Progress on processing GND evaluations

CSEWG Formats and Processing committee

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We are rewriting our processing codes to handle GND files.

- Monte Carlo support is complete
- Processing for deterministic codes is nearly complete
- Also working on access routines to read GND: Generalized Interaction Data Interface (GIDI)
  - For Monte Carlo, GIDI also does sampling
- We plan to release processing tools soon
  - LLNL verdict: no export control needed

For Monte Carlo codes, most work is done by GIDI

- Grouping, generating CDF and equal-probable bins are all fast, can be done at load time
  - More flexibility for users
- Doppler broadening is computationally intensive and should be done prior to library release
  - Fudge now includes cross section heating module
- We are working with LLNL's Mercury code team to integrate GIDI

For deterministic transport, we have a new tool for generating transfer matrices:

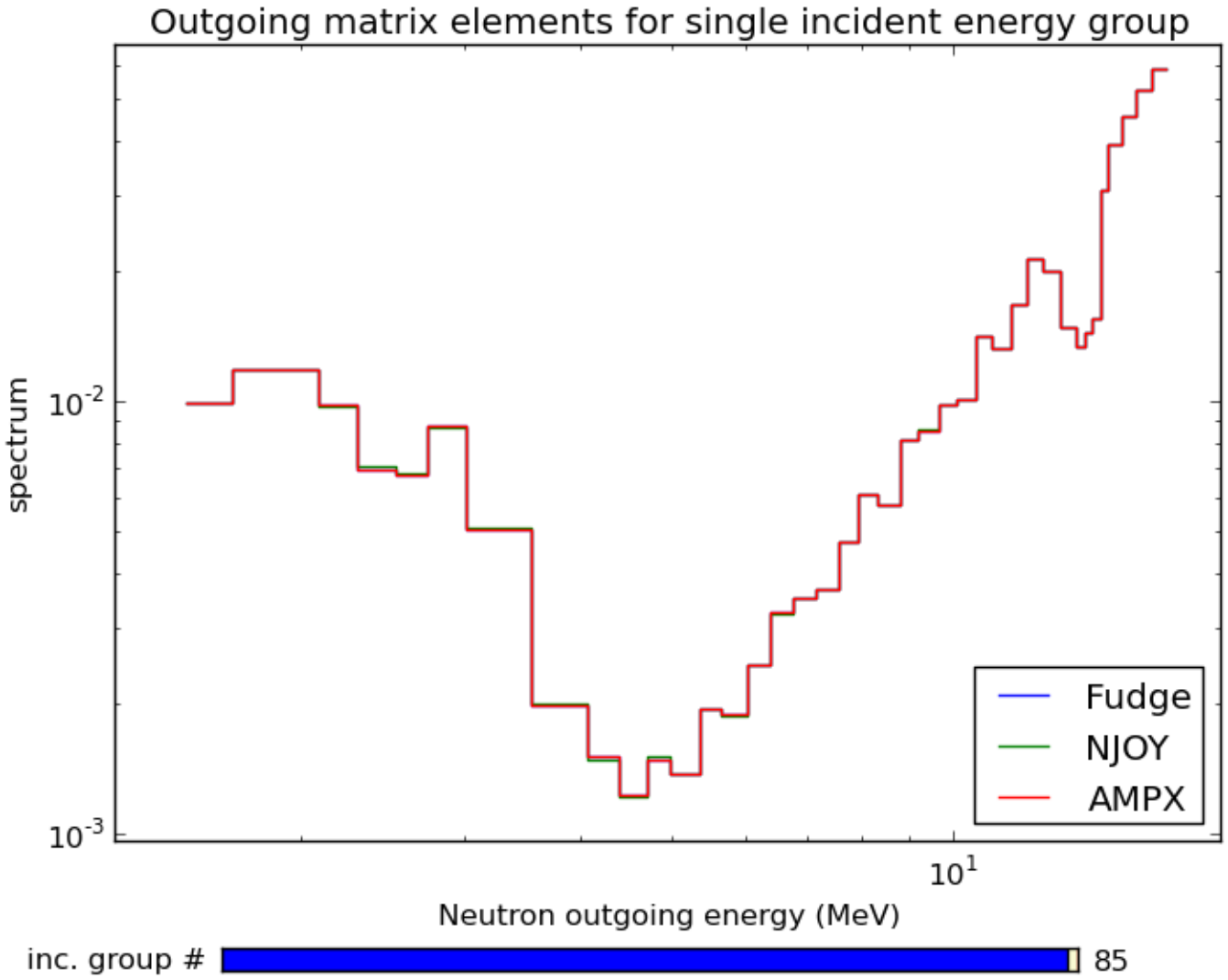
- C++ code ‘get_transfer’ written by G. Hedstrom
- Handles all types of distributions from ENDF and ENDL (although not all interpolation rules)
- Integrated with Fudge. After processing, transfer matrices are stored in GND along with the original (or ‘native’) data.

