle = \int_V \Sigma(\vec{r}) f(\vec{r}) dV$$

Average Flux and Cross Section

$$\langle f_g \rangle = \int_V f(\vec{r}) dV$$

$$\langle \Sigma_g \rangle = \frac{\int_V s(\vec{r}) f(\vec{r}) dV}{\int_V f(\vec{r}) dV}$$

Processed data files

Derived ENDF files

- Cross section reconstruction from resonance parameters
- Doppler broadening
- Internal format conversion (→ ENDF)

Reformatted files

- Format simplifications for more compact representation
  (e.g.: ACE = A Compact ENDF)

Summary

Nuclear Data Activities

- Basic nuclear Data Production
- Evaluation
- Processing (verification, validation)
- Application (benchmarking)

Data Clasification

- Basic nuclear Data
- Evaluated Nuclear Data
- Processed data (derived files)
- Averaged Data (energy/space)
  - Problem independent
  - Multigroup
  - Few-group (space averaged)


Selected topics
Data for Monte Carlo Codes
Data for Lattice Transport Codes
Data file Assembly and Verification

Data for Monte Carlo Codes (ACE)

- ACE = A Compact ENDF
- Continuous energy cross sections (i.e. no data reduction is necessary in principle)
- Cross sections given on a “union grid”
- “Thinning” of differential data
- Restrictions on representation of correlated energy/angle distributions (format conversion necessary)
- Single temperature in one library
- Not all ENDF file information transferred to ACE

Ace File Structure

- ASCII file
- Intermixed characters (C), integer pointer indices (I) and data (X)
- Indices point to other index tables or data
- Format designed for efficient reading and compactness
- “Eye reading” very difficult

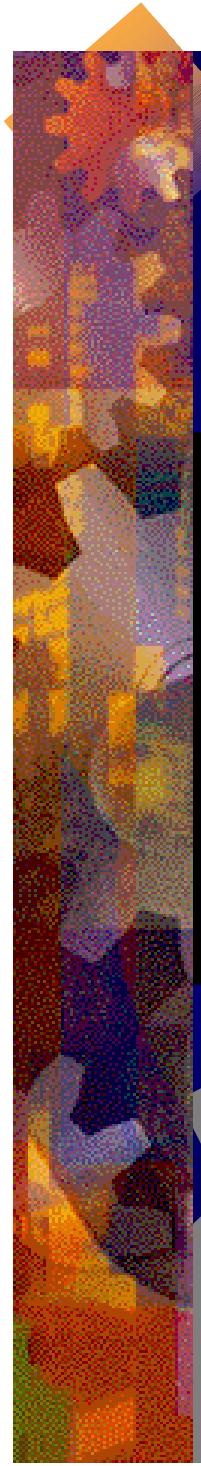
```
C  X  X  C
Comment
IX  IX  IX  IX
...
II  II  II  II
...
X   X   X   X
X   X   X   X
...
I   I   I   I
...
I   X   X   X
X   X ...
X   I   X   X
...
X   X   X   X
X   X   I ...
```

Data for Lattice Transport Codes (WIMS-D)

- Multigroup data representation with emphasis on thermal energy range
- Temperature-dependent thermal scattering data
- Resonance integral tables for fission yield and absorption (no scattering) for selected nuclides (fuel only); tabulation w.r.t. background cross section and temperature
- Single fission spectrum
- Restrictions on decay and capture branching
- P1 scattering for leakage only (4 materials only)

WIMS-D Library Update Project

- Completed in 2003
- Available on CD-ROM or web http://www-nds.iaea.org/wimsd/
- WIMSD-IAEA-69 and WIMSD-IAEA-172 (69- and 172-group libraries)
- (By-product: equivalent libraries based on JEF-2.2, JENDL-3.2, ENDF/B-VI.8)
- Benchmarked on > 200 test cases
- Draft documentation available, TECDOC in preparation



