WPEC SG38 and GND: Designing a New Format for Storing Nuclear Data

Presented at P(ND)^2

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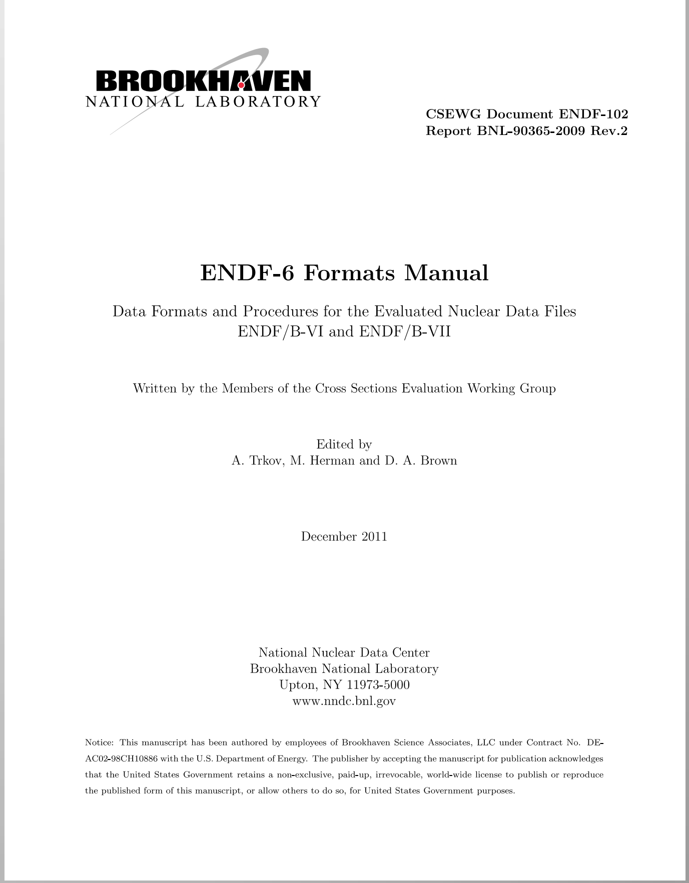
International collaboration (WPEC SG38) has been formed to design a new format for storing nuclear data, and to oversee the transition from ENDF-6 to the new format.

- Contents of this presentation:
  - Why is change needed?
  - How will it impact nuclear data evaluators and users?
  - What about infrastructure (processing, plotting etc.)?
  - Progress so far, and future work… and predictions!

Evaluated Nuclear Data condenses nuclear reaction theory and experimental data together into a set of recommended values.

- Includes cross sections, product multiplicities and distributions, covariances, etc.
- Stored in standard computer-readable form
  - Evaluated Nuclear Data Format (ENDF) has been that standard for nearly 50 years.



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CSEWG Document ENDF-102
Report BNL-90365-2009 Rev.2

ENDF-6 Formats Manual

Data Formats and Procedures for the Evaluated Nuclear Data Files
ENDF/B-VI and ENDF/B-VII

Written by the Members of the Cross Sections Evaluation Working Group

Edited by
A. Trkov, M. Herman and D. A. Brown

December 2011

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Why is change needed?
Reason #1: technical issues with ENDF-6.

- Hard precision limit: 11 digits including ‘.’, ‘+’, ‘-’, etc.

- Format is difficult to extend. The three digits allotted for reaction ids (MT numbers) are nearly used up.

- No standard way to store *processed* data, making code comparisons more difficult.

- My least-favorite line in the ENDF-6 format manual:
  - Section 6.2: “LIP: Product modifier flag. Its main use is to identify the isomeric state of a product nucleus… The exact meaning assigned to LIP should be explained in the File 1, MT=451 comments.”

Reason #2: ENDF-6 is hard to read. Bugs can and do lurk inside ENDF files undetected!

- ENDF-6 strongly influenced by punch-card origins:

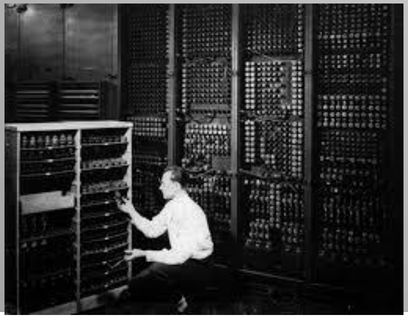
```
        ...
7.418400+4 1.823710+2          0          3         82          07437 6  5    1
1.000000+0 1.000000+0          0          1          1         457437 6  5    2
        45         2                                  7437 6  5    3
1.000000-5 0.000000+0 6.000000+6 0.000000+0 6.500000+6 9.700390-17437 6  5    4
        ...
1.150000+8 6.942060+0 1.300000+8 7.292060+0 1.500000+8 7.686070+07437 6  5   18
0.000000+0 0.000000+0          1          2          1         457437 6  5   19
        45        22                                  7437 6  5   20
0.000000+0 1.000000-5          0          0          4          27437 6  5   21
0.000000+0 2.000000+5 1.000000-5 0.000000+0                      7437 6  5   22
0.000000+0 6.000000+6          0          0          4          27437 6  5   23
0.000000+0 2.000000+5 1.000000-5 0.000000+0                      7437 6  5   24
        ...
```

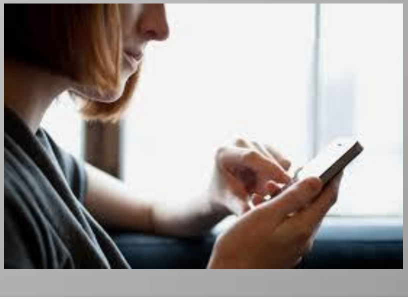
(Example is W184 from ENDF-VII.1, ~105K lines total)

- Not human-readable!
- Tools like FIZCON and PSYCHE are able to read and check ENDF files, yet errors continue to appear in evaluated libraries.