We are testing get_transfer by comparing results with NJOY and AMPX

- With each code we linearize data to 0.1%, heat to 0.1 K, and process into 87x87 transfer matrices up to L=5
- NJOY workflow: reconr, broadr, unresr, groupr
- AMPX workflow: polident, broaden, ..., y12, prell, x10, ..., simonize, ..., paleale
- We then compare resulting transfer matrices

ENDF-VII.1 neutron sublib processed with all three, results compared:

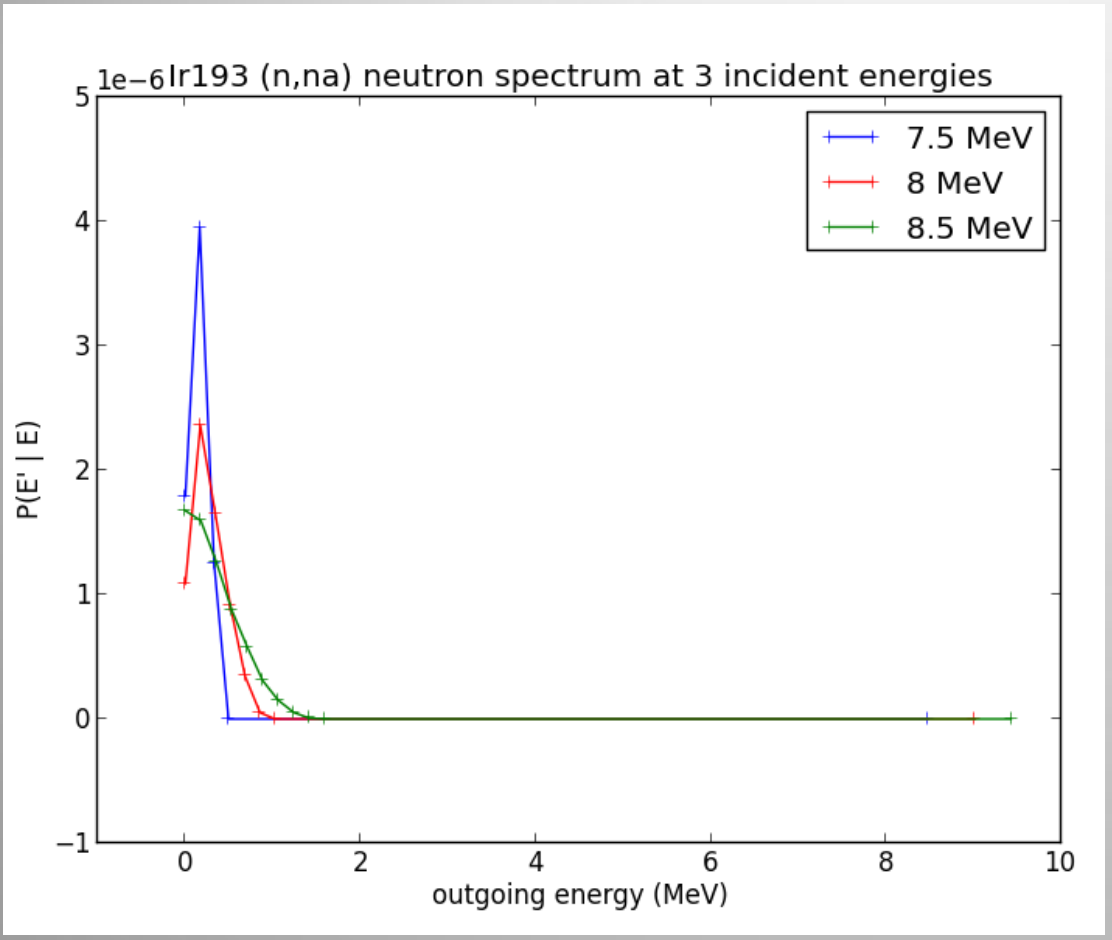
- Calculate absolute and relative differences for every matrix element
- Mask out relative differences if abs. diff < 1e-4
  - May also apply weighting strategies
- Sort remaining diffs, for now focus on L=0 terms
- Then use visual comparison tools to understand source of large differences


