Lawrence Livermore National Laboratory

Progress with Processing GND

Caleb Mattoon,
Bret Beck and Gerry Hedstrom

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Outline:

- Resonance reconstruction: comparison with RECENT
- Processing for deterministic transport
  - Comparing results with NJOY
- Processing for Monte Carlo transport
- Storing and sharing processed data with GND
- Future work

‘fudgeReconstructResonances’

- Now built into Fudge, reconstructs cross sections from res. parameters. Includes multiprocessing for speed
- Supports ENDF LRF 1,2,3,7 for RRR; LRF 1,2 for URR. No support yet for reconstructing angular distributions
- Building R-Matrix elements (for LRF 3 and 7) written in C for better performance
- How to use:

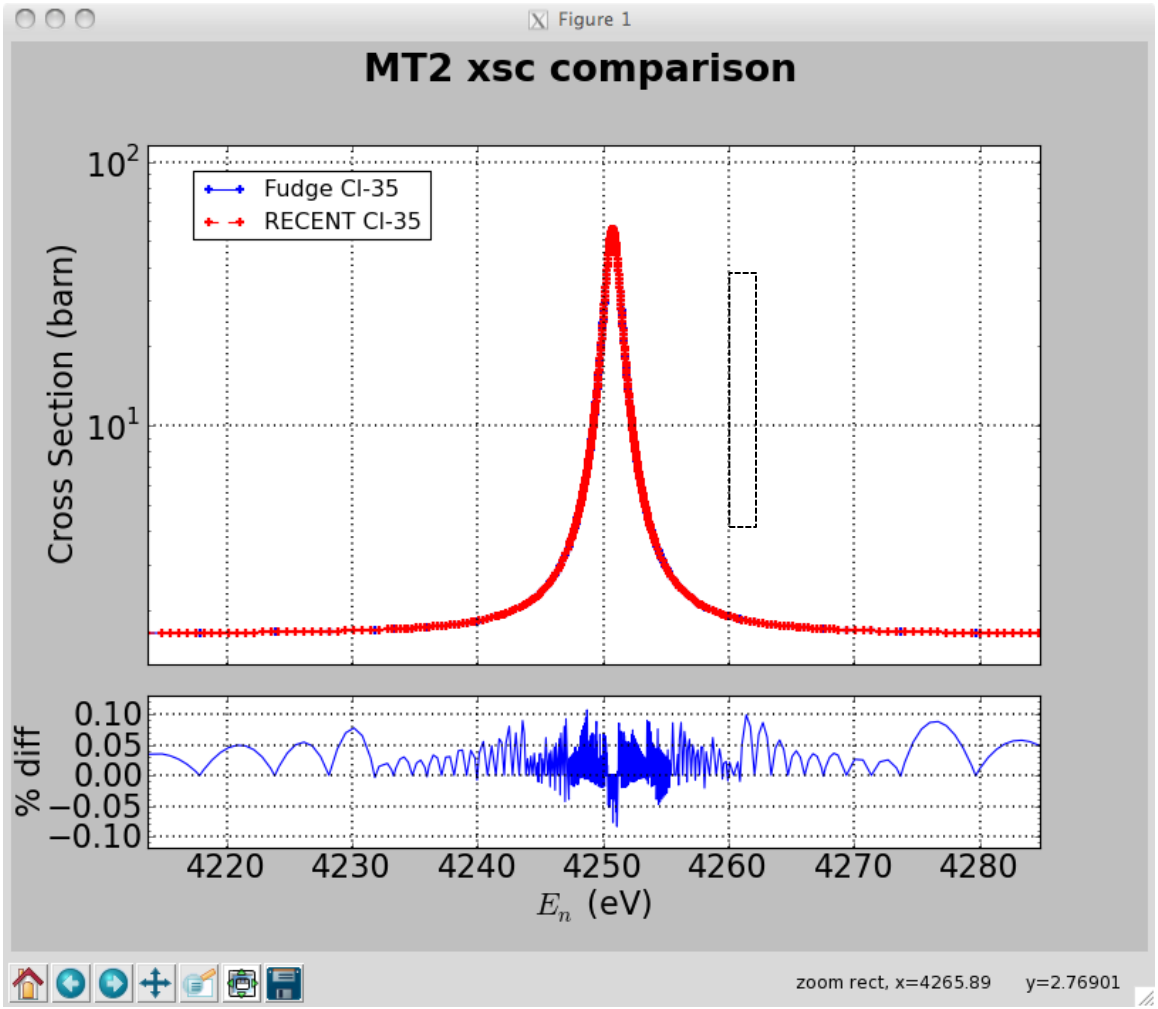
```
>>> from fudge.gnd import reactionSuite
>>> r = reactionSuite.readXML( “neutrons/n-092_U_238.xml” )
>>> r.reconstructResonances( accuracy=0.001, verbose=True )
```