Reason #3: we need to recruit new talent to replace retiring nuclear data experts!

- New generation prefer to use modern software tools and practices.
  - Just continuing to use old format + old infrastructure will *not* ensure reliable nuclear data.
  - Instead, adapt to new methods... while comparing rigorously to old codes for quality assurance!





Goal: design structure that builds on strengths of ENDF-6 but is more flexible, human readable and compatible with modern tools!

- LLNL already has a candidate: Generalized Nuclear Data or GND.
- LLNL can’t be isolated: to replace ENDF, GND must become an international standard, allow easy data exchange anywhere!
- Thus WPEC SG38 is leading the effort to turn GND into the new standard.

ENDF B-VII.1

JAEA NDC

NEA NUCLEAR ENERGY AGENCY

GND organizes data in a hierarchy. Most data are stored inside ‘reaction’ elements:

```
<reaction label=“...” date=“...” ENDF_MT=“...”>
    <crossSection nativeData=“...”> ... </crossSection>
        <!-- options: linear, piecewise, resonancesWithBackground, ... -->
    <outputChannel name=“...”>
        <product name=“...” label=“...” >
            <distributions>...</distributions>
            <multiplicity>...</multiplicity></product>
        <product>...</product>
        ...
    </outputChannel>
</reaction>
```

color code:

element   attribute   comment

Reactions involving same target/projectile are collected together in a ‘reactionSuite’:

```
<reactionSuite projectile=“...” target=“...” version=“...” temperature=“..”>
    <styles> e.g. ‘evaluated’ or ‘processed’ </styles>
    <documentations> support ascii, html, etc.</documentations>
    <particles> ground state, levels, gammas ... </particles>
    <resonances> resolved and/or unresolved ... </resonances>
    <reaction>...</reaction>
    <reaction>...</reaction>
    ...
</reactionSuite>
```

color code:

element   attribute   comment

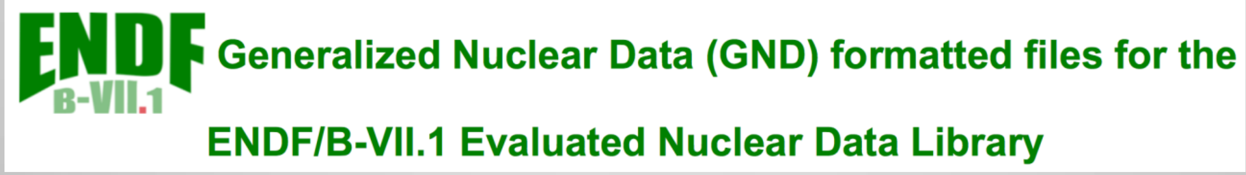
Make use of general-purpose low-level data containers

- Build on one of the strengths of ENDF-6: basic, flexible containers like ‘TAB1’ and ‘TAB2’
  - Capable of storing many different types of data
  - Support multi-dimensional data including interpolation rule(s)
- New containers should also support axis labels, units, etc.

```
<crossSection nativeData="linear">
 <linear xData="XYs" length="123" accuracy="0.001” interpolation="linear,linear">
  <axes>
   <axis index="0" label="energy_in" unit="eV”/>
   <axis index="1" label="crossSection" unit="b"/></axes>
  <data> 7894.169 0 8e3 0.03555347 9e3 0.2396638 ... </data></linear></crossSection>
```

GND-formatted data already accessible through data centers:

- ENDF-VII.1 available in GND from the NNDC:
  - http://www.nndc.bnl.gov/endf/b7.1/gndFiles.html



Generalized Nuclear Data (GND) formatted files for the ENDF/B-VII.1 Evaluated Nuclear Data Library

- Multiple libraries also available from IAEA NDS:
  - https://www-nds.iaea.org/exfor/servlet/E4sSearch2
  - To access, choose target/projectile, submit a search and then select the ‘extended’ button on results page