Outgoing matrix elements for single incident energy group
spectrum
10^{-2}
10^{-3}
10^{1}
Neutron outgoing energy (MeV)
Fudge
NJOY
AMPX
inc. group #
85

Transfer matrix differences help reveal bugs in codes *and* in nuclear data

- Code bugs:
  - Fudge incorrectly assumed that MF6 Legendre distributions always given in lab frame (fixed)
  - Fudge had problems with double-counting at boundary between different interpolations (fixed)
  - NJOY problem with error function complement erfc (reported, fixed in 2012.2 update)
- Data bugs:
  - When data are not clearly specified, codes make different assumptions.
  - Example: the Be7 evaluation only extends to 8.1 MeV. Group #65 (7.91 to 8.32 MeV) treated differently.
  - Also several issues with interpolation (see next slides)

Trailing zeros can cause trouble for unit-base interpolation!



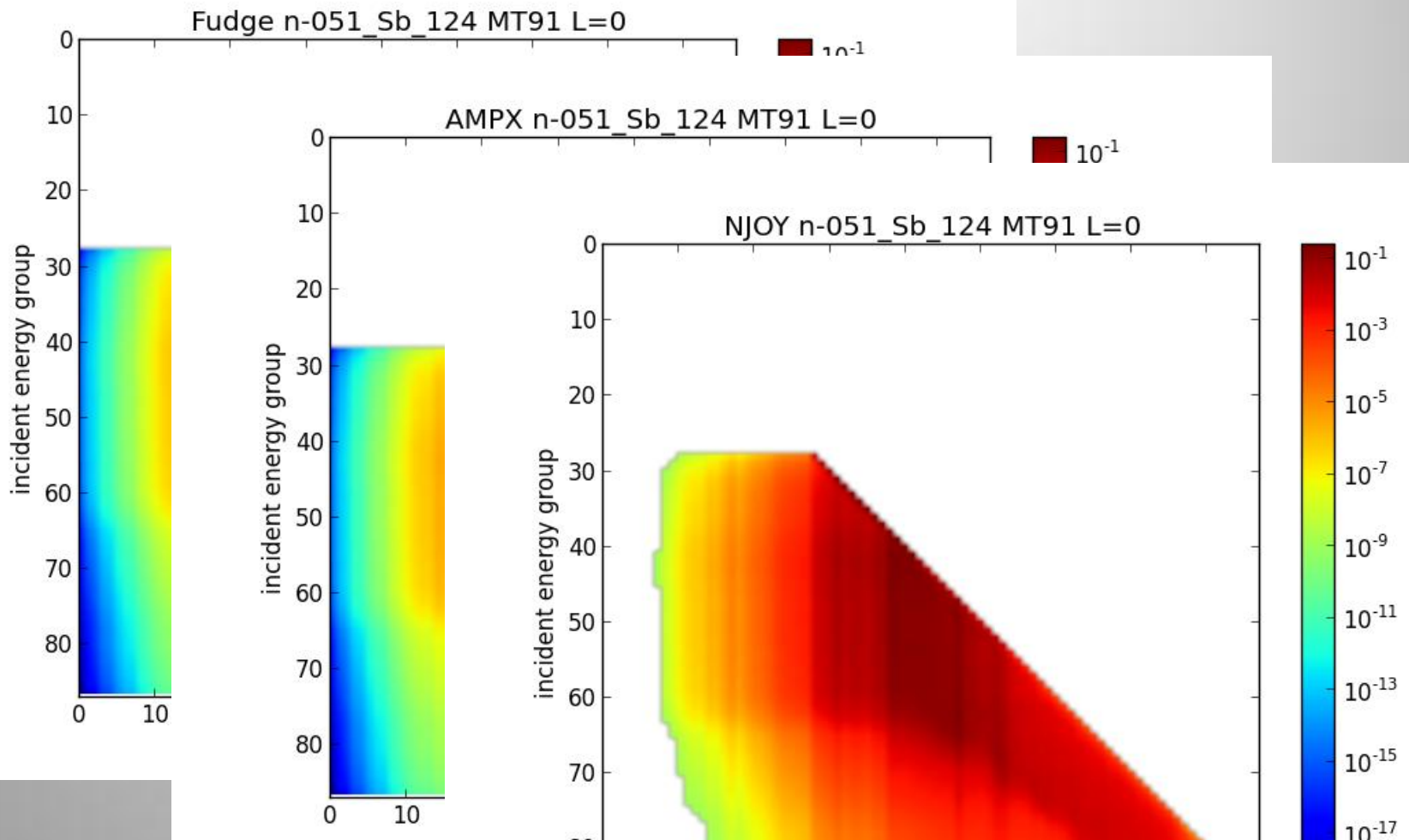
- What domain do we use for unit-base? Should it include trailing zeros or not?
- Removing trailing zeros would make data more clear.

Sb124 MT=91 (n,inelastic): distribution at threshold is far from conserving energy!

- In ENDF/B-VII.1, distribution at threshold extends to nearly 1 MeV! (GForge tracker 827)
- Energy imbalance warnings are raised... but the file still made it into ENDF-VII.1
- During processing, NJOY fixes with a cryptic warning, Fudge and AMPX process data as is

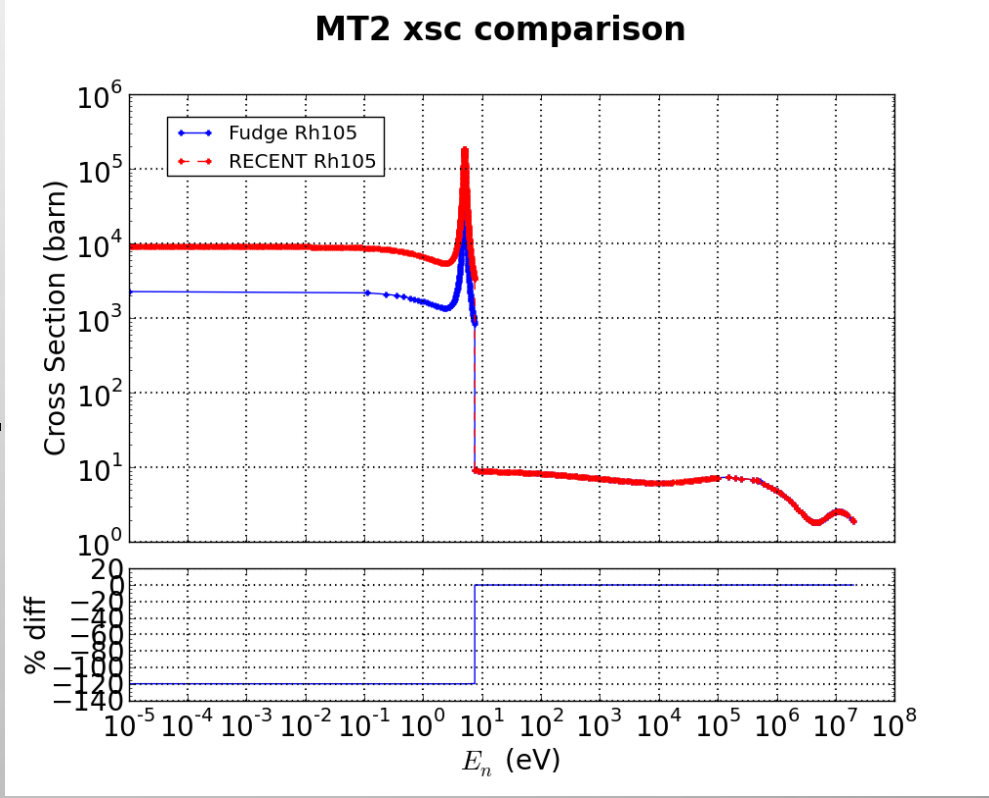
```
...
---message from getsed---upscatter correction   9.8457E-01
---message from getsed---additional messages supressed
```

