CINDER2008 – A New Version of CINDER

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The CINDER Development Team

- CINDER development is due to a large team which includes staff from both US National Laboratories and laboratories abroad
- Argonne National Laboratory
  - Brad Micklich
- Los Alamos National Laboratory
  - Shannon Holloway, Hannah Little, Bill Wilson, Charles Kelsey, Michal Mocko, Günter Muhrer, Eric Pitcher
- Oak Ridge National Laboratory
  - Franz Gallmeier, Erik Iverson, Wei Lu, Irina Popova, Phil Ferguson
- Paul Scherrer Institute (Switzerland)
  - Michael Wohlmuther, Daniela Kiselev

The CINDER Code Package

- CINDER has been developed since 1960, initially for reactor problems but more recently for accelerator problems
- The development team began in 2005 with the intent to package CINDER90 in a more user-friendly format
- The CINDER90 distribution from RSICC includes scripting tools in the Perl language to aid in preparing input for and running the code, and to construct an MCNP-compatible source deck for gamma-ray dose calculations
- These scripting tools will be discussed in the following presentation

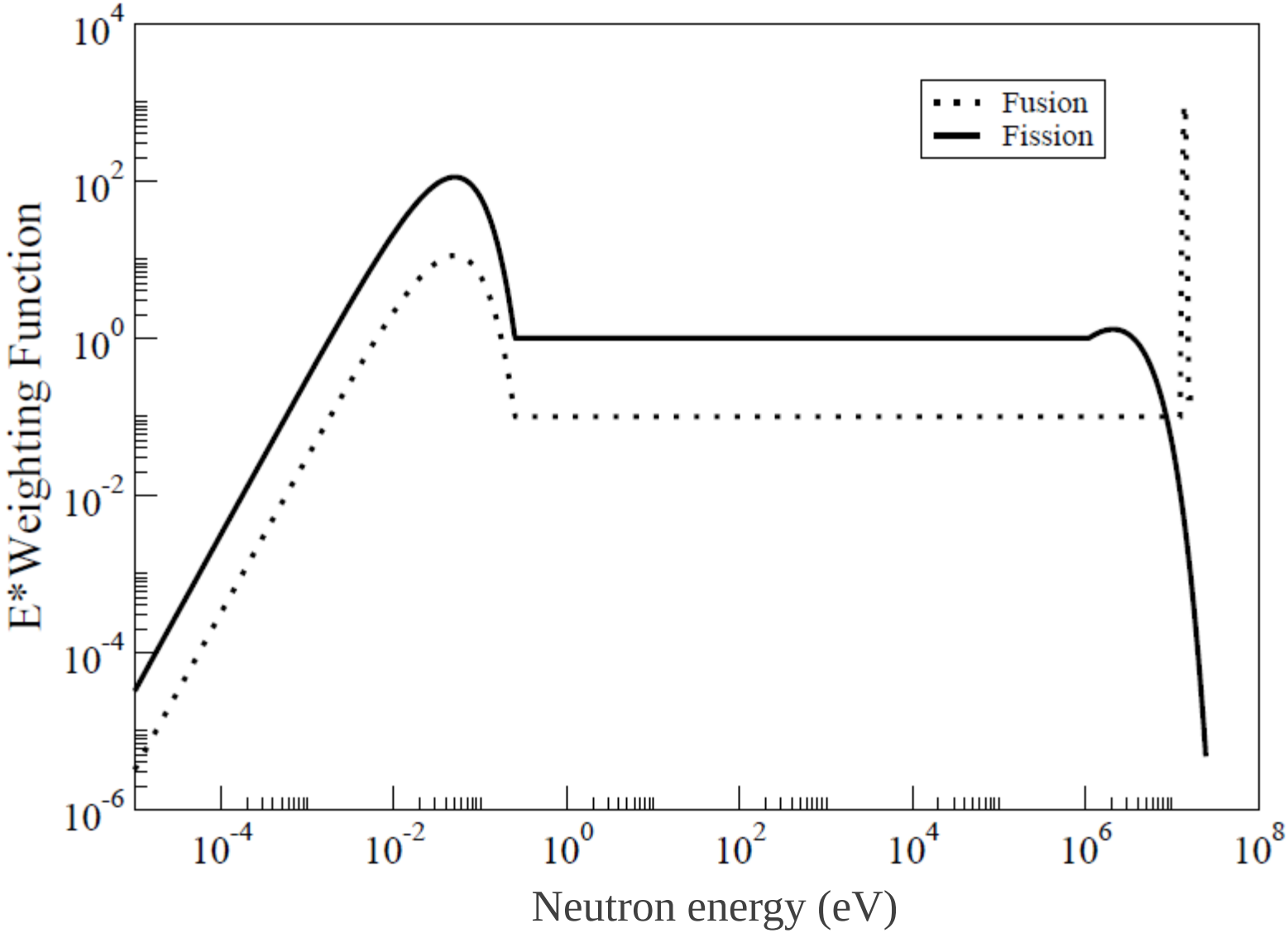
CINDER Code Upgrades

- CINDER2008 is a significant upgrade in capability from CINDER90
- Improvements include
  - Modern programming language and methods
  - New algorithms to more accurately solve the underlying differential equations
  - New extended data libraries using fission, fusion, and flat weighting functions
  - A new data library development tool
  - Automatic post-processing capabilities
  - Accident analysis tools
  - NAMELIST input option
  - Constant power approximation
  - High-fidelity β-delayed gamma spectra
- We expect that CINDER2008 will be released to RSICC sometime later in 2015

CINDER Data Libraries

- CINDER comes with an extensive library of neutron-induced reactions
- There has been thought from time to time about developing photon-induced and proton-induced cross section libraries, but these are still a future project
- The neutron cross section libraries were completely reformulated for CINDER2008
- The CINDER90 library used 63 groups from 10^{-11} MeV to 25 MeV
  - Cross sections collapsed from pointwise ENDF using a hybrid fission-fusion weighting function
- CINDER2008 has three reaction libraries covering energies 10^{-11} to 25 MeV (20 MeV)
  - 66-group fission-weighted library has the same group structure as the 63-group library, except the lowest group ($E_n < 10^{-9}$ MeV) has been broken into four groups
  - 321-group flat-weighted library, based on 315-group TRIPOLI group structure; this library is expected to provide the best results overall due to higher fidelity
  - 175-group fusion-weighted library, in the VITAMIN-J group structure; this library doesn't have many groups at low energy and is probably best reserved for special problems for which the fusion spectrum serves as a good approximation to the actual neutron flux in the system
  - Maximum energy for each cross section is that from the respective reference data

CINDER Data Libraries – Weighting Functions

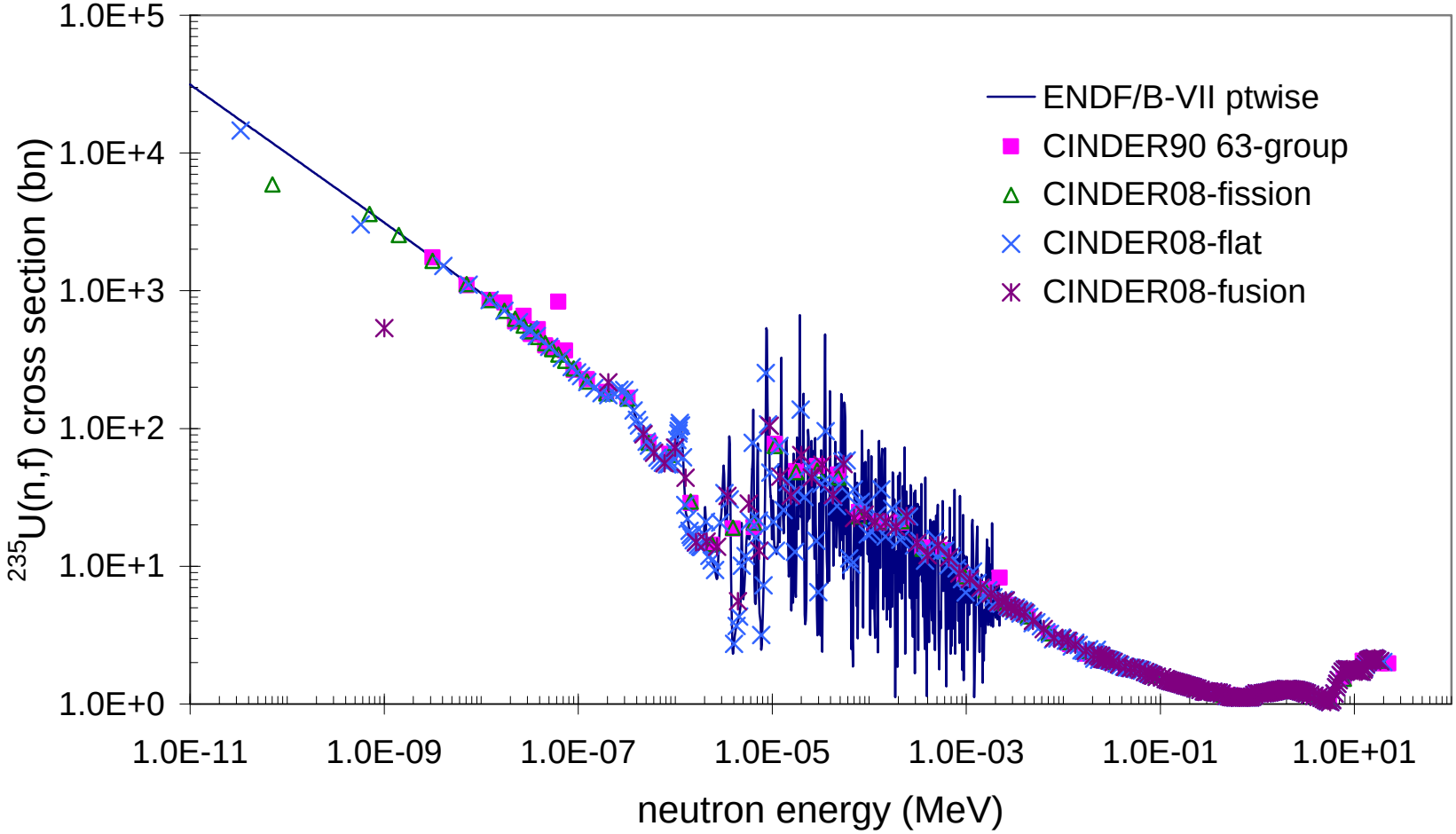


CINDER Data Libraries

- The group order of the cross sections given in the CINDER2008 library files runs from high to low – this is different from the ordering in the CINDER90 library, where the group order was from low to high
- This reduces the library file size because only the non-zero group constants are included for threshold reactions
- A library maker code is included with the CINDER2008 package so that the user can make their own group-averaged cross section library if desired
  - The library maker package will also be discussed in a later presentation
- It is the user's responsibility to select a library with the appropriate spectral weighting!
- The neutron flux must be specified using the same energy bin structure as the cross section library that you intend to use