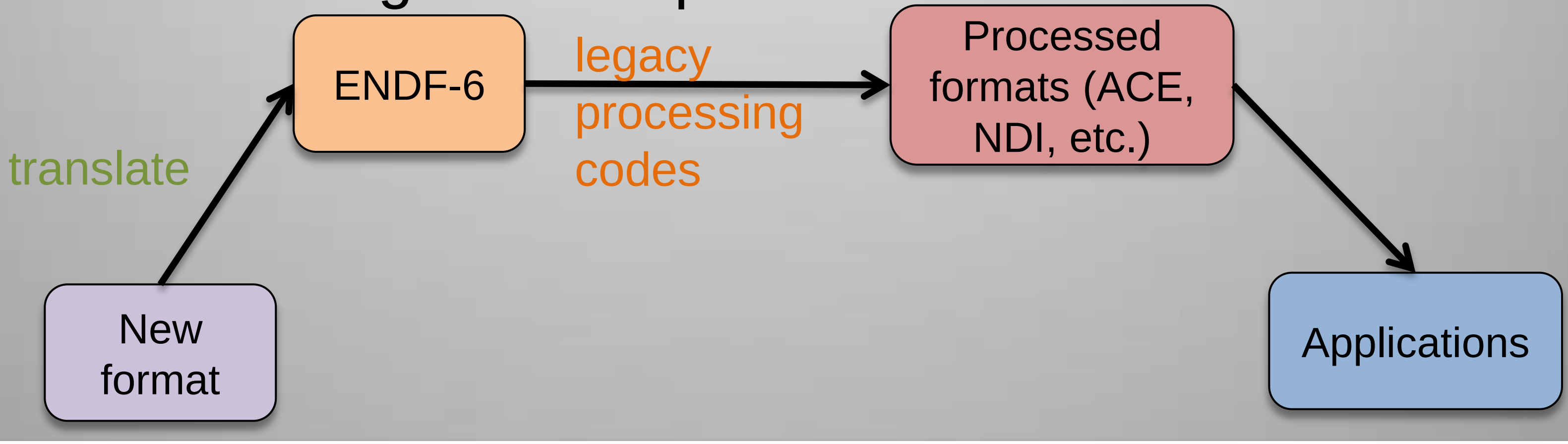
What will be the impact on nuclear data users?

- In the short term, not much impact: backwards-compatibility with ENDF-6 is an SG38 *requirement*
    - Support translating back to ENDF-6, or exporting directly to processed formats like ACE, NDI, etc.

- In longer term, applications codes should access data directly from new format.
    - Will facilitate exchanging data, comparing codes

Major goal for SG38: Support backwards compatibility with ENDF-6 as long as possible

- ENDF-6 and new format will need to co-exist for several years. This means:
  - Support translation back and forth.
  - Extend codes that currently handle ENDF to also handle the new format.
  - Lots of testing and comparison!



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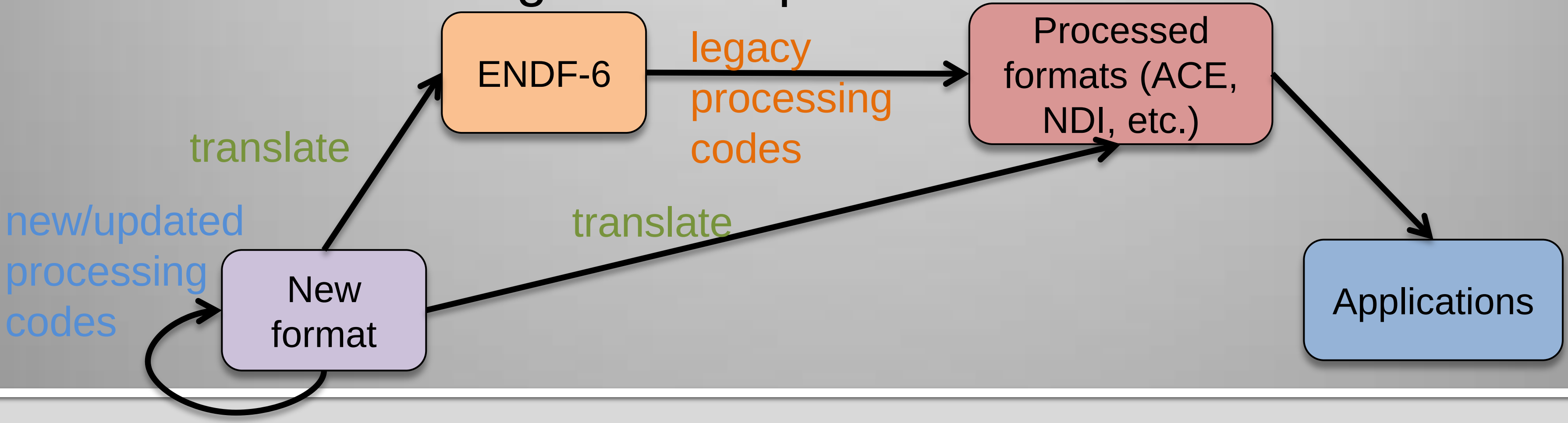
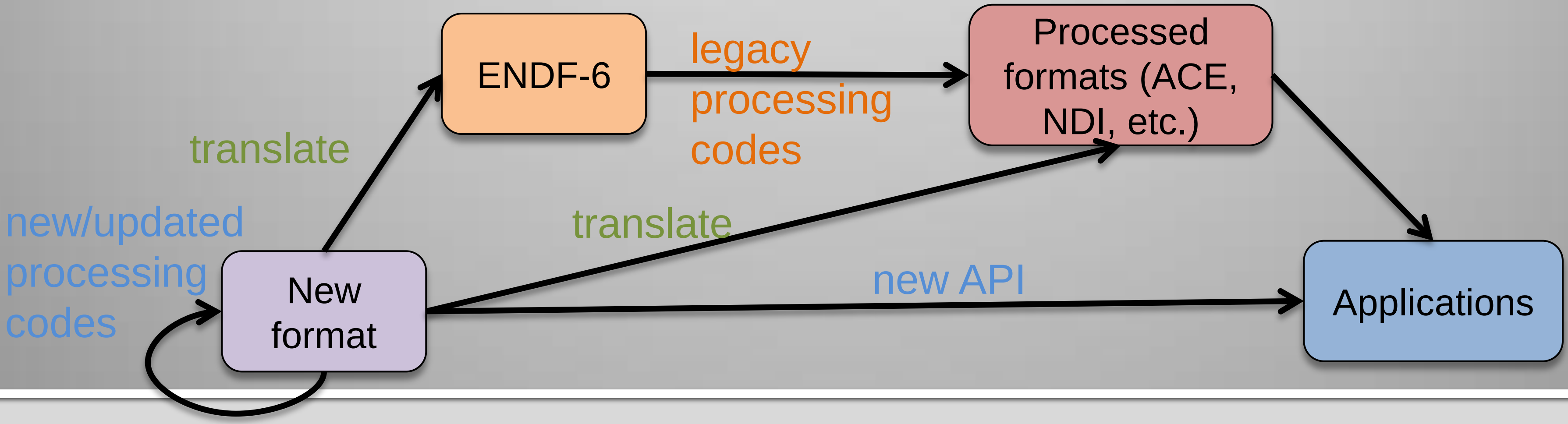