Comparing results to RECENT

- Test: reconstruct same file with both RECENT and fudgeReconstructResonances, to same accuracy, compare results

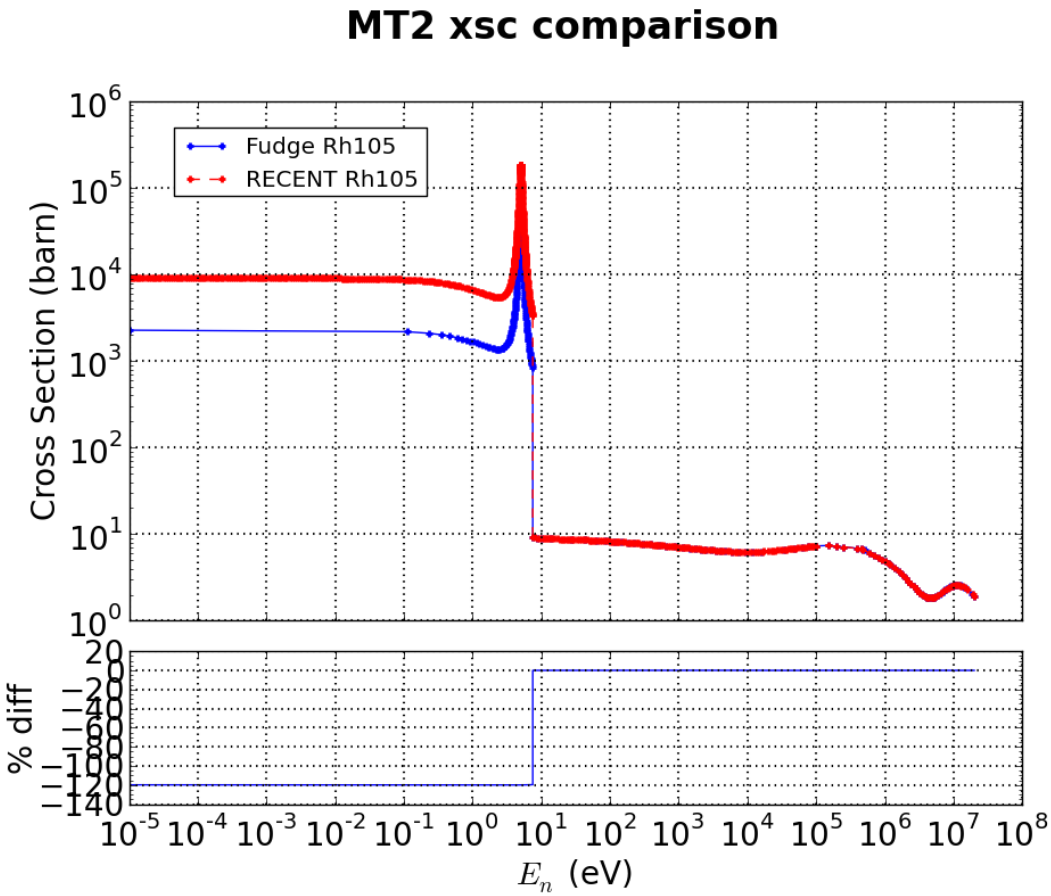
- New tool compareCrossSections (similar to COMPLOT) helps with comparison

Comparing results to RECENT



Comparing results to RECENT

- Trouble in Rh-105
- Cause: conflicting spin assignments in the evaluation!