ENDF Data File Assembly Verification and Validation

Data to be assembled

- Task requirements
- Codes

File verification

- Requirements
- Codes

Data validation

- Processing and verification
- Benchmarking

ENDF Data File Assembly Verification and Validation

Make use of available codes:

- **ENDF Utility Codes**
- **ENDF Pre-Processing Codes PrePro2000**
- **ENDF verification support package ENDVER**
- **Various small utilities (Evaluators' tools)**
- **Production codes NJOY**

File Assembly

Data to be assembled

- Resonance parameters (up to ~keV region)
- Nuclear model code results (above ~keV)
- Results of statistical averaging of experimental data

File Assembly (cont.)

Examples of data operations:

- **Extract sections of ENDF data (e.g. cross sections in 2-column format)**
- **Manipulate extracted cross sections**
- **Insert partial data sections into ENDF blocks (e.g. replacement of cross sections over a limited E-range)**
- **Merge/replace complete sections in an ENDF file.**

File Assembly (cont.)

Evaluators' tools (examples)

- ENDTAB extracts from ENDF file selected cross sections over specified energy range with output in 2-column format.
- FLUCTU performs various operations on data in 2-column format
- EDENDF edits ENDF cross sections in a given energy range from data in 2-column format
- DDXTHR corrects thresholds of MF4, MF6 data in an ENDF file …
- GRUPINT calculates integral parameters.

File Assembly (cont.)

Standard Codes: Pre-Pro

- LINEAR, RECENT basic tools from the Pre-Pro series.
- MERGER extracts/inserts complete sections in an ENDF file.
- FIXUP has useful checking functions.
- DICTION can generate the dictionary section in file MF1.
- EVALPLOT displays the contents of an ENDF file.
- COMPLOT compares two ENDF files.

File Assembly (cont.)

Standard Codes: ENDF Utility Codes

- CHECKR checks file formal correctness.
- FIZCON makes simple checks of physical consistency.
- PSYCHE makes advanced checks of physical consistency.
- STANEF makes uniform appearance of numbers, generates dictionary section, etc.

Running ENDF utility codes is ESSENTIAL before release of any partial or complete ENDF file!

File Verification

Checking sequence (example):

- **Check format and internal consistency**
- **Compare with starter file (if applicable).**
- **Compare with other evaluations.**
- **Compare against experimental data.**
- **Compare simple (integral) parameters**
  - **Thermal cross sections**
  - **Resonance integrals**
  - **Fiss.spect.aver. cross sections**
  - **14 MeV cross sect. values, etc.**

Be careful about definitions!

File Verification (cont.)

Checking procedure (example):

- Run CHECKR, FIZCON, PSYCHE on the new file.
- Run LINEAR, RECENT, FIXUP for additional messages (-ve x-sect., thresholds, etc.).
- Run COMPLOT comparing outputs of RECENT and FIXUP to check redundant cross sections.
- Run COMPLOT to compare new file with the starter.
- Run COMPLOT to compare new file with other evaluations.