Longer term goal: Define Application Programming Interfaces (APIs) for reading and writing data in the new format.

- Using an API:
  - provides a standard way to access data, and
  - protects applications from future changes in the format.



What about infrastructure? How can we replace all the codes that currently use ENDF-6?

- LLNL’s FUDGE is a good start:
  - For Updating Data and Generating an Evaluation
  - Supports
    - Reading/Writing GND data
    - Conversion of ENDF to GND and vise-versa
    - Visualization of data – e.g., plotting and printing
    - Manipulation of data
    - Checking of data
    - Processing of data
      - Resonances reconstruction
      - Cross section heating
      - Grouping of data (mainly for Sn as grouping is done on recast in GIDI for MC)
      - Sn transfer matrices

Translating ENDF←→GND

```
>python rePrint.py ENDF-B-VII.1/neutrons/n-001_H_001.endf
```

```
   2 [3, 4, 33] : MF=4, LTT = 1
 102 [3, 6, 33] : MF=6 : ZAP=0, LAW=2, LANG=0 : ZAP=1002, LAW=4
   1 [3, 33]
    processing MT1 gammas
```

ENDF to GND

```
n + H1 -->
      n + H1
        n: label = n: to ENDF6:
        H1: label = H1: to ENDF6:
      H2 + gamma
        gamma: label = gamma: to ENDF6:
        H2: label = H2: to ENDF6:
      summed reaction: total
```

GND to ENDF

```
>ls -lh
37K   test.endf6.xml
4.9K  test.endf6-covar.xml
50K   test.endf6.noLineNumbers
50K   test.endf6.orig.noLineNumbers
50K   test.endf6.orig.noLineNumbers.cleanAndFixed
```

resulting files after translation

Status of ENDF translation to GND

- For ENDF-VII.1 sub-libraries:
  - Can translate:
    - — neutrons/ protons/ deuterons/ tritons/ helium3s/ gammas/ standards/ electrons/ photoat/ atomic_relax/

Evaluations “H1 + H2” and “H2 + H3” have bad data

  - Can be translated into GND-like format, these are not yet integrated with FUDGE:
    - — nfy/ sfy/ thermal_scatt/
  - Currently not supported:
    - — Decay/

Status of translation for other libraries (incident neutrons only):

- JEFF-3.1.2
  - 328 / 381 successfully translated
  - 371 / 381 with the 'skipBadData' option
- JENDL-4
  - 385 / 406 successfully translated
  - 406 / 406 with skipBadData
- We are submitting bug reports to library maintainers
  - Fudge is now part of pre-release testing for TENDL

Processing codes are changing with computer architecture. Processing includes:

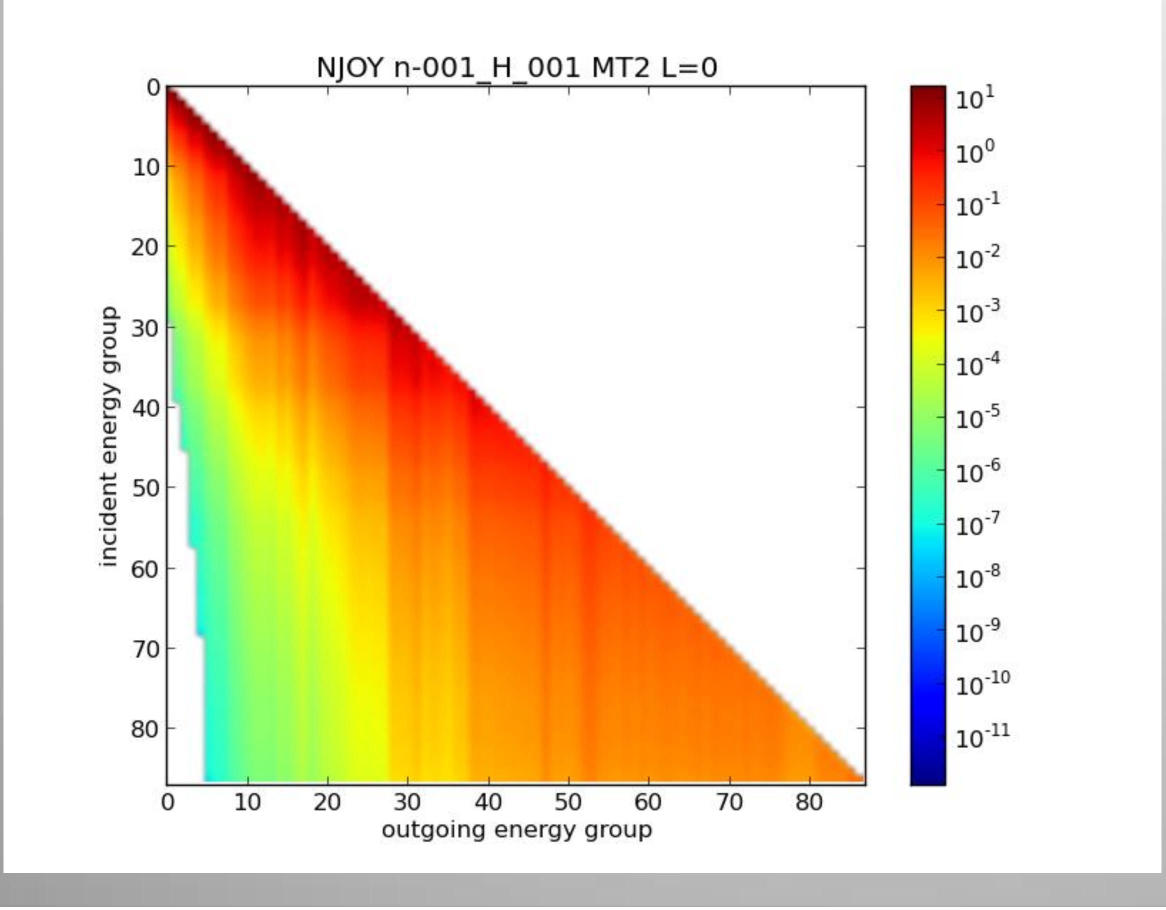
- Fast data transformations, can happen when data are read in by user code:
  - Grouping cross sections, flux weighting
  - Converting pdf→cdf

- More computer-intensive, done off-line:
  - Reconstructing cross section from resonances
  - Doppler broadening
  - Generating transfer matrices

- Processed data should be stored in GND (facilitate sharing data)

Transfer matrices: outgoing angle/energy spectra averaged over incident energy bins