Sb124 results:

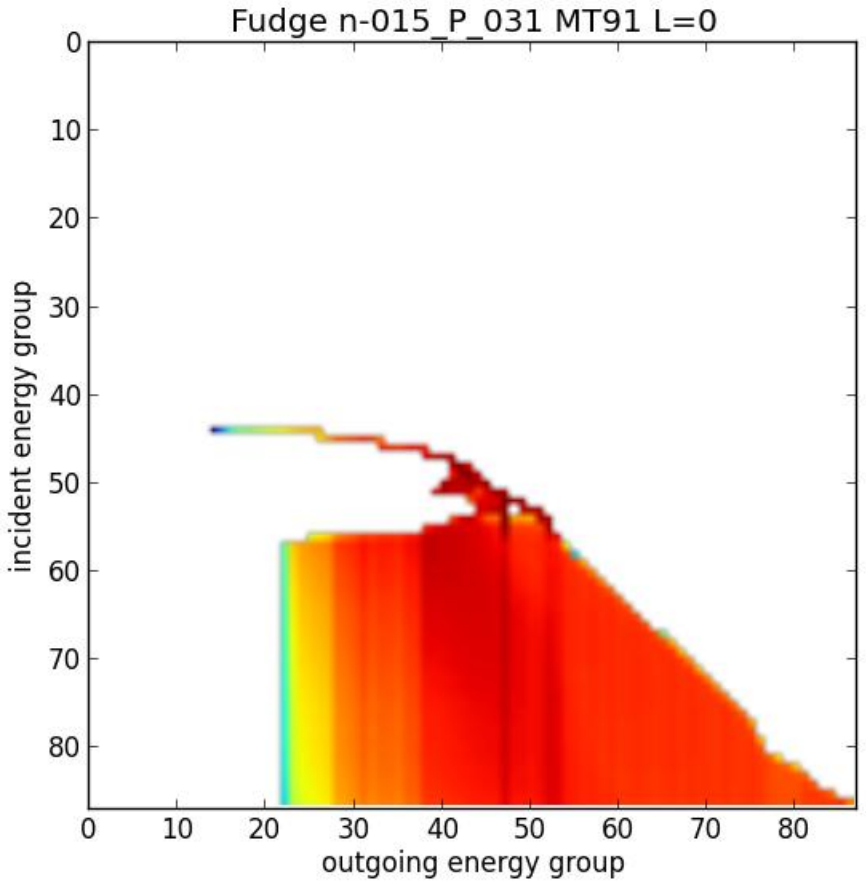


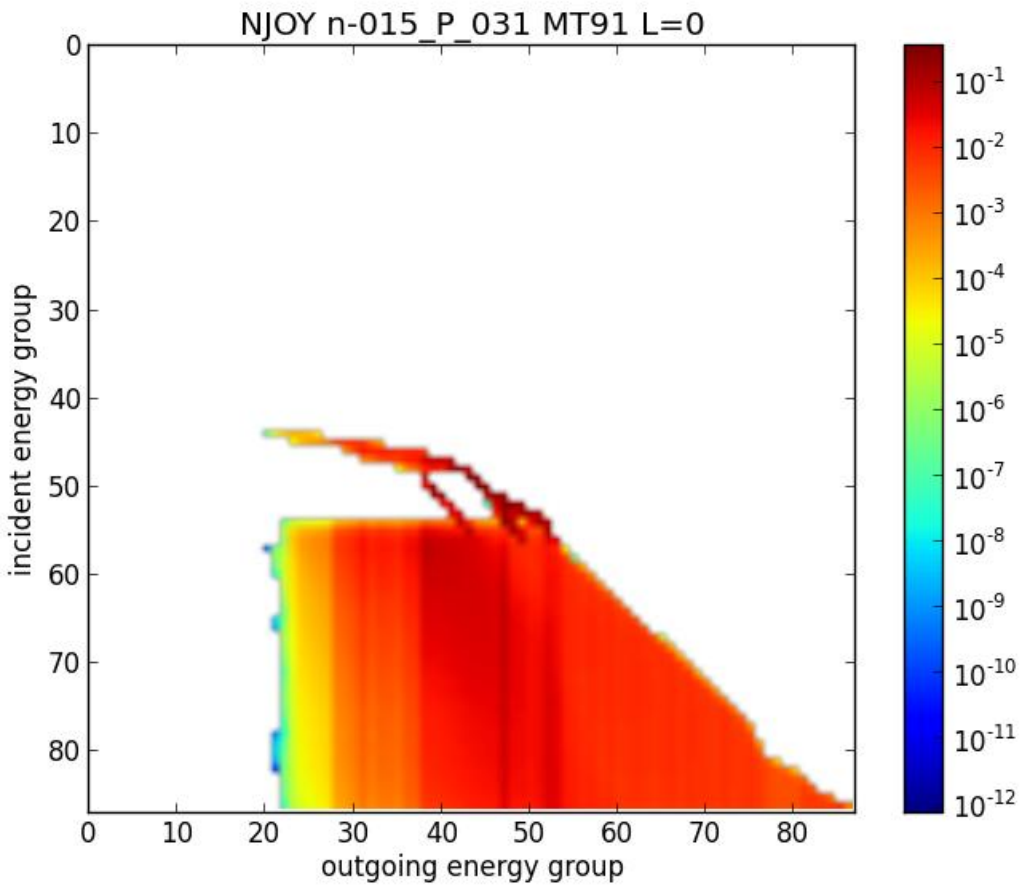
Inconsistent spins for Rh105. GForge tracker item #710 submitted, not yet fixed

- Resolved region claims spin 1/2 but URR claims 7/2!
- GND only has room for one particle spin...
- File adopted from JENDL-3.3... adopt JENDL-4 instead?