Comparing results to RECENT

- Rh-105 evaluation originally taken from JENDL-3.3. Spin assignments for RRR and URR differ:

```
 4.510500+4  1.040000+2          0          0          1          04531 2151
 4.510500+4  1.000000+0          0          0          2          04531 2151
 1.000000-5  7.500000+0          1          1          0          04531 2151
 5.000000-1  6.200000-1          0          0          1          04531 2151
 1.040050+2  0.000000+0          0          0         12          24531 2151
-5.000000+0  1.000000+0  1.610000+0  1.450000+0  1.600000-1  0.000000+04531 2151
 5.000000+0  1.000000+0  4.900000-1  3.300000-1  1.600000-1  0.000000+04531 2151
 7.500000+0  1.000000+5          2          2          0          04531 2151
 3.500000+0  6.207500-1          0          0          3          04531 2151
 1.040050+2  0.000000+0          0          0          2          04531 2151
 3.000000+0  0.000000+0          5          0        174         284531 2151
 0.000000+0  0.000000+0  0.000000+0  1.000000+0  0.000000+0  0.000000+04531 2151
 7.500000+0  3.410700+1  0.000000+0  1.500700-3  1.500000-1  0.000000+04531 2151
```

- ENSDF agrees with 7/2 assignment
- Evaluation re-done in JENDL-4, with yet another spin assignment (3/2). Should we adopt that?

Other resonance region issues

- Common problem in evaluations: invalid interpolations!
- Sample from U236, trying to use log-log interpolation in URR:

# energy	competitive	fission
1500.0	0.0	0.00034
		...
45000.0	0.0	0.00034
50000.0	2.03e-05	0.00034
60000.0	0.000333	0.00033
		...

- Other stuff?

Processing for deterministic transport

- Boltzmann equation:

$$\frac{1}{v}\partial_t\phi(E,\Omega)+\Omega\cdot\Delta\phi(E,\Omega)+\rho\sigma_t\phi(E,\Omega)=\frac{\rho}{4\pi}\int_{\Omega'}d\Omega'\int_0^\infty dE'K(E,\Omega\cdot\Omega'|E')\phi(E',\Omega')$$

- Kernel ‘K’: probability that incident particle with incident energy and direction E’,Ω’ produces outgoing particle at E,Ω

- For each Legendre order, produce transfer matrix:

$$J_{gh,\ell,r}=\frac{\int_{\varepsilon'_g}dE'\sigma_r(E')M_r(E')\phi_\ell(E')\int_{\varepsilon_h}dE\int_\mu d\mu P_\ell(\mu)\pi_r(E,\mu|E')}{\int_{\varepsilon'_g}dE'\phi_\ell(E')}$$