Angular dependence is in Legendre expansion



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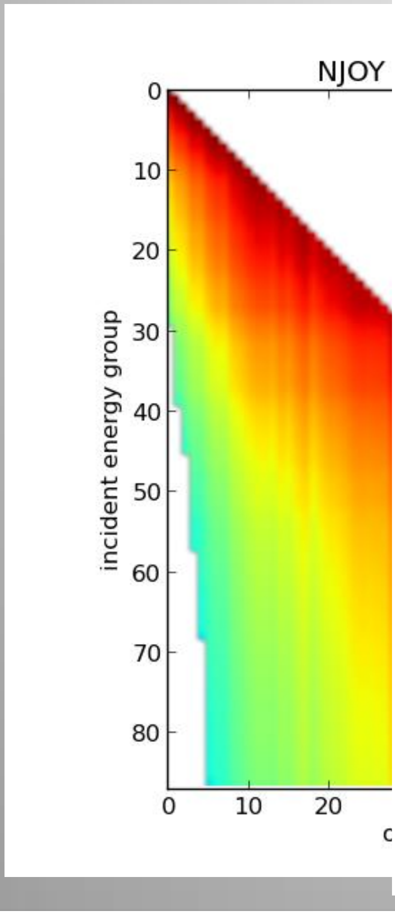
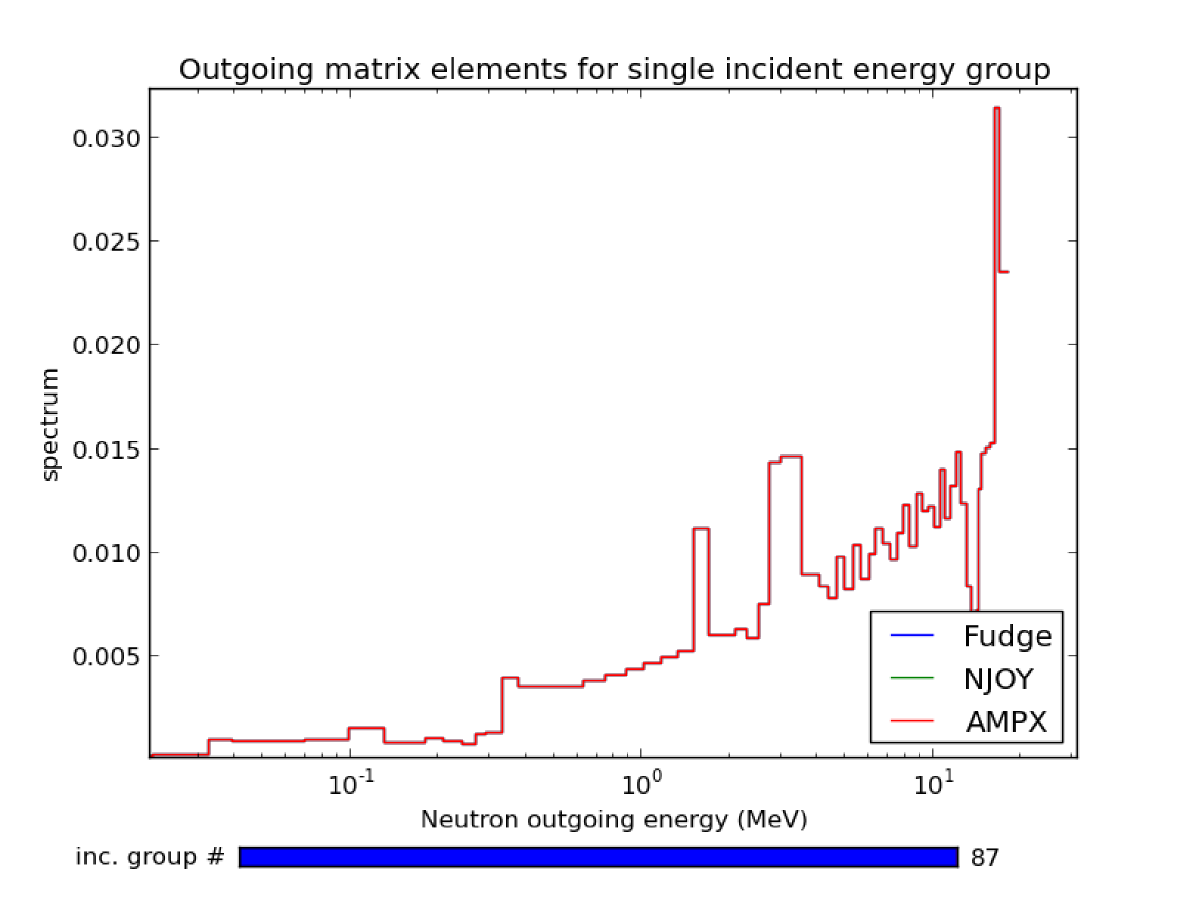
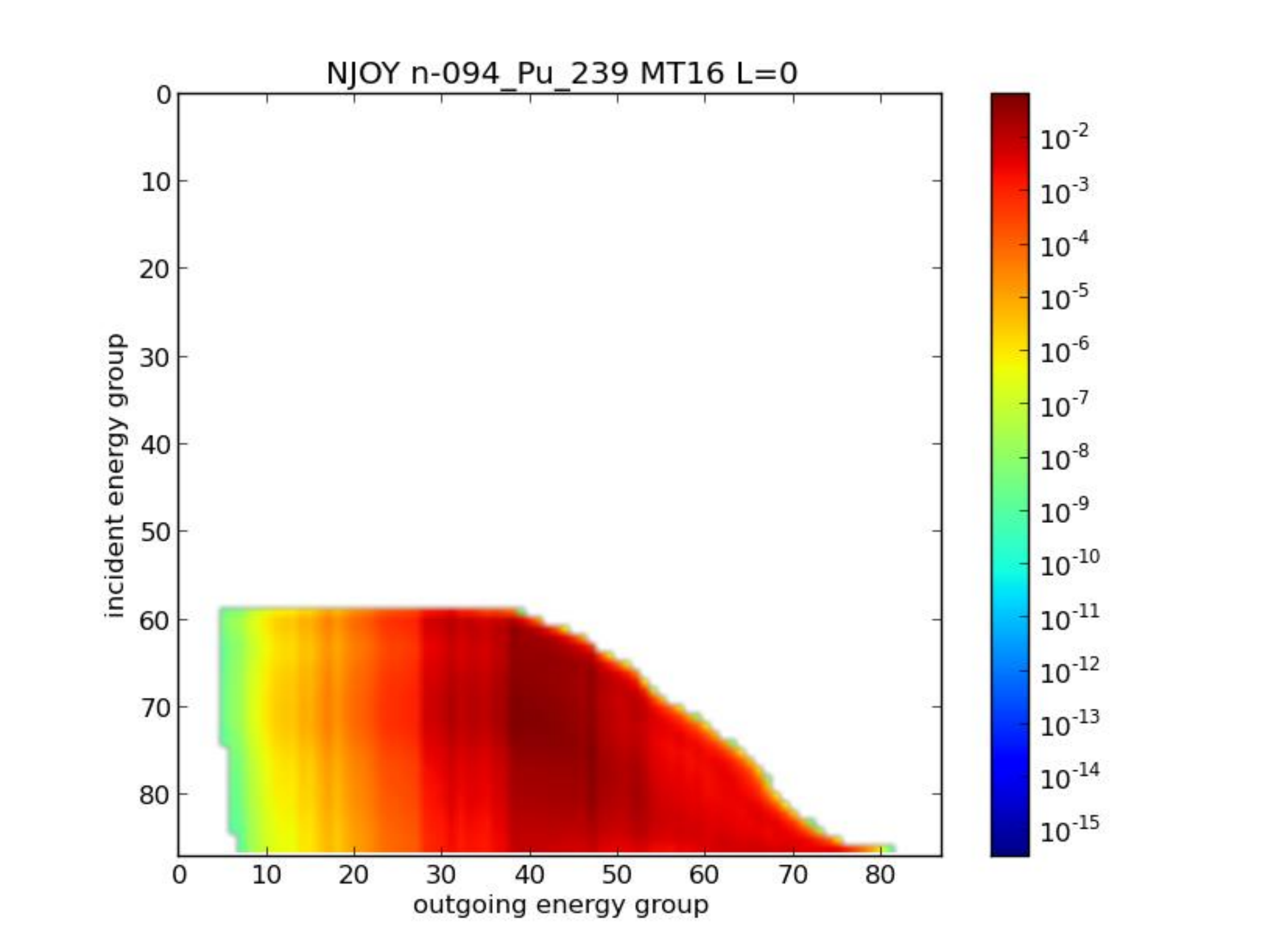