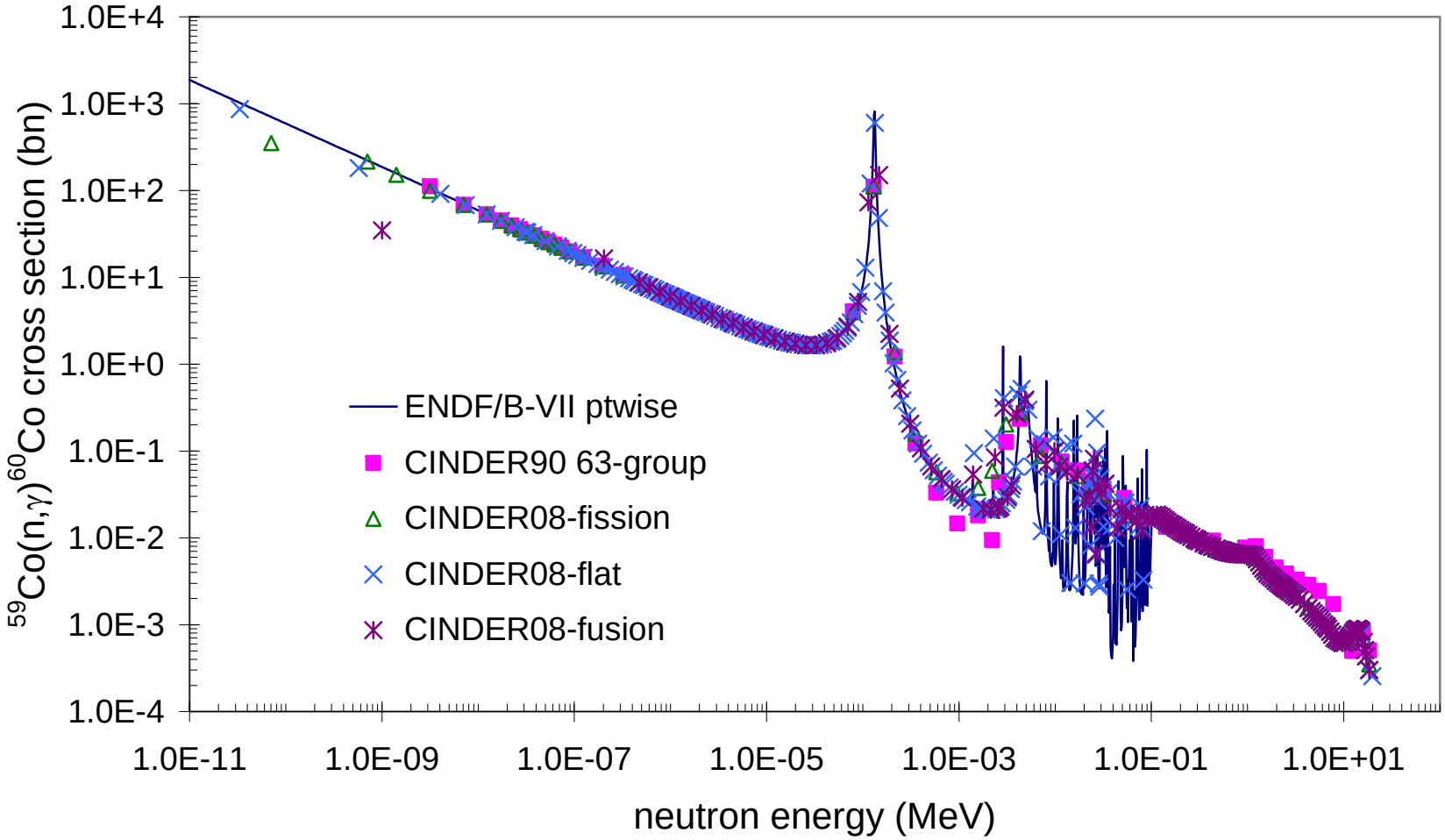
CINDER Data Libraries Example - $^{235}U(n,f)$

- CINDER90 library gave 10% greater $^{235}U(n,fission)$ rate in a well-moderated system compared to CINDER2008 fission library
- Fusion-weighted library has only one point for energies < 10^{-7} MeV



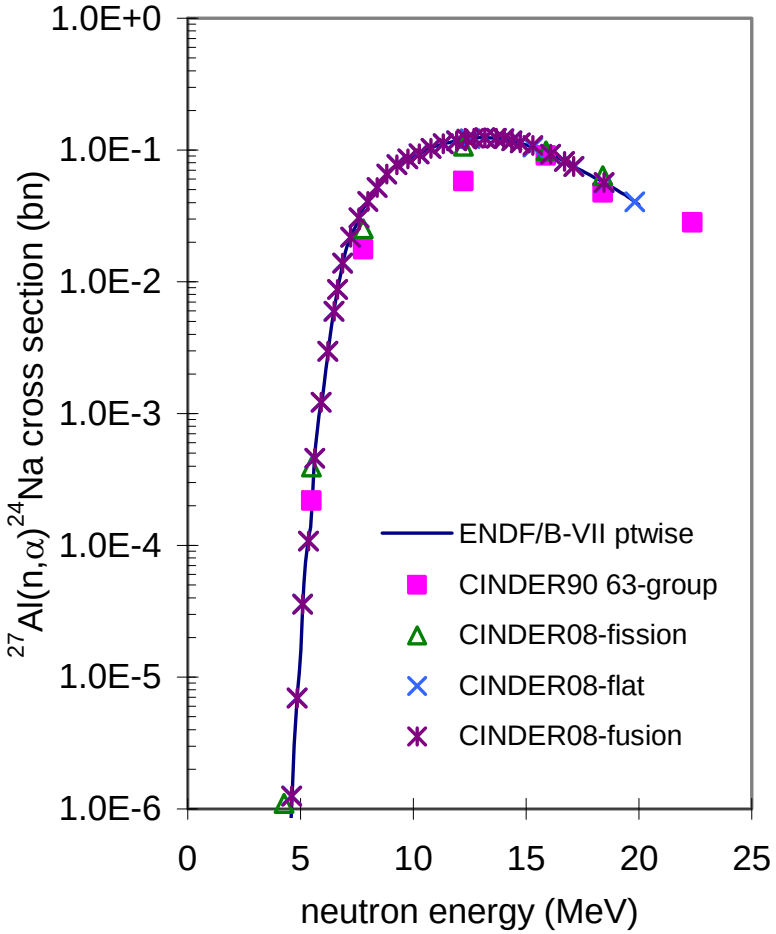
CINDER Data Libraries Example - $^{59}Co(n,\gamma)^{60}Co$

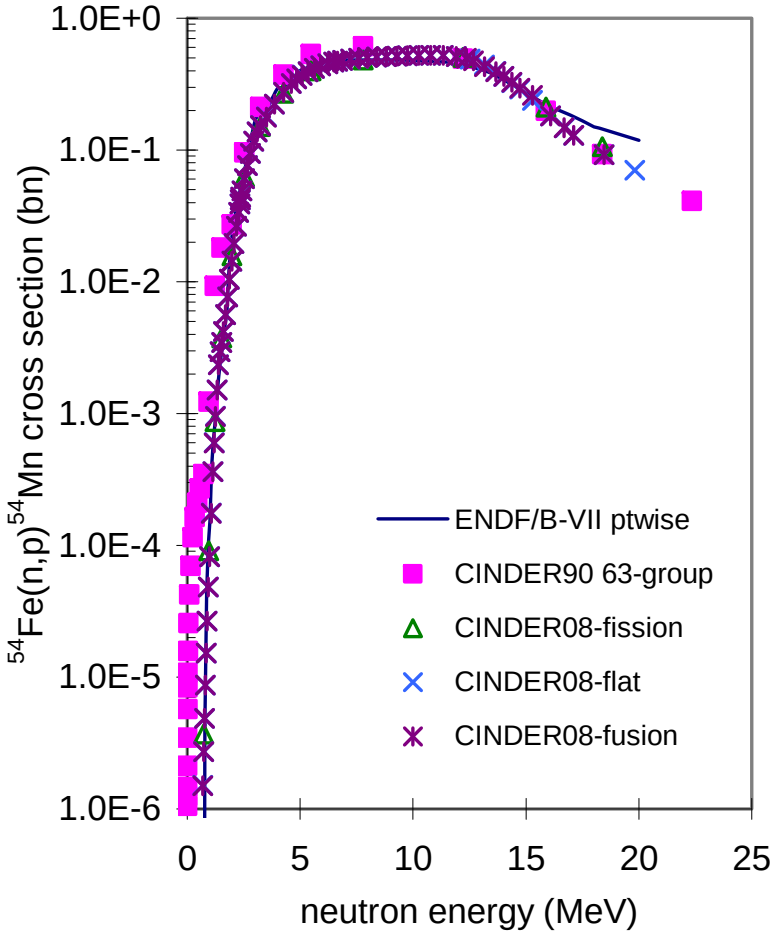
- Lowest-energy group for both fission- and fusion-weighted libraries has cross section significantly lower than ENDF/B-VII