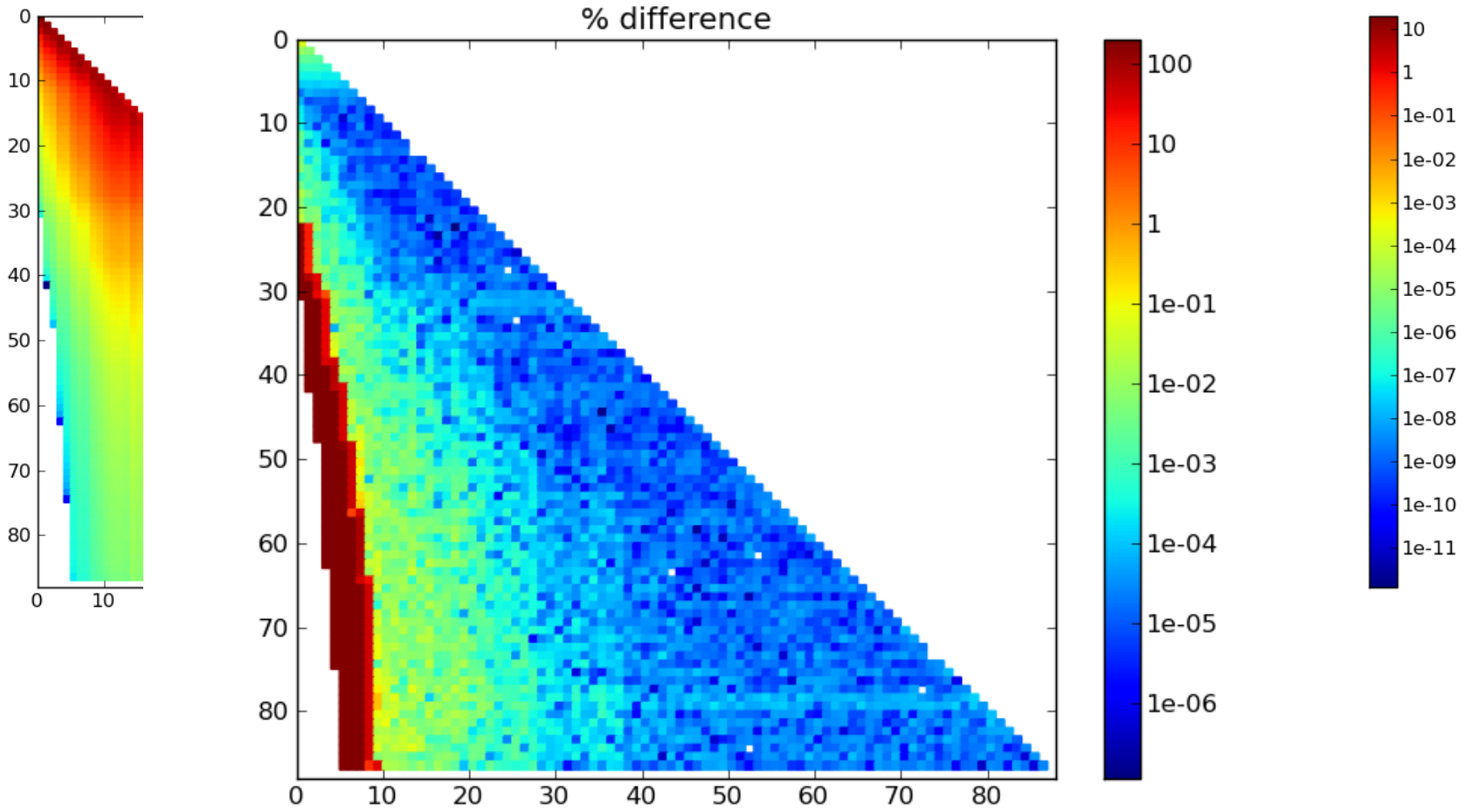
Generating transfer matrices from GND:

- LLNL's new code *get_transfer*: produce transfer matrices from nearly any distribution supported by ENDF-6*
  - c++ code, primarily written by G.Hedstrom
  - integrated into Fudge, permits
- Now testing *get_transfer* by comparing to results from NJOY's GROUPR module