Processing codes don’t always agree, especially for double-differential distributions:



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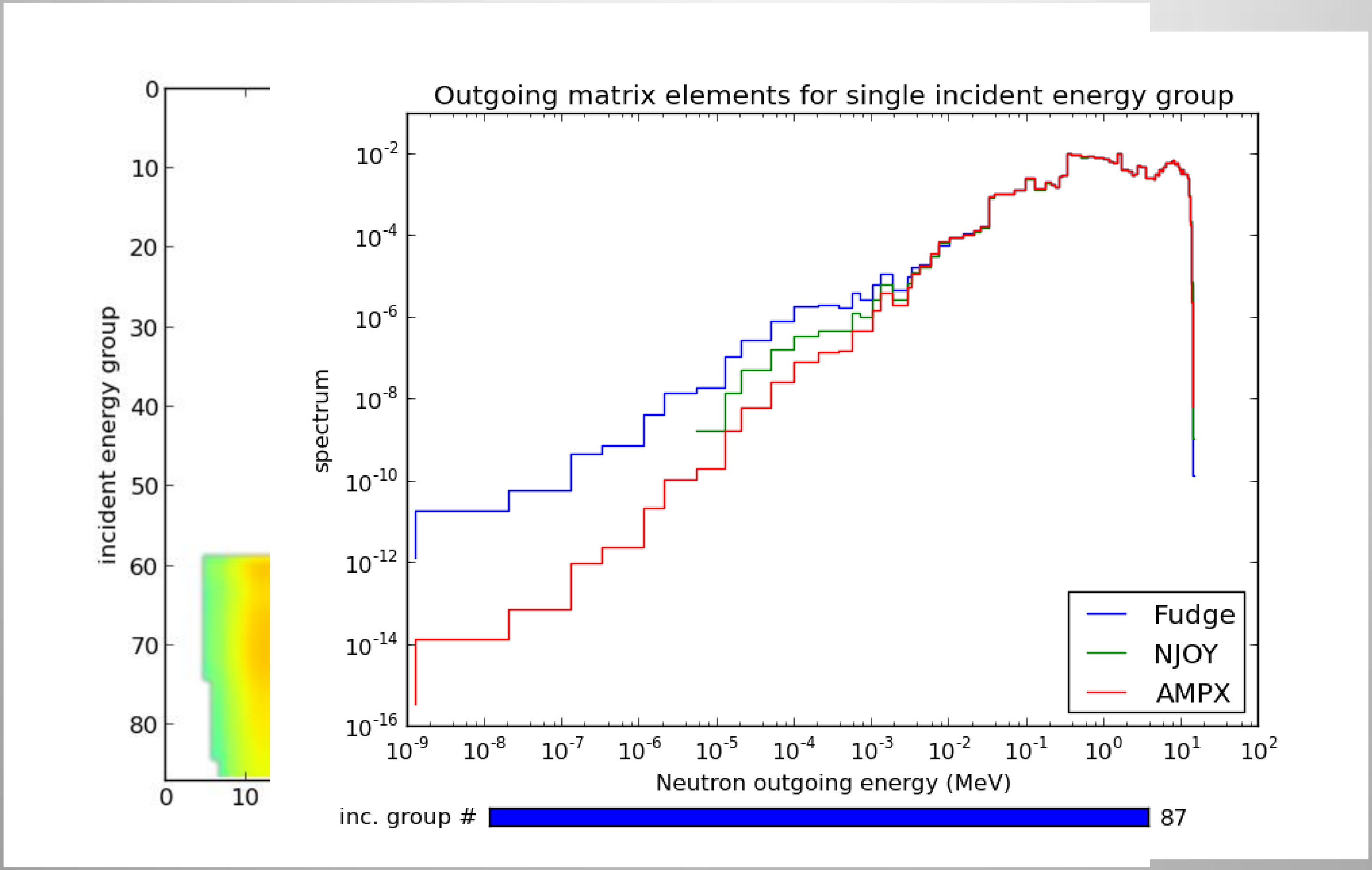