CINDER Data Libraries – $^{27}Al(n,\alpha)^{24}Na$ and $^{54}Fe(n,p)^{54}Mn$

- Fast-neutron threshold reactions are well represented by the new CINDER08 libraries
- CINDER90 library based on earlier reference data sets, so the cross sections don't necessarily agree with ENDF/B-VII



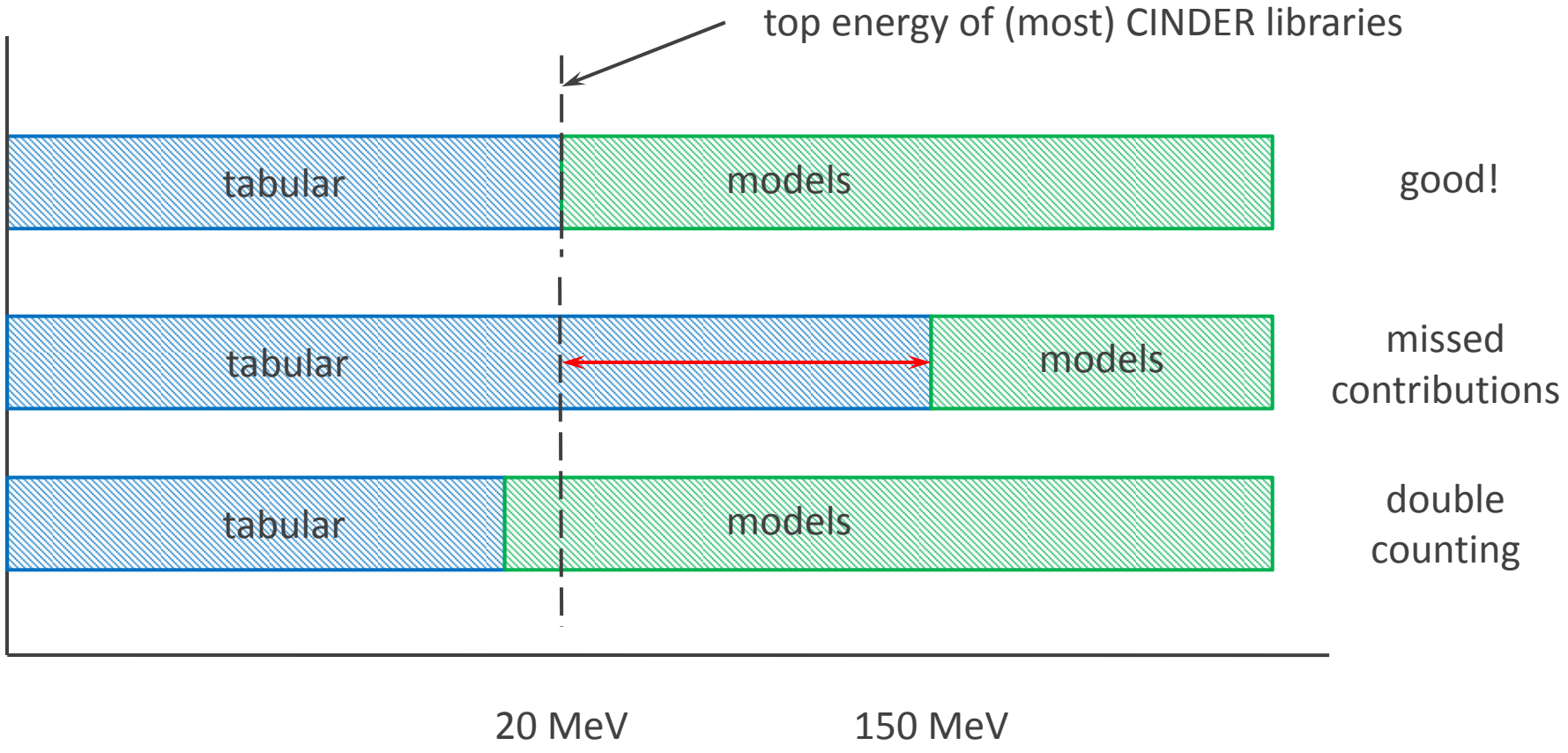


CINDER Data Libraries

- CINDER libraries have cross sections only for neutrons
- In MCNP/X, nuclide transmutation due to photons/hadrons/mesons can be accounted for by using nuclear models
- MCNP writes the results of model interactions to an optional histp file
- histp can be processed to extract the nuclide formation and destruction rates
- Contributions are only made to the histp file in the model physics regime
- histp will also contain contributions from neutron-induced reactions in the model physics regime (above the top of the tabular regime)
- The user must also pay special attention to the crossover between physics models and tabular data to avoid double counting, or not counting at all!
- In MCNPX, the maximum neutron energy to be used in the tabular regime should be set to the highest energy in the respective CINDER library (e.g. on the phys:n card)
- Example – using the default mix-and-match behavior in MCNP means that you can lose the production/destruction of nuclides due to neutrons with energies 20-150 MeV!

Tabular vs. Model Regimes

- The transition between tabular and model physics should coincide with the highest energy in the CINDER cross section library to be used



Running CINDER

- The CINDER90 package consisted of three distinct codes
  - CINDER – buildup/depletion calculation
  - TABCODE – generates table of photon spectra, decay power, radionuclide hazards, etc.
  - ALLCODE – generates selected tables summed over all regions of a problem; results ranked at a selected time step
  - The latest CINDER90 version was 7.4.2
- The CINDER 2008 package has two codes
  - CINDER – combines the functions of CINDER and TABCODE from the previous package
  - POST – generates tables for a single region, or a group of regions, for spectra, radionuclide hazards, power, dose equivalents, CAT-3 fractions, etc. (can generate the TABCODE tables if they weren't requested earlier)
  - Post-processing can now be initiated automatically by setting certain input variables

Running CINDER

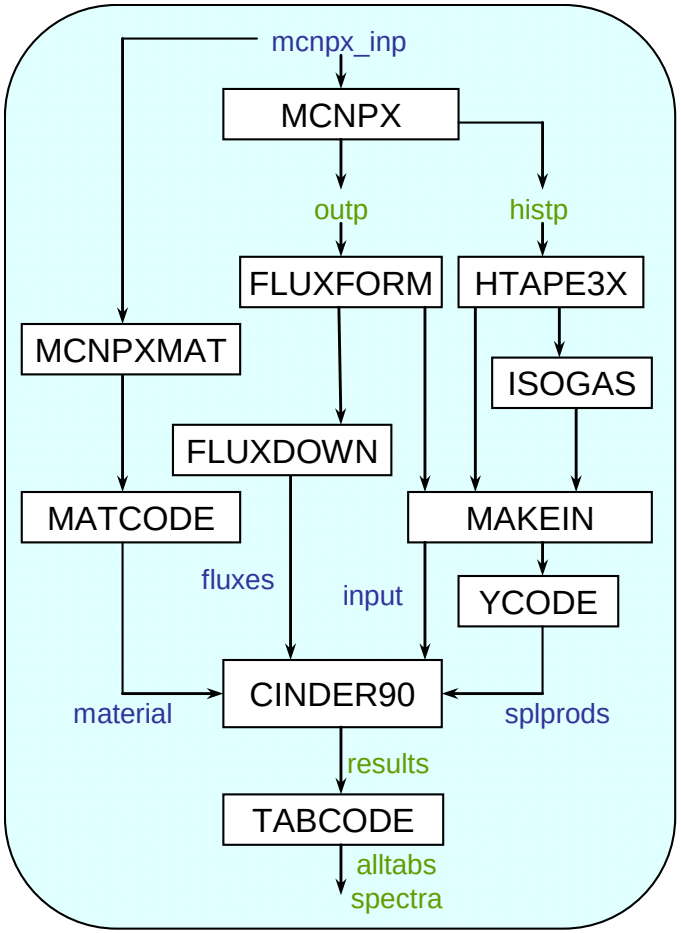
- CINDER has four required input files …
  - input – identifies flux, material, temporal history, and other problem parameters
  - fluxes – multigroup fluxes for one or more homogenized regions
  - material – initial nuclide atom densities for one or more material regions
  - library – file with neutron reaction cross sections
- … and a number of optional input files
  - splprods – constant production/depletion rates of nuclides from reactions outside the particle/energy domain of the CINDER reaction library
  - cxupdate – multigroup cross section data that replaces or adds to the reactions in the data library
  - locate – gives paths to the CINDER library and cxupdate files
  - dnz – contains the results of a CINDER calculation for earlier times and a different irradiation history