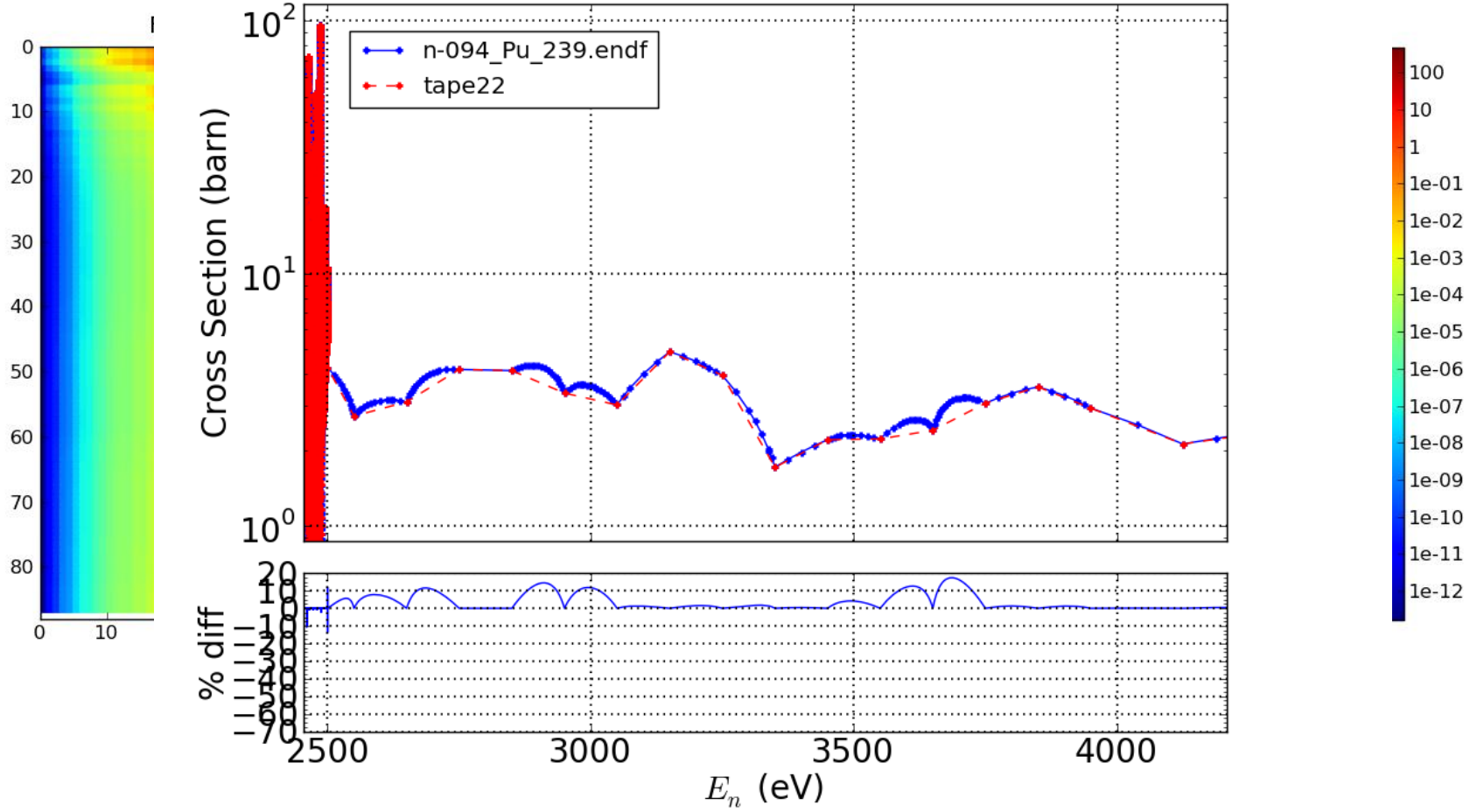
*exception: Madland-Nix parameterization

Transfer matrix comparison:

H1 (n, elastic) L=0 transfer matrices:

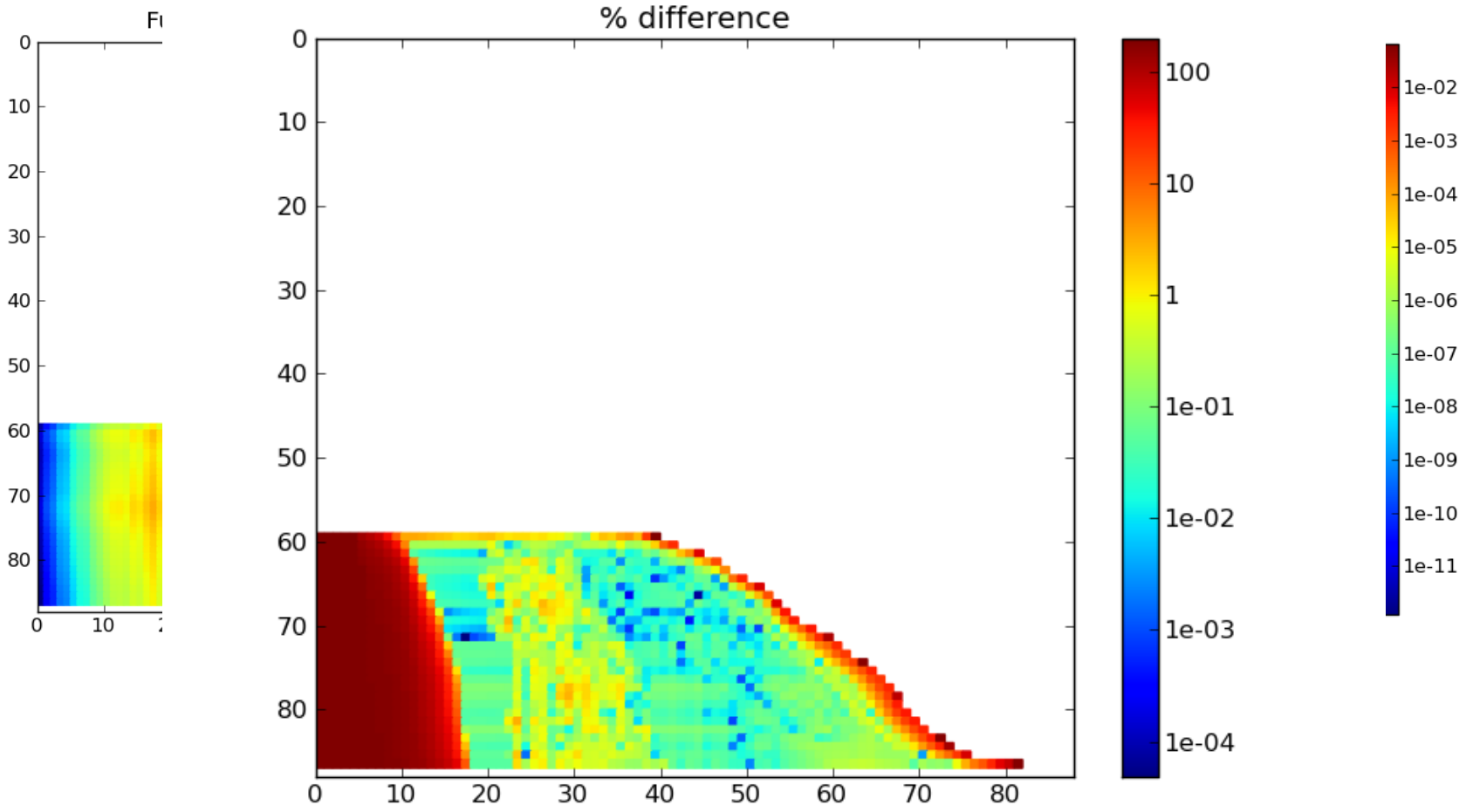


Comparing processing capability:



Comparing processing capability (Kalbach-Mann):

Pu239 (n, 2n) prompt neutron L=0 transfer matrices:



Processing for Monte Carlo codes:

- Two ways of handling MC data:
  - at LLNL, we are moving towards ‘minimal’ MC processing, with most of the work done by access routines
  - legacy codes, however, will continue to need pre-processed data

‘Minimal processing’

- Tasks when processing and using nuclear data:
  - Doppler broadening, generating transfer matrices (expensive)
  - grouping, equiprobable binning, cdf-ing, reaction-specific transfer matrix summing (cheap)

- To give users more freedom, trying to move ‘cheap’ tasks to happen at run-time, through access routines

Future work and legacy support:

- Heating cross sections: have code, need to link it into Fudge
- Continued testing against other processing codes: outgoing gammas, higher L-orders, various temps, comparing MC data...
- Translating to other formats: ACE, LLNL's legacy MCF/NDF, etc.

Sharing processed data

- GND could enable better sharing of data
- Common processed format, perhaps to be translated into site-specific (binary) forms?
- Format sample:

```
<grouped xData="matrix" size="87,87">
        <axes>
          <axis index="0" label="energy_in" unit="eV" interpolation="linear,flat" frame="lab"/>
          <axis index="1" label="energy_out" unit="eV" interpolation="linear,flat" frame="lab"/>
          <axis index="2" label="C_l(energy_in,energy_out)" unit="b" frame="lab"/></axes>
        <l value="0">
          <matrix rows="87" columns="87" form="sparse_asymmetric">
            0 0 1 8.04765353
            1 0 2 0.0128888641 7.59496411
            2 1 2 0.0385045077 8.95273144
            3 2 2 0.0592808172 11.3596173
            4 3 2 0.109015267 9.60703412
            5 4 2 0.0470416286 8.87828991
            ...
```

Conclusions:

- Processing is an essential requirement before GND can fill the vital role of ENDF in nuclear data
- Much progress has already been made on processing GND files; more is needed especially to support legacy codes
- We will continue to compare to NJOY, AMPX, etc. as we implement new processing codes
- Hopefully other codes will be able to handle GND as well!

87-group structure (abbreviated):

group #	lower bound (eV)
0	1.3068e-3
10	102.45
20	4233.9
30	98.909e+3
40	632.470e+3
50	2.5299e+6
60	6.0425e+6
70	10.12e+6
80	14.407e+6
87	18.134e+6