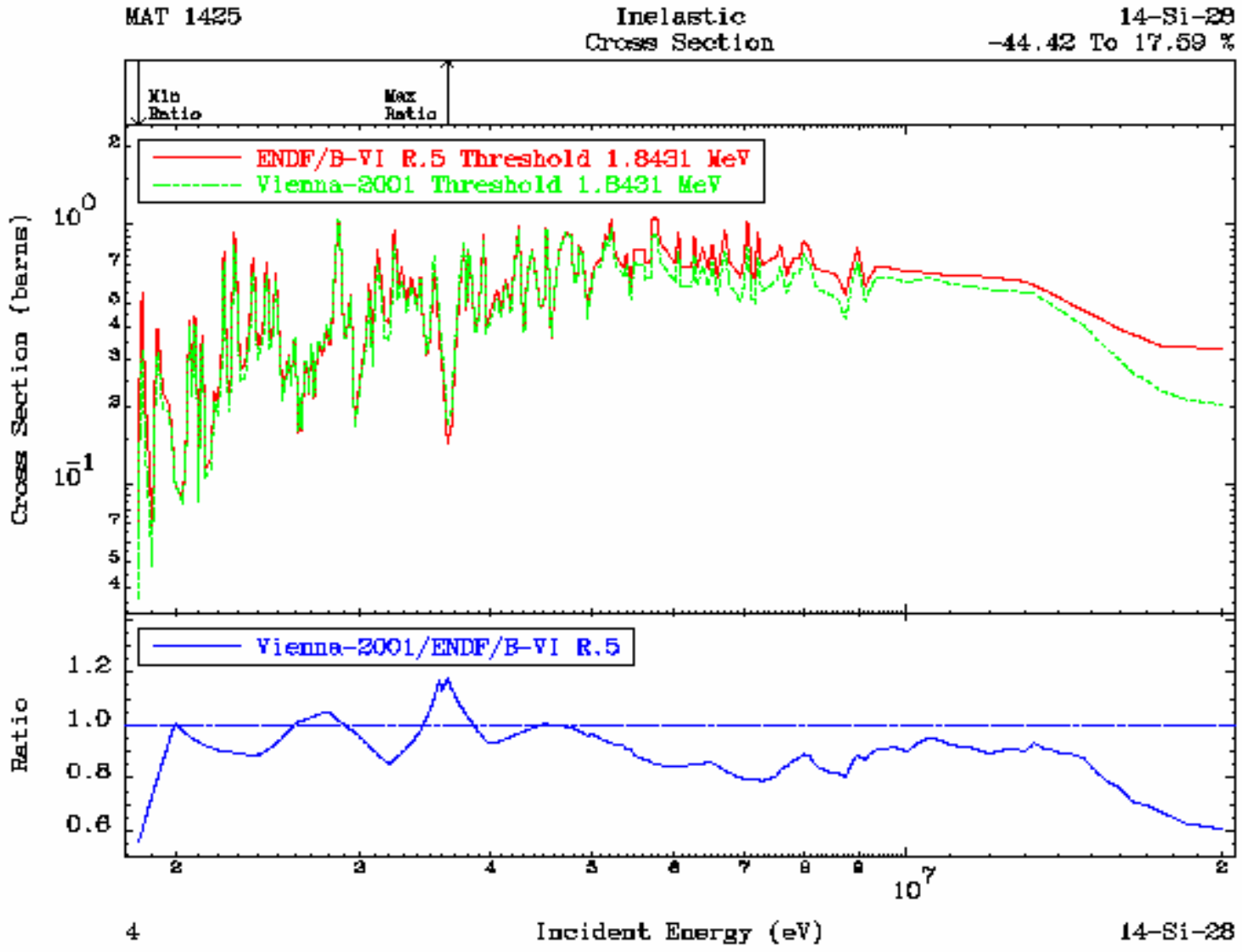
File Verification (cont.)