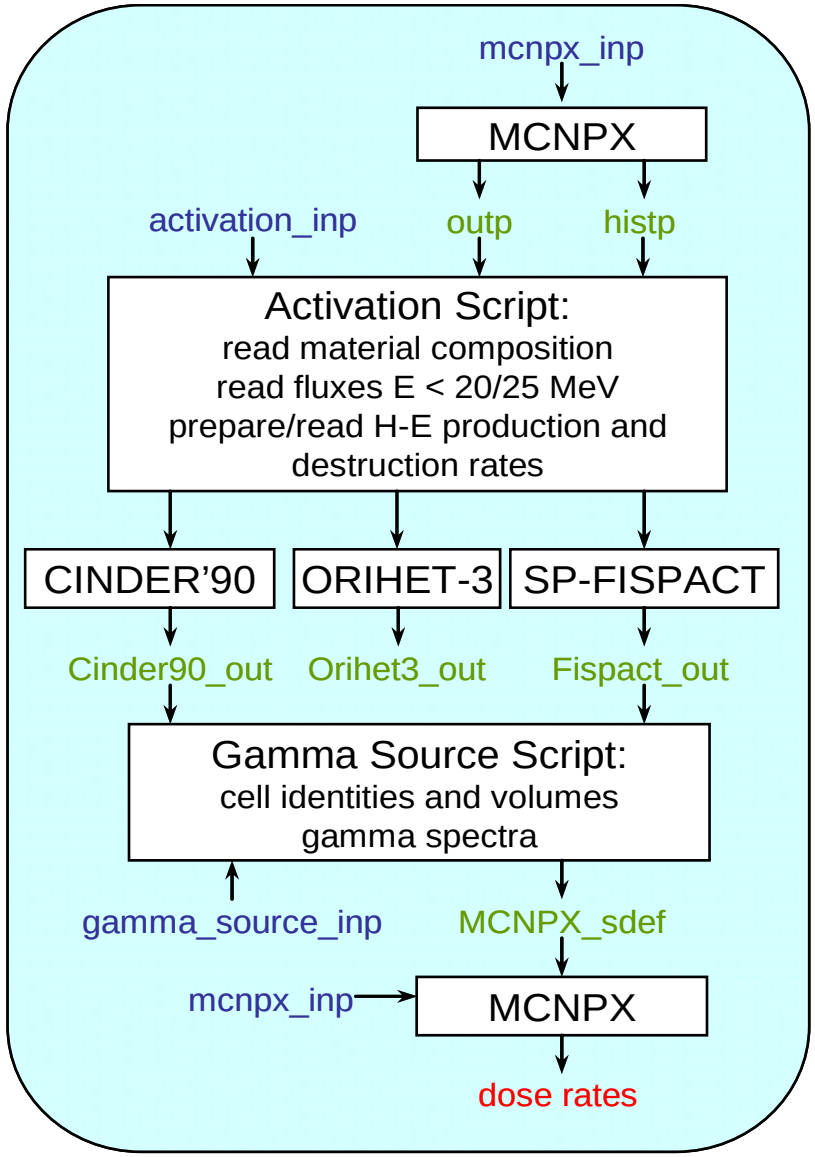
Running CINDER

- CINDER produces a number of output files, including
  - results – the main output file provides initial nuclide inventories and, for each nuclide, the atom density, activity density, and delayed neutron production at the end of each time step; also decay rate, absorption rate, spontaneous fission rate and fission rate
  - alldnz – a binary file giving the atom densities of all nuclides present initially or produced during the calculation at each time step
  - newshort – a binary file containing the library data used with flux-integrated reaction data

Activation Script

- Scripting tools written in Perl facilitate preparing CINDER input and running the code





CINDER input files

- CINDER offers the use of list-directed or namelist input
- General rules for list-directed CINDER input files
  - Input values are separated by commas, slashes, or at least one blank
  - A data value which is to be repeated n times may be given a repeat count n* (e.g. 3*4)
  - If there is no data value between successive separators, the default value of the parameter is used
- The namelist input, which is keyword driven, may be more suitable for newer users

CINDER input files

- input – identifies flux, material, temporal history, and other problem parameters
  - alphanumeric problem identification
  - flux and spallation scaling [the same energy dependence is used for the entire problem, but the normalized level can change)
  - Fission neutron spectrum selection
  - Region volume, material name, flux name, and alphanumeric information for table production
  - Selection of numerical parameters controlling the precision of calculations
  - Temporal history specifying "campaigns" in which the flux magnitude is unchanged, but may involve a number of time steps
  - Post-processing specifications

Record	Format	Variables
1	A80	calculation
2	free-form	volcc, flxmlt, flosig, signif, epsm, epsn, exponmax, kabc, kchn, klib, nfe, ltsdnz, nlintl, nosame, tabopt, timeout, gasopt, run_tab, suffix, fine_dg, coarse_dg, fine_dn, coarse_dn
3	A80	description repeated nlintl+1 times
4	A8	fluxname
5	A6	matname
Records 6 & 7 are repeated for each campaign.		
6	free-form	if(flxmlt < 0.0) jts, factor, cp, dcp
	free-form	if(flxmlt > 0.0) jts, factor
7	free-form	deltat(i), iubt(i), (i=1, jts)
8	A20, I4	vols_info, itsord

CINDER *input* file

Record	Format	Variables
1	A80	calculation
2	free-form	volcc, flxmlt, flosig, signif, epsm, epsn, exponmax, kabc, kchn, klib, nfe, ltsdnz, nlintl, nosame, tabopt, timeout, gasopt, run_tab, suffix, fine_dg, coarse_dg, fine_dn, coarse_dn
3	A80	description repeated nlintl+1 times
4	A8	fluxname specifies a flux from *fluxes* file
5	A6	matname specifies a material from *material* file
Records 6 & 7 are repeated for each campaign.		
6	free-form	if(flxmlt < 0.0) jts, factor, cp, dcp
	free-form	if(flxmlt > 0.0) jts, factor
7	free-form	deltat(i), iubt(i), (i=1, jts)
8	A20, I4	vols_info, itsord

Used to specify a constant-power approximation

Time step at which to rank quantities

Controls post-processing

Example of CINDER *input* file

- Examples are from a CINDER example problem for a DT neutron source in the center of a spherical polyethylene moderator

```
  DT source
1.93732e+004,1.00000e+000,0.000e+000,,,,,0,0,0,2,-1,2,0,,,1,1,'  ',10000,2000000/
  act04 -- D-T neutron source test problem
  cell 9
 using libarary:
tally  4
mat  1
1 1.0
    30.0   'd'
```

specifies tally 4 from *fluxes* file

specifies material 1 from *material* file

one time step, normalization 1.0 (a decay step has normalization of 0)

time step of 30 days

CINDER *fluxes* file

Record	Format	Variables
1	A72, I4	title, ngnx
Records 2 & 3 are repeated for each flux in the file.		
2	A8, 42X, E12.0	fxlbname, sumflx
3	8E10.0	flux(i),i=1,ngnx

title	Descriptive information on the regions with fluxes in this file.
ngnx	Number of neutron energy groups used in fluxes. Must be consistent with ngn of *library* file.
fxlbname	Name assigned to flux in this region. Must agree with fluxname read from the *input/input_nl* file.
sumflx	Sum of neutron multi-group flux values in this region.
flux	Fluxes are given ngnx groups in increasing energy order.

… even though the cross sections are given in decreasing order

Example of CINDER *fluxes* file

175 energy groups

```
  DT source                                                                  175    0
tally  4     Integral of Rebinned flux is          1.3316e+05
5.227e+0047.902e+0033.034e+0022.881e+0022.844e+0022.603e+0022.594e+0022.504e+002
2.430e+0022.427e+0022.500e+0022.505e+0022.390e+0022.487e+0022.579e+0022.613e+002
2.549e+0022.592e+0022.470e+0022.530e+0022.402e+0022.489e+0022.530e+0022.550e+002
2.550e+0022.623e+0022.569e+0022.538e+0022.587e+0022.654e+0022.584e+0022.457e+002
2.750e+0022.607e+0022.561e+0022.701e+0021.109e+0021.025e+0025.317e+0015.602e+001
1.107e+0021.091e+0021.093e+0021.613e+0022.778e+0022.781e+0022.641e+0021.671e+002
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2.102e+0025.598e+0022.856e+0022.712e+0022.962e+0023.052e+0023.108e+0023.250e+002
3.452e+0023.520e+0023.286e+0023.716e+0023.517e+0023.927e+0023.941e+0024.135e+002
2.623e+0021.313e+0026.619e+0016.175e+0012.870e+0024.840e+0024.566e+0024.593e+002
4.325e+0025.122e+0024.804e+0029.659e+0021.050e+0031.086e+0036.033e+0026.038e+002
6.106e+0026.381e+0027.266e+0027.036e+0027.180e+0024.582e+0022.575e+0028.700e+002
8.725e+0026.975e+0027.884e+0029.235e+0021.010e+0031.102e+0038.168e+0029.293e+002
1.073e+0031.246e+0031.259e+0036.545e+0027.279e+0021.998e+0032.627e+0031.734e+004
1.448e+0010.000e+0000.000e+0000.000e+0000.000e+0000.000e+0000.000e+000
```

Monoenergetic source at 14.06 MeV – higher energy groups have zero flux!

CINDER *material* file

- initial nuclide atom densities for one or more material regions

Record	Format	Variables
1	A80	Descriptive information regarding fluxes in this file.
2	A6, I4, E10.0	mtlbname, nzero, atoms
Record 3 is repeated for each of the nzero nuclides.		
3	I7, E13.0	jazs, fracatj