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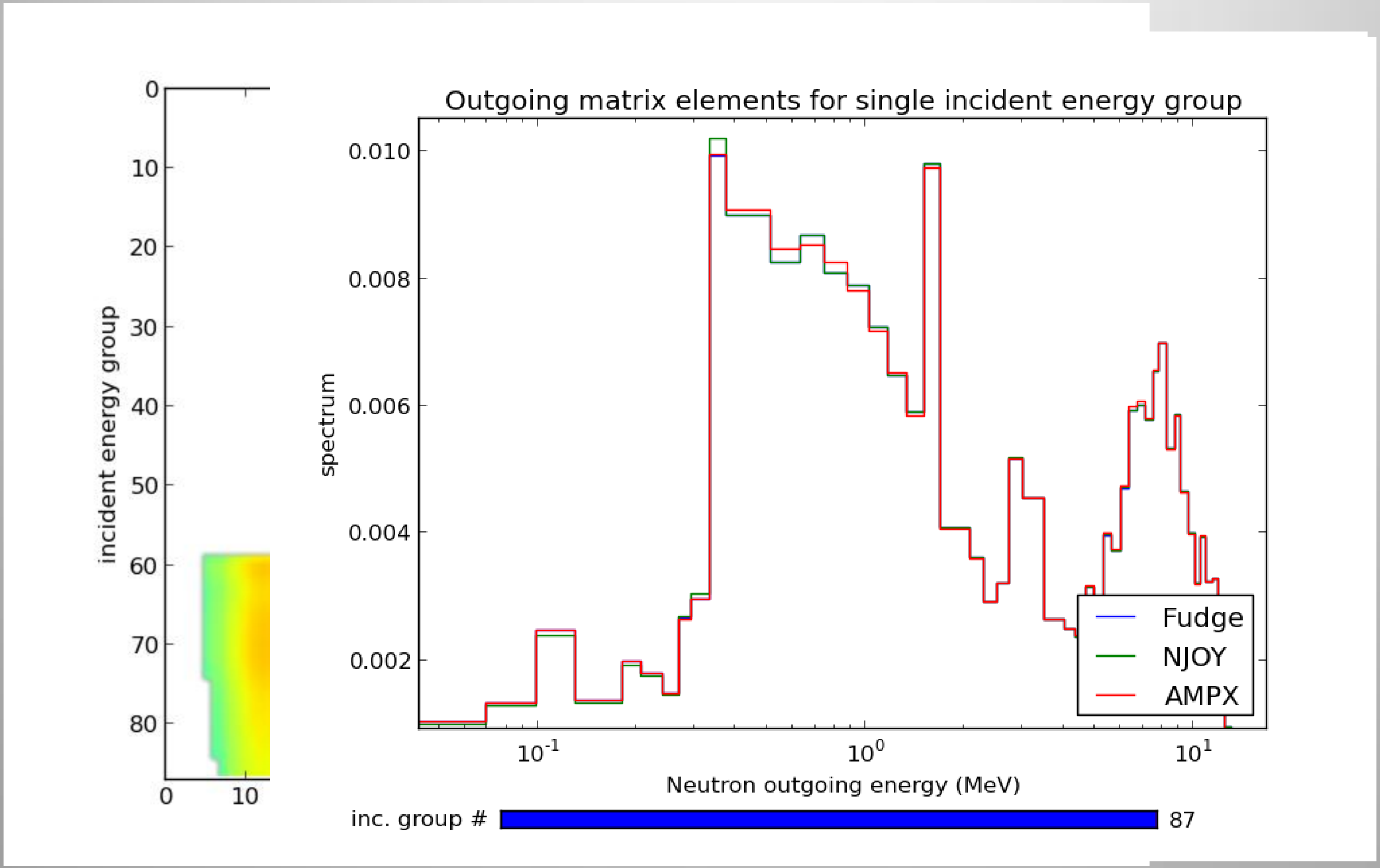
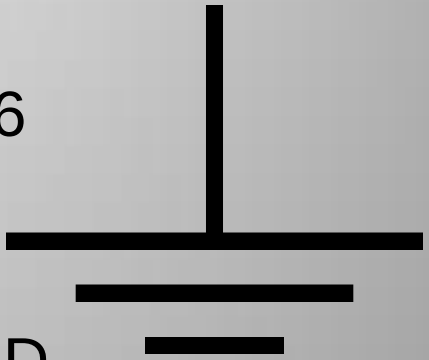


GND infrastructure is freely available. More testing and feedback are needed!

- GND 1.3 plus supporting infrastructure now available for download:
  - https://ndclx4.bnl.gov/gf/project/gnd/
- The package includes:
  - Translation tool 'rePrint.py' to move ENDF-6 data to and from GND
  - Infrastructure for reading, writing, plotting, physics testing and basic processing of GND files.
- Please test it out and give us feedback!



GIDI (General Interaction Data Interface)

- An API for GND we are developing
  - Deterministic GND data
    - Reading
    - Collapsing
  - Monte Carlo GND data
    - Reading data
    - Sampling data

- Beta version currently in GEANT4
- Being tested in LLNL stand-alone Monte Carlo code Mercury
  - Testing with critical assemblies and ‘broomsticks’

Future work:

SG38 still working to finalize specifications for how data will be stored in GND.

- SG38 plans to create ‘final’ draft of specifications for the new format by December 2015.
- GND and Fudge will be modified as specifications evolve.
- Ongoing work: extending the API, testing and QA, assisting transition away from ENDF-6

Main perspective for the next decade:

- Libraries officially released in both ENDF-6 and in the new format
- Formats will coexist, but new evaluations will begin to add data types not supported by ENDF. Possibly new sub-libraries only available in GND?
- Existing codes gradually extended to handle GND, new codes use it directly

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