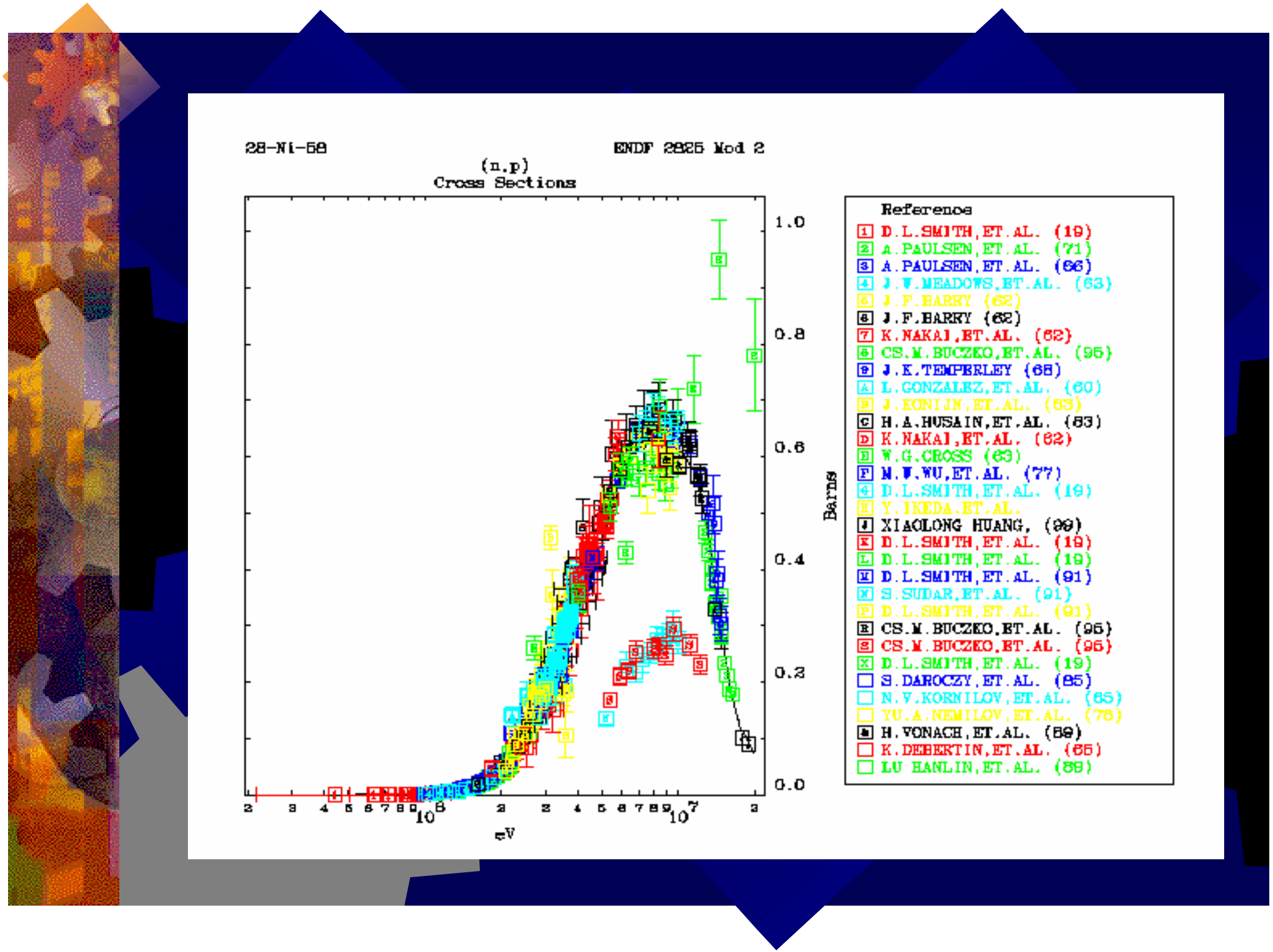
Checking procedure (example):

- Make EXFOR retrieval and run ENDVER codes to compare (LINEAR, RECENT, SIGMA1 output) with measurements.

  WARNING: EXFOR entries require careful consideration and review!
- Run GRUPINT (on GROUPR output, 640 groups) to compare simple (integral) parameters with measurements (thermal cross sections, resonance integrals, etc.).

  WARNING: Be careful about definitions!