Example of CINDER *material* file

- initial nuclide atom densities for one or more material regions (in this case, polyethylene)

material name

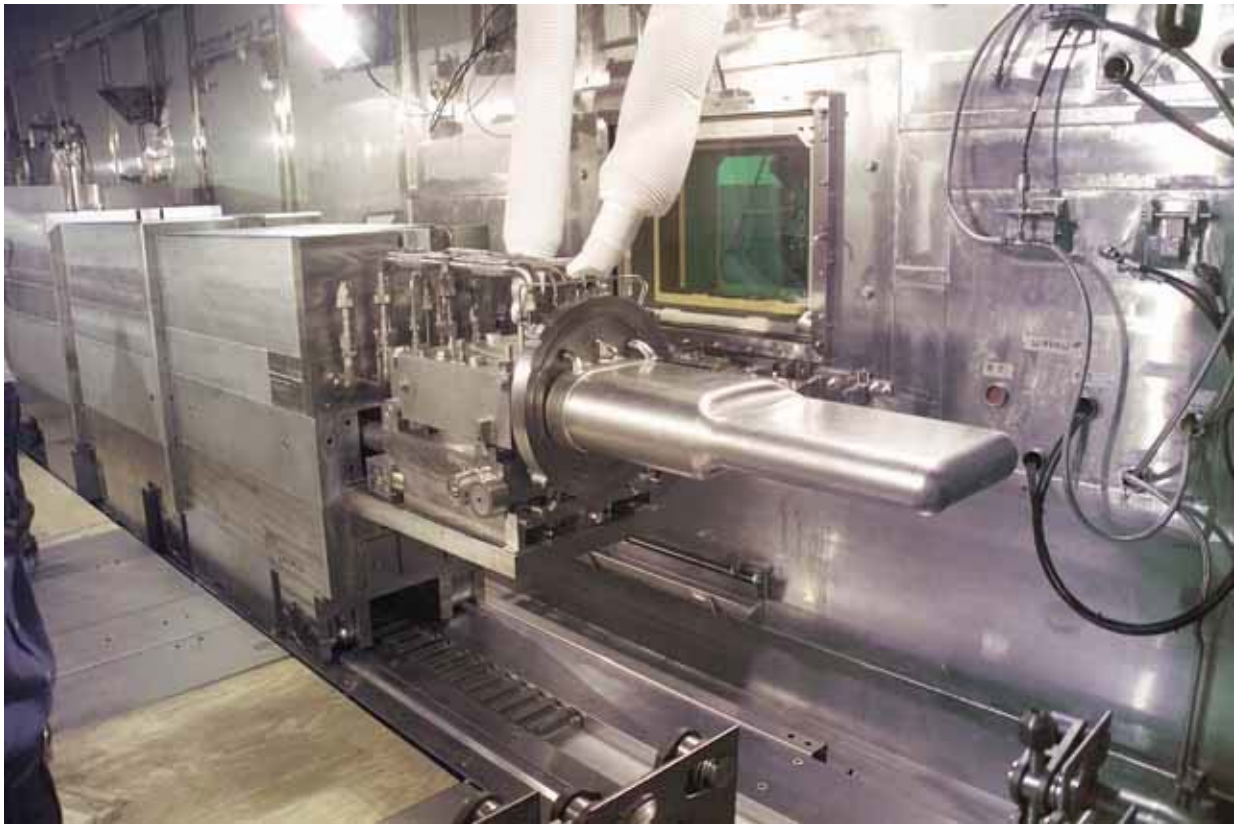
4 nuclides in list

```
   DT source
 mat   1    40.12235600
   10010    6.666e-001
   20010    1.000e-004
  120060    3.297e-001
  130060    3.667e-003
```

Atom density in atoms/bn-cm

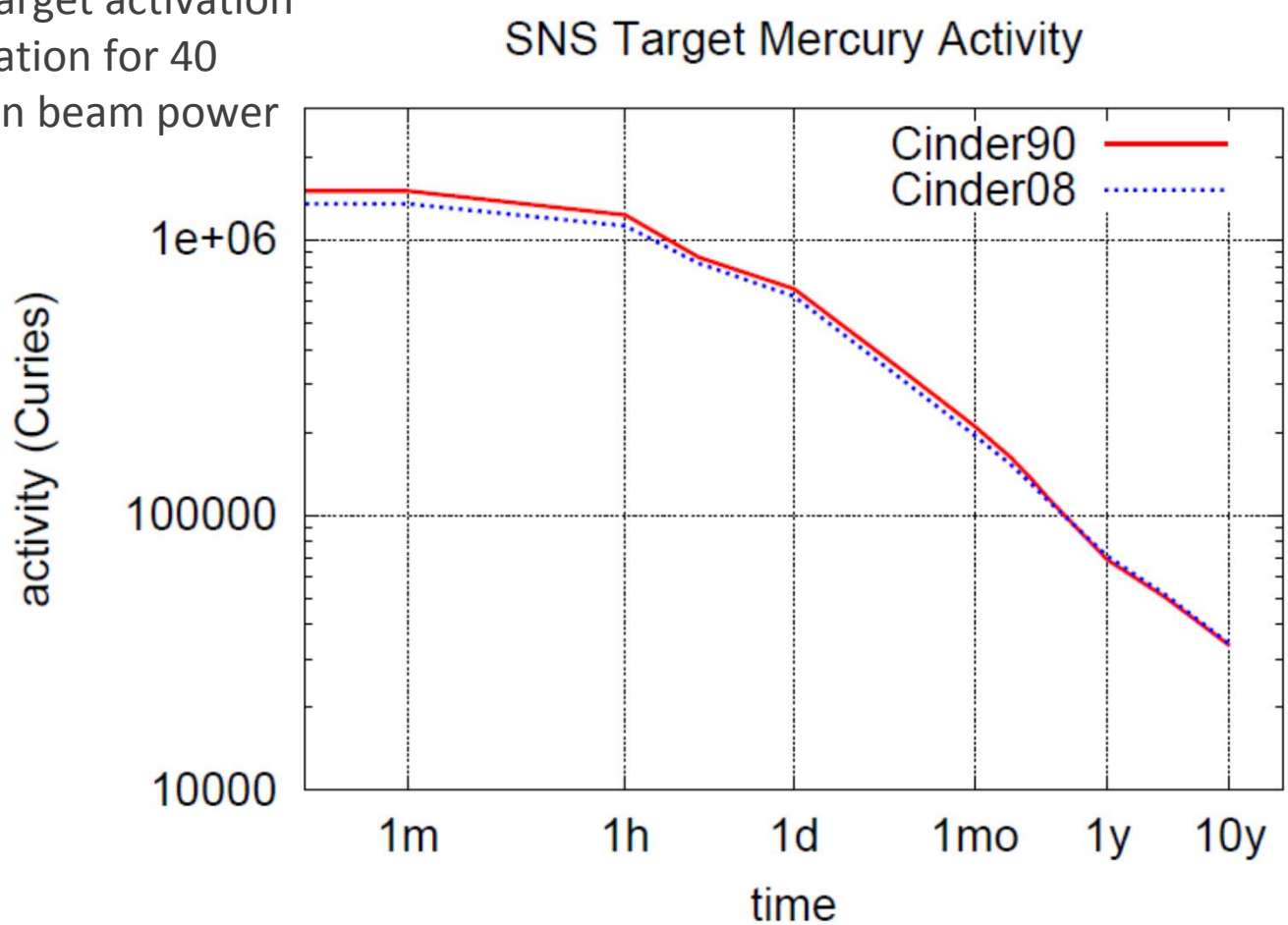
CINDER90 vs CINDER2008 – SNS Mercury Target

- The Spallation Neutron Source uses a liquid mercury target (high Z, high density, liquid at room temperature) to generate neutrons for use in experiments in condensed matter and fundamental physics



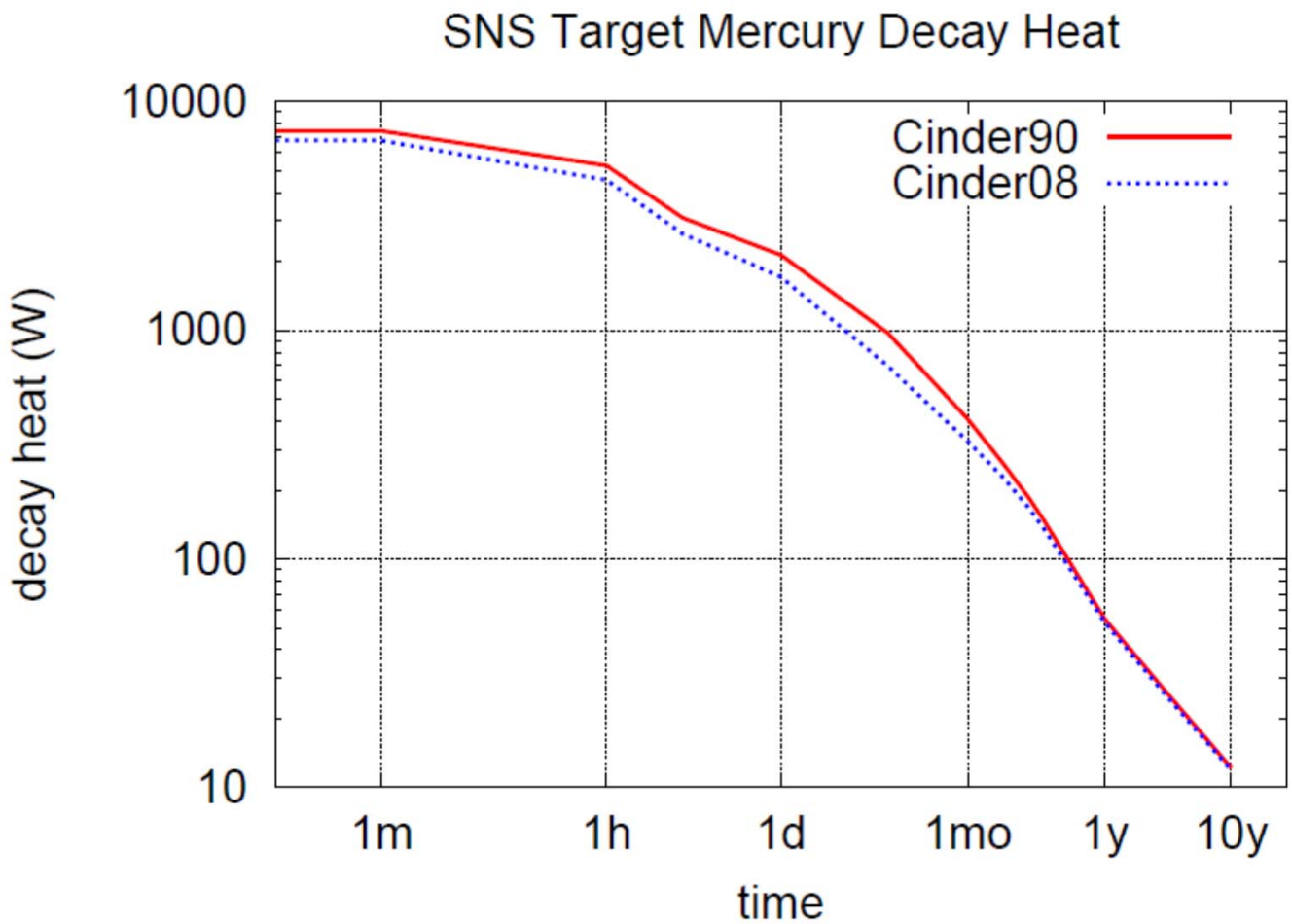
CINDER90 vs CINDER2008 – SNS Mercury Target