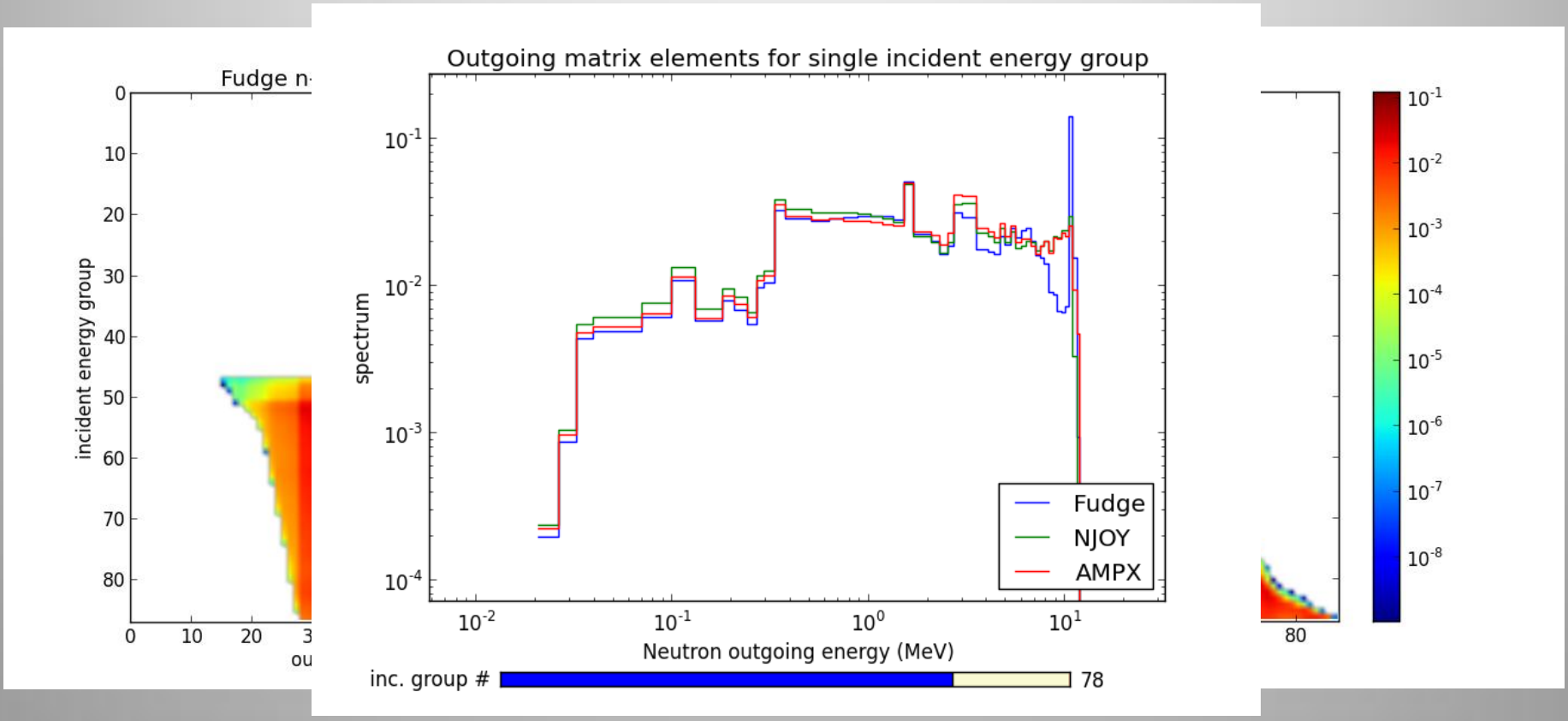
P31 MT=91 (n,inelastic), NJOY differs from Fudge/AMPX:





Be9 (n,2n) angular-energy distributions: P(mu,energy_out | energy_in)

- Here Fudge is the outlier:



Summary of deterministic processing:

- Still 48 materials have at least 5% relative difference (with NJOY) *and* at least 1e-4 absolute difference for one or more reactions.
- Working to understand these differences. Often I can trace them back to data issues.
- Note: mainly looking at L=0 matrices for now.
- Still TBD: correction for thermal up-scattering

Can we use Fudge as a platform for other processing codes?

- Other institutions have expressed interest in basing new processing capability on Fudge.
- We are looking for a general solution to allow this without adding too many methods to the main GND class definitions
- What we don't want:
  - r = reactionSuite.readXML("n-094_Pu_239.xml")
  - r.processLLNL()
  - r.processKAPL()
  - r.processIRDC()
  - ...
- One proposal: make a generic process() that accepts a dictionary of functions as an argument

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