MAT 1425
Inelastic
Cross Section
14-Si-28
-44.42 To 17.59 %
Min Ratio
Max Ratio
ENDF/B-VI R.5 Threshold 1.8431 MeV
Vienna-2001 Threshold 1.8431 MeV
Cross Section (barns)
Vienna-2001/ENDF/B-VI R.5
Ratio
Incident Energy (eV)
14-Si-28


28-Ni-58
ENDF 2825 Mod 2
(n,p)
Cross Sections
1.0
0.8
0.6
0.4
0.2
0.0
Barns
eV
Reference
D.L.SMITH,ET.AL. (19)
A.PAULSEN,ET.AL. (71)
A.PAULSEN,ET.AL. (66)
J.W.MEADOWS,ET.AL. (63)
J.F.BARRY (62)
J.F.BARRY (62)
K.NAKAI,ET.AL. (62)
CS.M.BUCZKO,ET.AL. (95)
J.K.TEMPERLEY (68)
L.GONZALEZ,ET.AL. (60)
J.KONIJN,ET.AL. (63)
H.A.HUSAIN,ET.AL. (63)
K.NAKAI,ET.AL. (62)
W.G.CROSS (63)
M.W.WU,ET.AL. (77)
D.L.SMITH,ET.AL. (19)
Y.IKEDA,ET.AL.
XIAOLONG HUANG, (99)
D.L.SMITH,ET.AL. (19)
D.L.SMITH,ET.AL. (19)
D.L.SMITH,ET.AL. (91)
S.SUDAR,ET.AL. (91)
D.L.SMITH,ET.AL. (91)
CS.M.BUCZKO,ET.AL. (95)
CS.M.BUCZKO,ET.AL. (95)
D.L.SMITH,ET.AL. (19)
S.DAROCZY,ET.AL. (85)
N.V.KORNILOV,ET.AL. (65)
YU.A.NEMILOV,ET.AL. (78)
H.VONACH,ET.AL. (89)
K.DEBERTIN,ET.AL. (65)
LU HANLIN,ET.AL. (89)

Data Validation

- **Processing into test applications libraries**
- **Verification of processed libraries**
- **Modelling of integral benchmark experiments**

Benchmark databases (examples):

- **SINBAD (shielding)**
- **ICSBEP (criticality safety)**

Links for further information:

- **http://www-rsicc.ornl.gov/rsic.html**
- **http://www.nea.fr/**

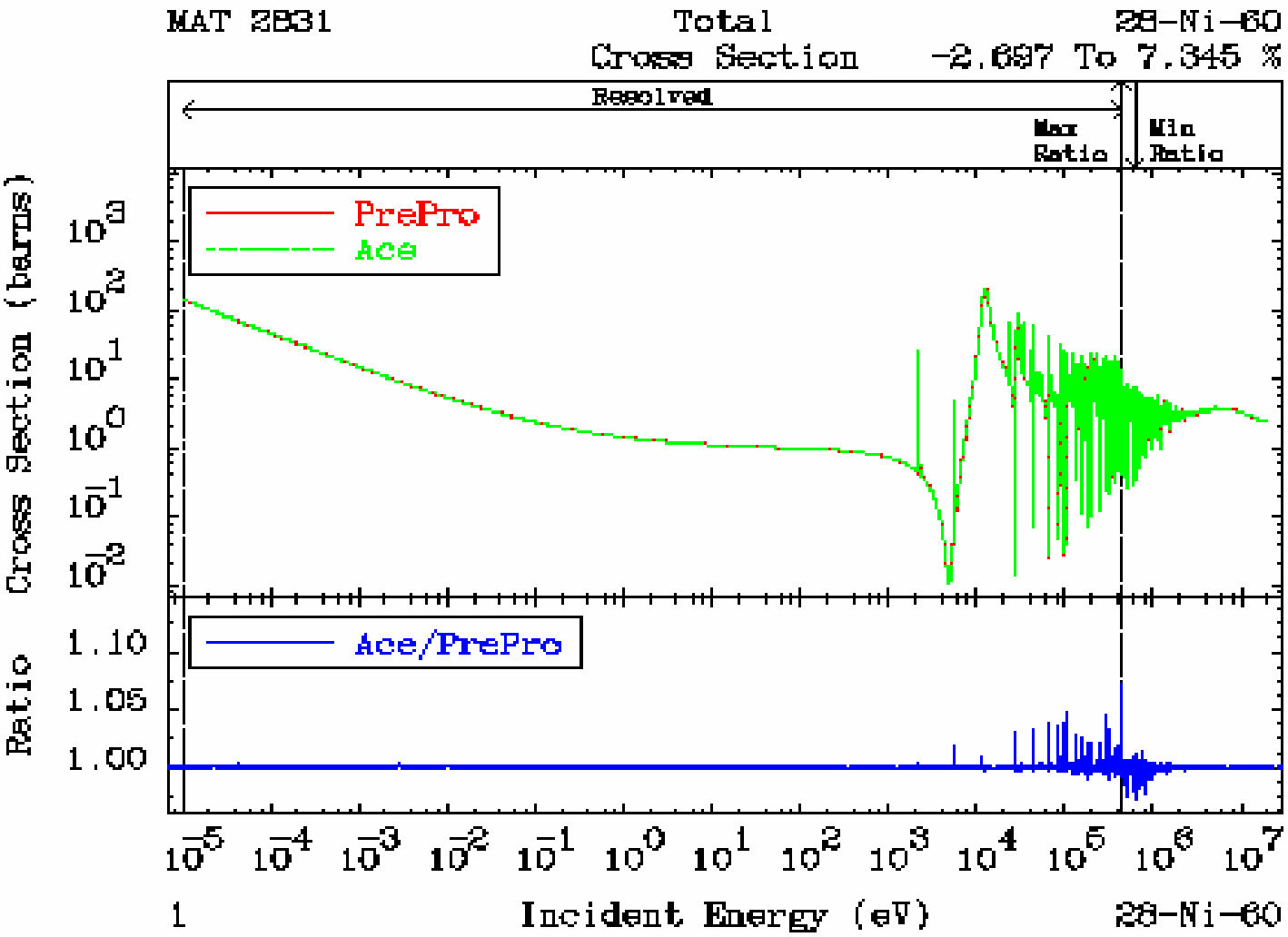
Data Validation (cont.)

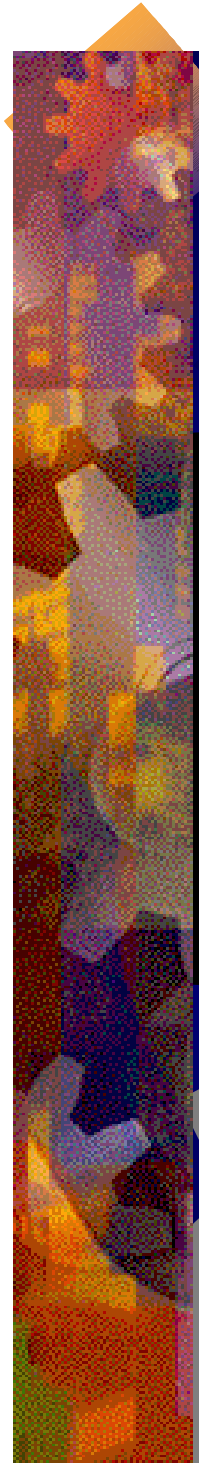
Processed library verification

(Ace library example)

- **Run Pre-Pro codes from the same source data to the same temperature.**
- **Convert Ace library to ENDF (using ACELST code).**
- **Compare Pre-Pro output with data converted from Ace (using COMPLOT).**

WARNING: Only cross sections are verified!


MAT 2831
Total
Cross Section
28-Ni-60
-2.697 To 7.345 %
Resolved
Max Ratio
Min Ratio
PrePro
Ace
Cross Section (barns)
Ace/PrePro
Ratio
Incident Energy (eV)
28-Ni-60



Summary

- File assembly, verification and validation
  - Data to be assembled
    - Task requirements
    - Codes
  - File verification
    - Requirements
    - Codes
  - Data validation
    - Processing and verification
    - Benchmarking