- All CINDER calculations use the same MCNPX output and the CINDER90 and CINDER08_fission libraries
- SNS liquid mercury target activation for 5000 hrs/yr operation for 40 years at 2 MW proton beam power



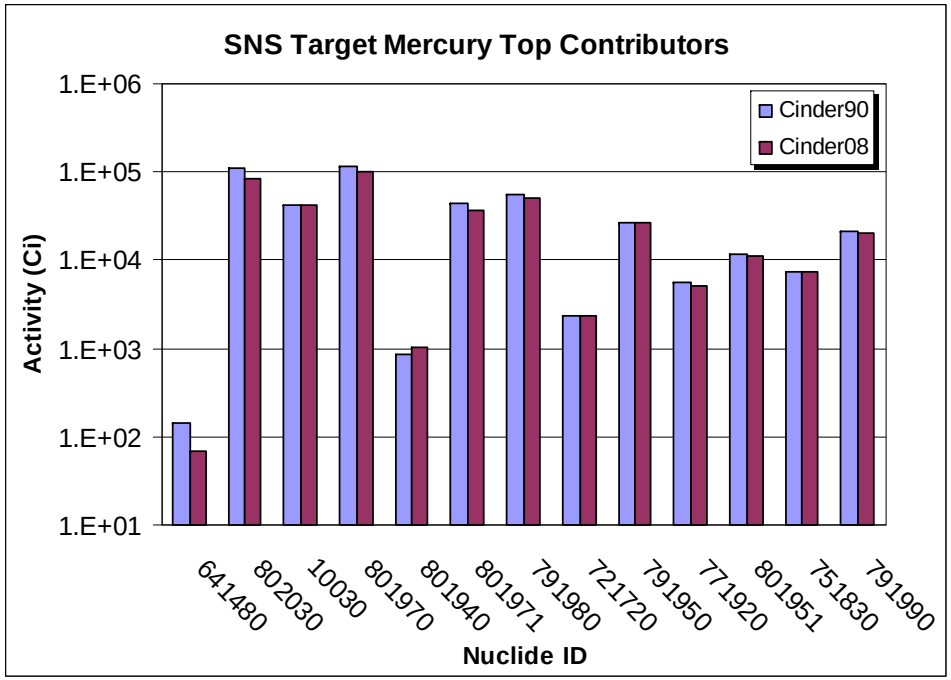
CINDER90 vs CINDER2008 – SNS Mercury Target

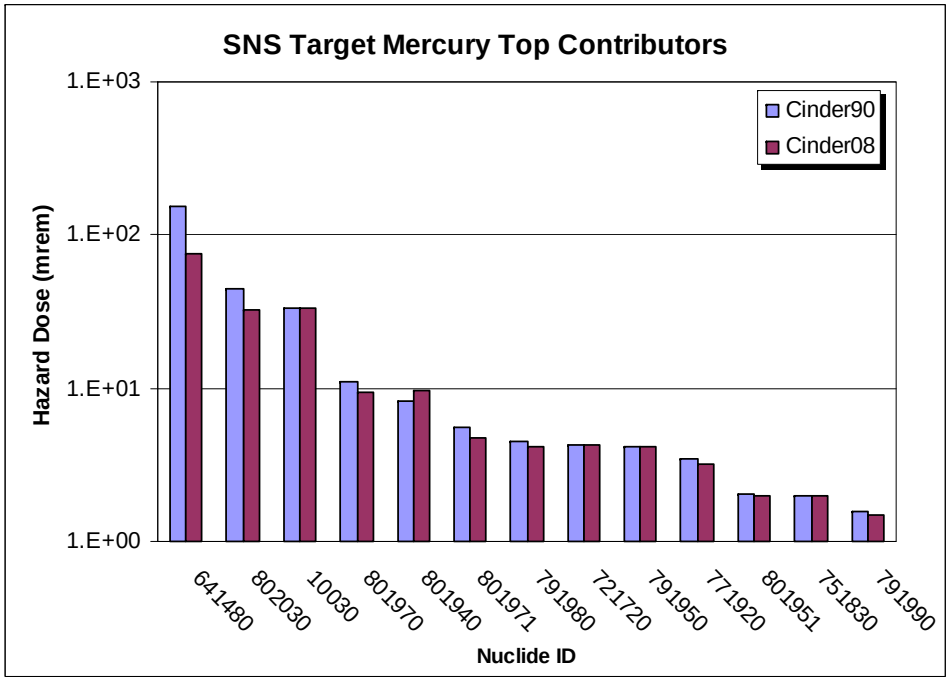
- SNS liquid mercury target decay heat for 5000 hrs/yr operation for 40 years at 2 MW proton beam power



CINDER90 vs CINDER2008 – SNS Mercury Target

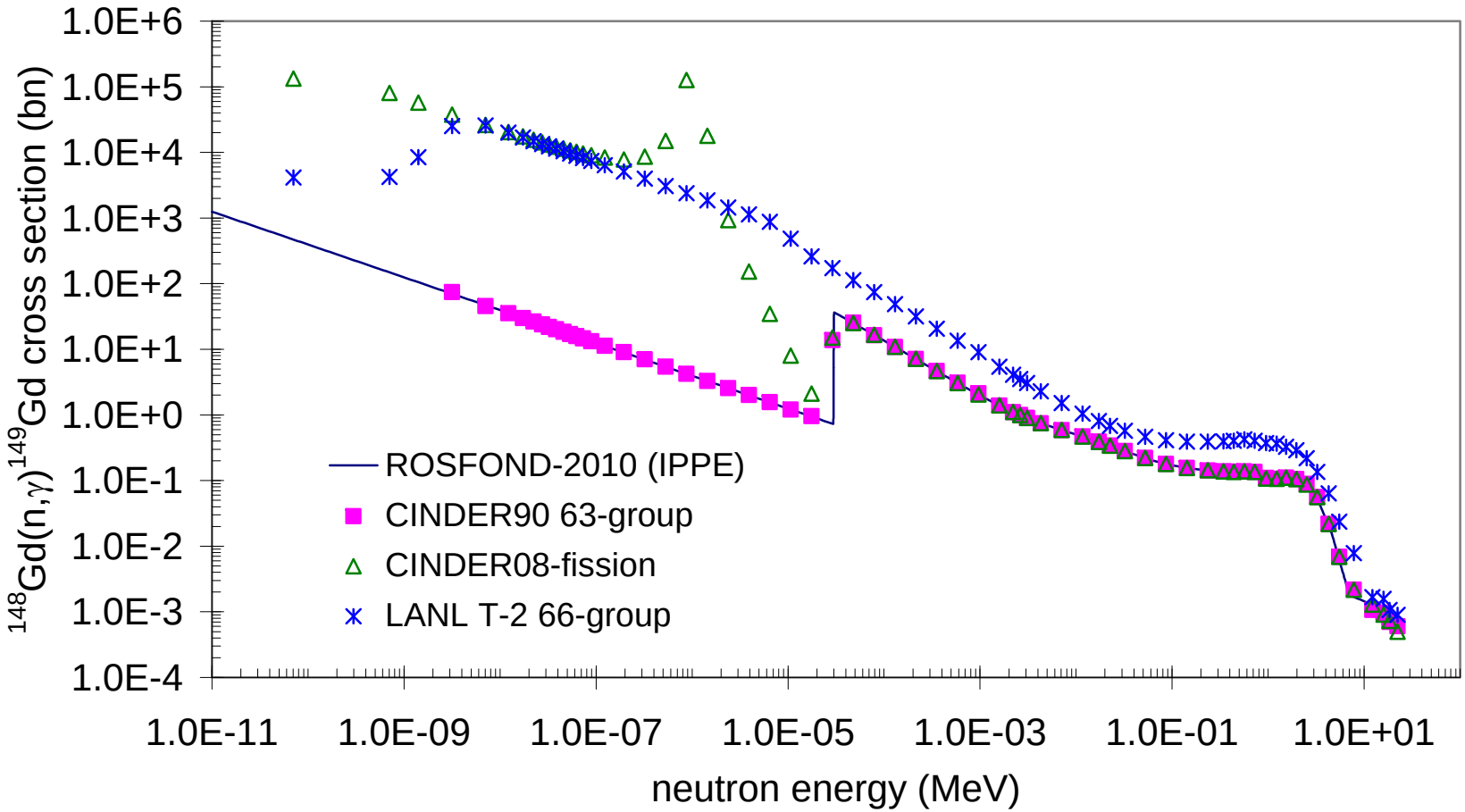
- Radioactivity release due to loss of heat sink
- Hazard comparison based on release fractions, inhalation dose conversion factors, dispersion and breathing factors, and 30 minutes decay time following release





CINDER90 vs CINDER2008 – SNS Mercury Target

- Difference in ^{148}Gd contribution due to difference in destruction rates
- ^{148}Gd(n,γ) xsecs from CINDER90 and CINDER08 don't agree, and different from T-2 evaluation



Use of CXUPDATE File

- New reaction cross sections can be input to CINDER using a file named cxupdate
- Energy group structure for cxupdate must be the same as the main library being used for that problem (there are no checks to make sure this is the case)

Record	Format	Variables
1	free-form	azst, azsp, scale, xx(i), (i=1,ng)

azst	AZS value of target nuclide
azsp	AZS value of product nuclide (for fission set to 0)
scale	Cross section scaling factor used, for example, to scale input cross section data to barns, as used in the library.
xx	Flux weighted multi-group cross sections
ng	Number of energy groups.

```
1480640 1490640 1.000
8.9493E-04  1.0667E-03  1.5702E-03  1.6806E-03  7.8323E-03  2.3622E-02  6.4067E-02
1.3534E-01  2.1908E-01  2.9038E-01  3.2633E-01  3.6382E-01  3.7434E-01  4.0380E-01
4.2347E-01  4.0460E-01  3.9497E-01  3.9038E-01  3.9379E-01  4.1288E-01  4.6544E-01
5.7277E-01  6.8059E-01  8.1054E-01  1.0492E+00  1.5188E+00  2.2813E+00  3.0616E+00
3.5396E+00  4.0829E+00  5.4404E+00  9.0522E+00  1.3451E+01  2.0585E+01  3.1696E+01
4.8571E+01  7.4105E+01  1.1336E+02  1.7300E+02  2.5920E+02  4.8444E+02  8.8005E+02
1.1352E+03  1.4478E+03  1.8550E+03  2.3932E+03  3.0746E+03  3.9792E+03  5.1008E+03
6.3649E+03  7.4472E+03  8.2328E+03  8.9210E+03  9.5939E+03  1.0397E+04  1.1365E+04
1.2369E+04  1.3442E+04  1.4857E+04  1.6851E+04  1.9928E+04  2.5620E+04  3.7749E+04
5.7418E+04  8.1010E+04  1.3257E+05
```

Use of CXUPDATE File

- Recall that the CINDER data libraries go from highest energy to lowest, and don't have all neutron groups for reactions with thresholds
- When inputting data using CXUPDATE, you have to use all energy groups
- An example for ^{204}Pb(n,n') ^{204m}Pb with the fission-weighted cross

cross section = 0 in 20-25 MeV group

```
2040820 2040821 1.000
0.0000E+00  1.5088E-01  4.6221E-01  5.4320E-01  3.9339E-01  2.7524E-01  1.8103E-01
9.1403E-02  4.2336E-02  2.0971E-02  1.1232E-02  7.8810E-03  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
0.0000E+00  0.0000E+00  0.0000E+00
```

Use of CXUPDATE File

- Recall that the CINDER data libraries go from highest energy to lowest, and don't have all n groups for reactions with thresholds
- When inputting data using CXUPDATE, you have to use all energy groups
- To change the ^{235}U fission cross section in the 58-67 meV energy group, you would use this CXUPDATE file (in CINDER90)

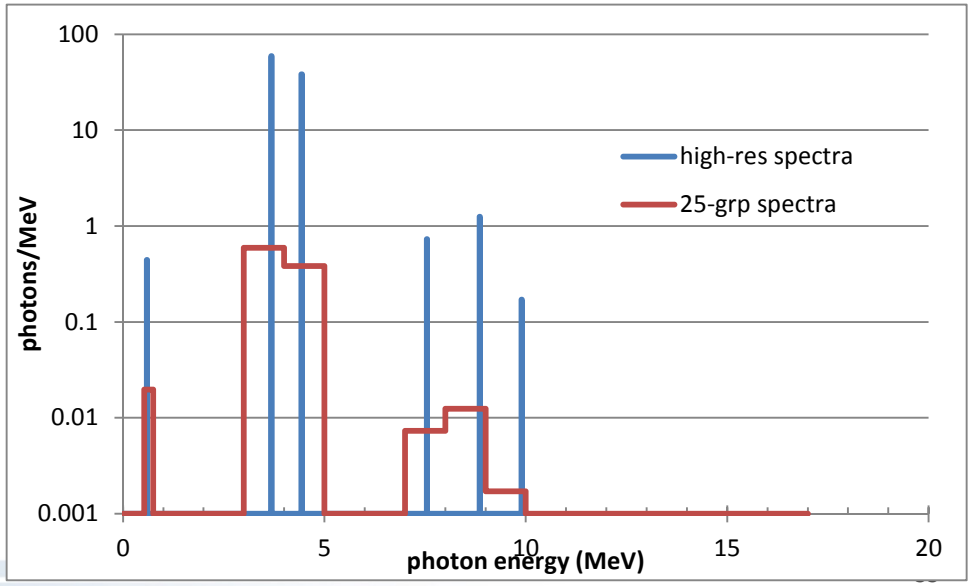
An entry of zero here denotes a fission cross section

New value for 58-67 meV group

```
2350920   0  1.0
1.7478E+03  1.0957E+03  8.5472E+02  8.2191E+02  5.9611E+02  6.5582E+02  4.8543E+02
5.2496E+02  4.0107E+02  3.8406E+02  3.7701E+02  3.6851E+02  2.6693E+02  2.2771E+02
1.8375E+02  1.6702E+02  7.9628E+01  6.5383E+01  2.8785E+01  1.4351E+01  1.8771E+01
1.9271E+01  7.7268E+01  4.9074E+01  5.3224E+01  4.6268E+01  2.4777E+01  2.0813E+01
2.0772E+01  1.3680E+01  1.3099E+01  8.2349E+00  6.8170E+00  8.2630E+00  5.2332E+00
4.9688E+00  4.3224E+00  3.2622E+00  2.7185E+00  2.3153E+00  2.1683E+00  1.9867E+00
1.8030E+00  1.6187E+00  1.4698E+00  1.3211E+00  1.2381E+00  1.1894E+00  1.1519E+00
1.1381E+00  1.1847E+00  1.2202E+00  1.2564E+00  1.2929E+00  1.2685E+00  1.1982E+00
1.1200E+00  1.0656E+00  1.5322E+00  2.0617E+00  2.1007E+00  1.9677E+00  1.9677E+00
```

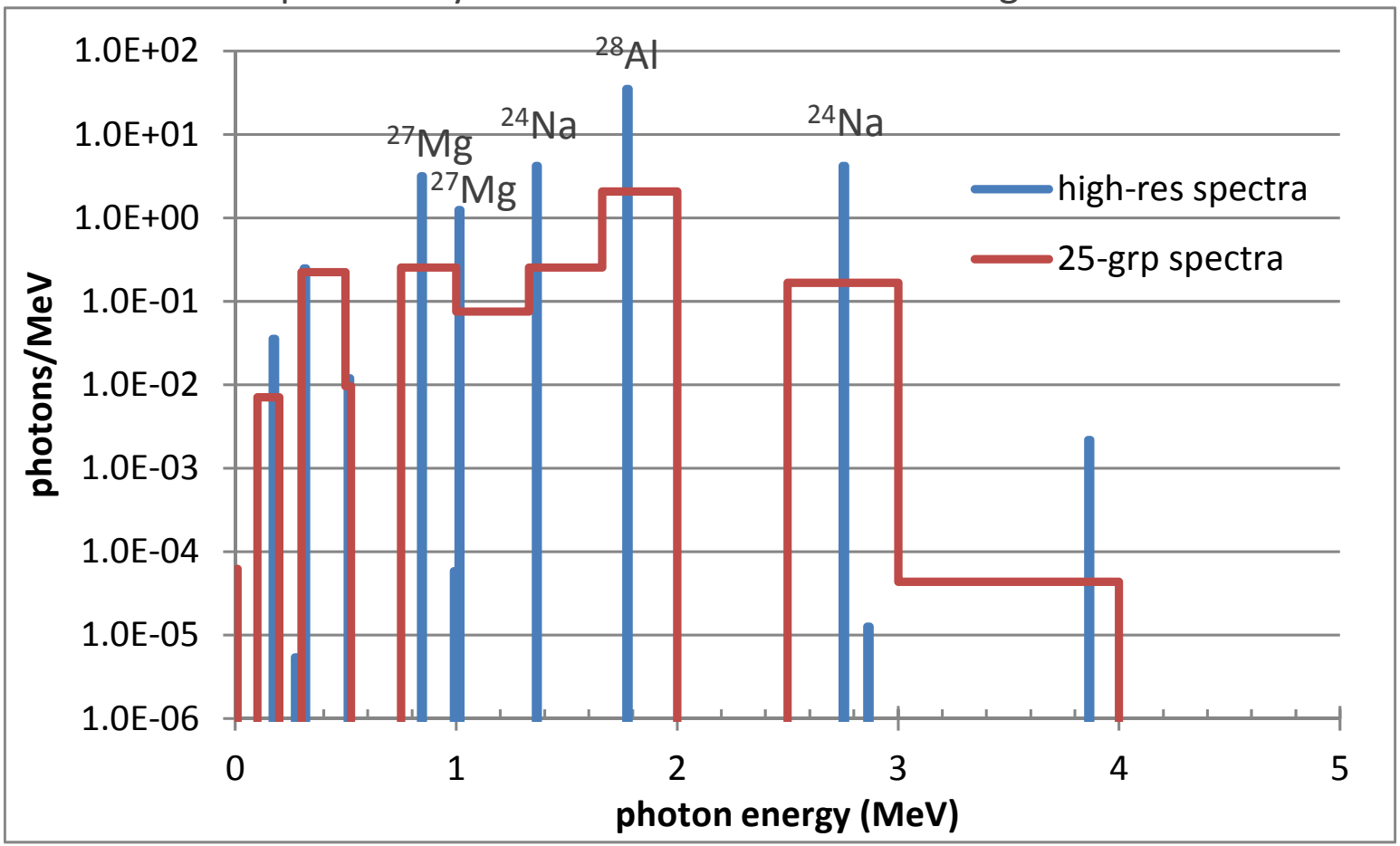
Gamma Spectra from CINDER

- CINDER90 output decay gamma spectra in a 25-group energy structure
- This output is maintained, but the user can also request high-resolution gamma decay spectra using the discrete and continuous source data in the library *cindergl.dat*
- The energy grid structure is defined by the user with variables fine_dg and coarse_dg (these have the default values 1000 eV and 10000 eV
  - Start with the finest bin structure as given by fine_dg
  - Group the discrete data using the fine group structure
  - Combine empty bins on the fine grid structure into a coarser grid, with the largest bin size limited to coarse_dg
  - Group the continuous energy spectra on the new variable-grid energy structure
- As an example, consider the decay gamma spectra from neutron capture in polyethylene
- If you look at the output files and see a lot of zero entries, it might be a good idea to increase coarse_dg



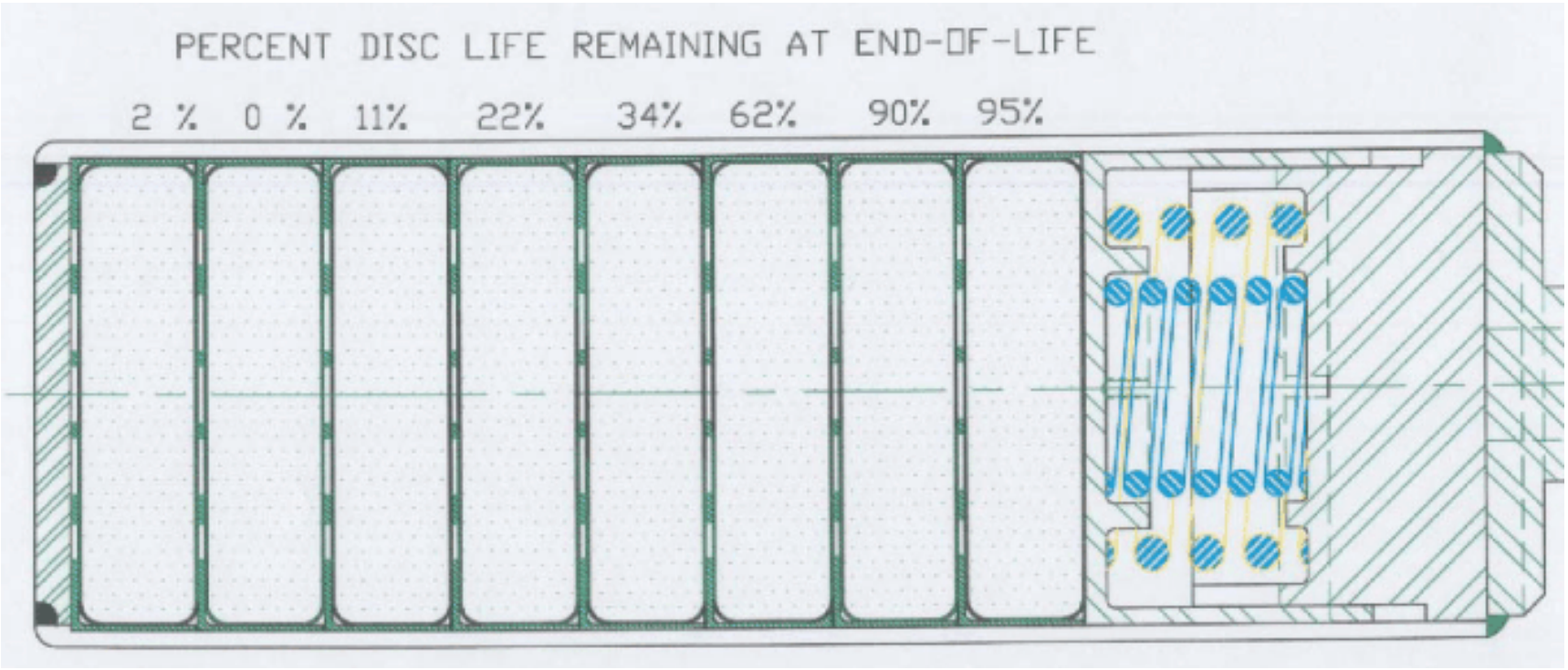
Gamma Spectra from CINDER

- Another example – neutrons irradiating aluminum
- The fine detail allows one to identify specific radionuclides in the spectrum
- The extra detail is potentially much more useful in modeling radiation detectors



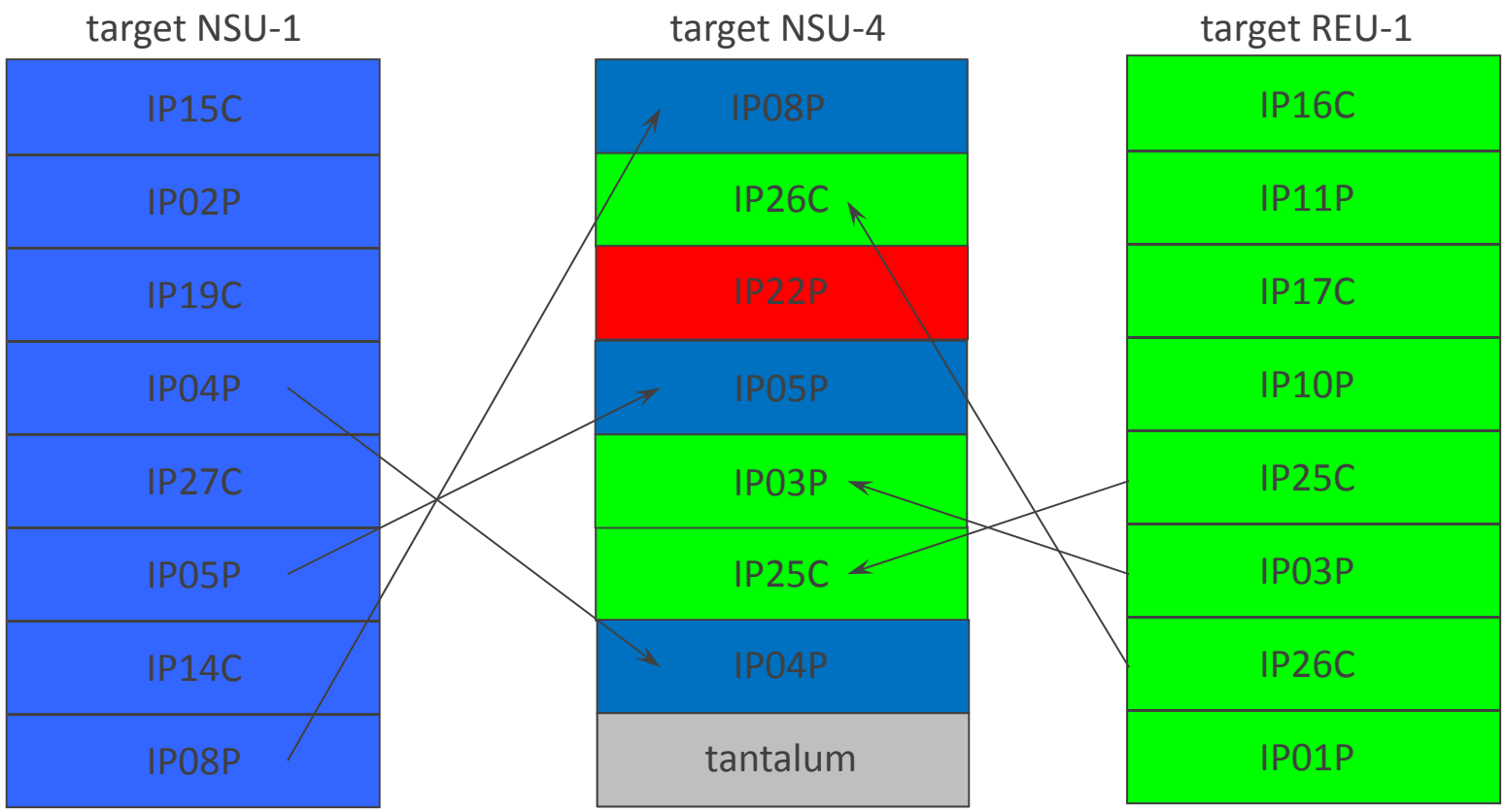
Use of *dnz* File in CINDER – IPNS Target

- The spallation target in use at IPNS at final shutdown included some depleted uranium disks that had been recycled from a previous target
- The proton beam stopped in the fourth disk, and the disks in the rear half of the target had remaining lifetime
- Calculation based on fissions as an indicator of disc power was performed to estimate remaining life



Use of *dnz* File in CINDER – IPNS Target

- Disks from the back half of two spent targets were used to make another target



Use of *dnz* File in CINDER – IPNS Target

- Radionuclide inventories for the disks in target NSU-4 were calculated in two steps
- Initial run to calculate the radionuclide inventories in the disks in their initial positions with the irradiation histories of their respective targets
- The alldnz output files for each disk were used as an input file to a second calculation
- The second calculation used the irradiation history for target NSU-4 and the neutron flux for the new disk position

Record	Format	Variables
1	A80	calculation
2	free-form	volcc, flxmlt, flosig, signif, epsm, epsn, exponmax, kabc, kchn, klib, nfe, ltsdnz, nlintl, nosame, tabopt, timeout, gasopt, run_tab, suffix, fine_dg, coarse_dg, fine_dn, coarse_dn
3	A80	description repeated nlintl+1 times
4	A8	fluxname
5	A6	matname
Records 6 & 7 are repeated for each campaign.		
6	free-form	if(flxmlt < 0.0) jts, factor, cp, dcp
	free-form	if(flxmlt > 0.0) jts, factor
7	free-form	deltat(i), iubt(i), (i=1, jts)
8	A20, I4	vols_info, itsord

Time step from previous calculation from which the calculated nuclide inventory in the dnz file should be read and used as the initial inventory of the present calculation (default = -1, do not use)

Summary

- CINDER2008 is a significant upgrade from CINDER90 – a different (and better) code, not merely an update
- CINDER2008 has undergone substantial development and testing
- The code comes with completely new reaction libraries with three different spectral weighting functions
- A number of examples for using CINDER2008 were discussed, but there are many others
- CINDER2008 runs under Linux, Windows, and MacOS, and can be compiled with Intel, Portland, Lahey, and gfortran compilers