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# AARE Activation Library Developments

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U.S. DEPARTMENT  
of **ENERGY**

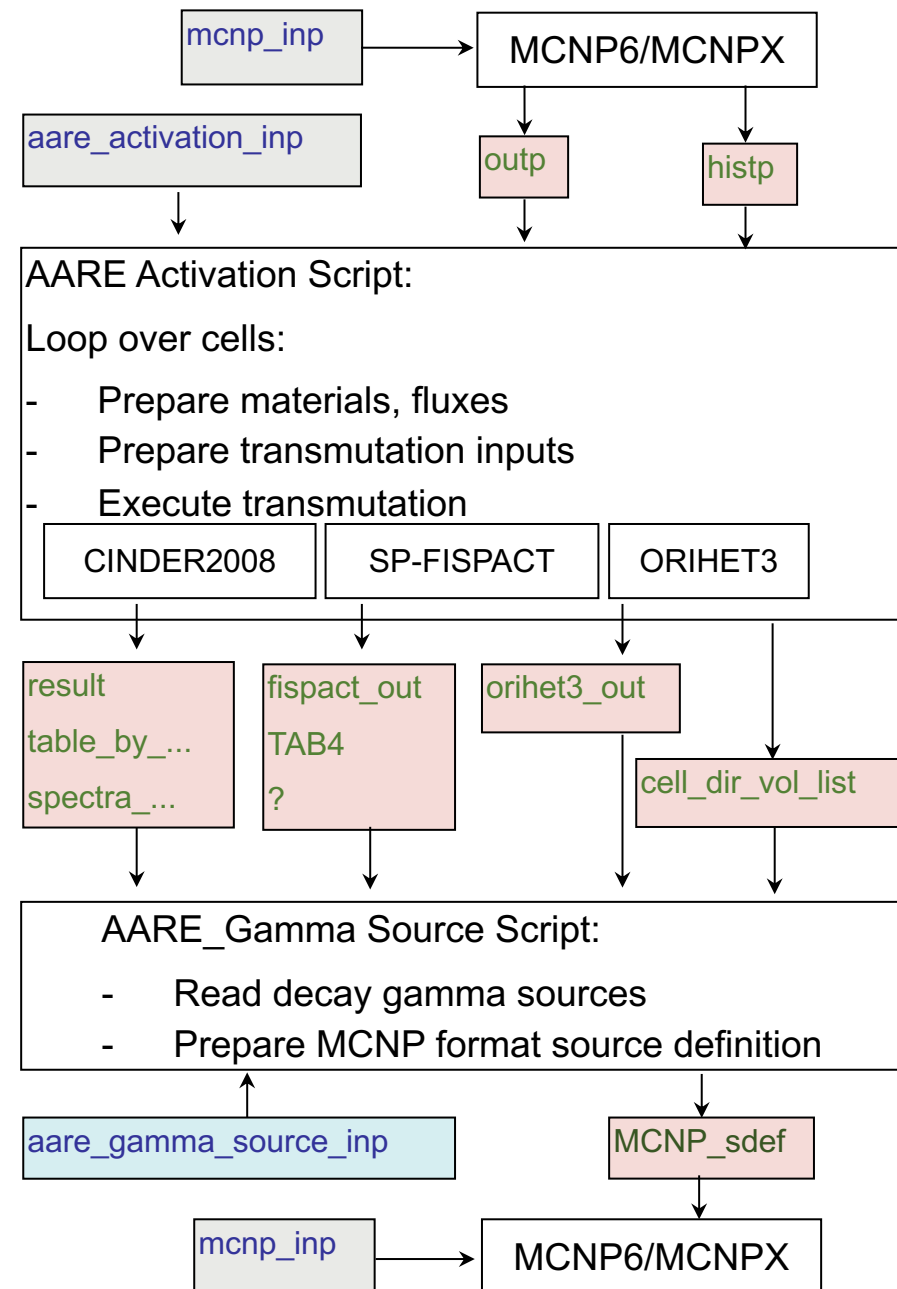
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# Layout

- AARE introduction
- Motivation
- AARE development roadmap
- CINDER library development overview
- Decay information updates
- Cross section updates
- Fission fragment yield updates
- Forging of the libraries
- Overview of library contents

# The AARE workflow

- Workflow geared around MCNP analyses of accelerator driven systems
- Generate radionuclide inventory information
- Generate decay gamma sources
- Perform decay gamma dose rate analyses
- RSICC Packages
  - CINDER\_1.05 (2008)
  - AARE\_1.0 (2018)



# Motivation

- MCNP evolved from MCNP5 -> MCNPX -> MCNP6
  - Neutron cross section libraries extended to 150 and 200 MeV with mix-and-match using models where no data are available
  - Charged particle cross section libraries introduced
- Nuclear data developments:
  - Progress in evaluated data: ENDF/B-VI -> ENDF/B-VII -> ENDF/B-VIII also JEFF, JENDL, KAERI ...
  - Nuclear reaction modeling provides large-volume libraries
- Make use of these developments to improve predictive capability

# AARE2 Development Roadmap

- New activation libraries
- Modernized CINDER code
- Update MCNP RNUCS tally
- Converting workflows to Python
- Develop mesh-based activation
- Develop plotting

# Here we cover CINDER Library Developments

- Update decay data basis
- Update activation cross section data
- Generate new charged-particle-induced and gamma-induced cross section libraries
- Extend the fission fragment distributions
- Merge all parts into a complete library

# Decay libraries provide:

- nuclide spin, parity, energy-level, half-life
- decay schemes
- decay products and their energy distributions

# Update decay library

- ENDF/B-VIII.0 as the basis, which gives the largest coverage among the evaluated data libraries
  - for 3742 nuclides
- Supplemented by data from various other sources
- Summing up to 5711 nuclides from 4084 in CINDER2008

# Cross section data libraries provide:

- Cross section data bases of pointwise data in ENDF-6 format
- Reaction cross sections for 200 explicit reaction channels to 30 MeV energy
- Radionuclide production cross sections above 30 MeV energy
- Fission cross sections

# New Activation cross sections for CINDER libraries

- Extending neutron libraries to 150 MeV energy
- Develop charged-particle-induced and gamma-induced activation libraries
- Starting out with TENDL cross section libraries (TENDL-2021, TENDL-2023, latest release TENDL-2025 not used yet)
- TENDL offers cross sections to 200 MeV energy for
  - 2850 nuclides
  - Neutrons, protons, deuterons, tritons, helions, alphas, gammas
- Supplemented by other sources to cover low mass nuclei for which TENDL uses ENDF/B-VIII with lower upper energy

# Library preparation steps

- Using NJOY2016 process pointwise library data into multigroup representations
  - of 339 groups for neutrons
  - of 47 groups for charged particles and gammas
  - Flat weighting spectrum for group collapsing
- TENDL2023 data for 2835 nuclides
- Neutron library supplemented by
  - 16 nuclides from TENDL2021
  - 3 nuclides from ENDF/B-VIII.1
  - 7 nuclides from JENDL5
  - 9 nuclides from IEAF2001
- Proton library supplemented by 4 nuclides from JENDL5

# Fission Fragment Yields

- Listing of fission fragment nuclides with abundance per fission event

# Fission fragment yields

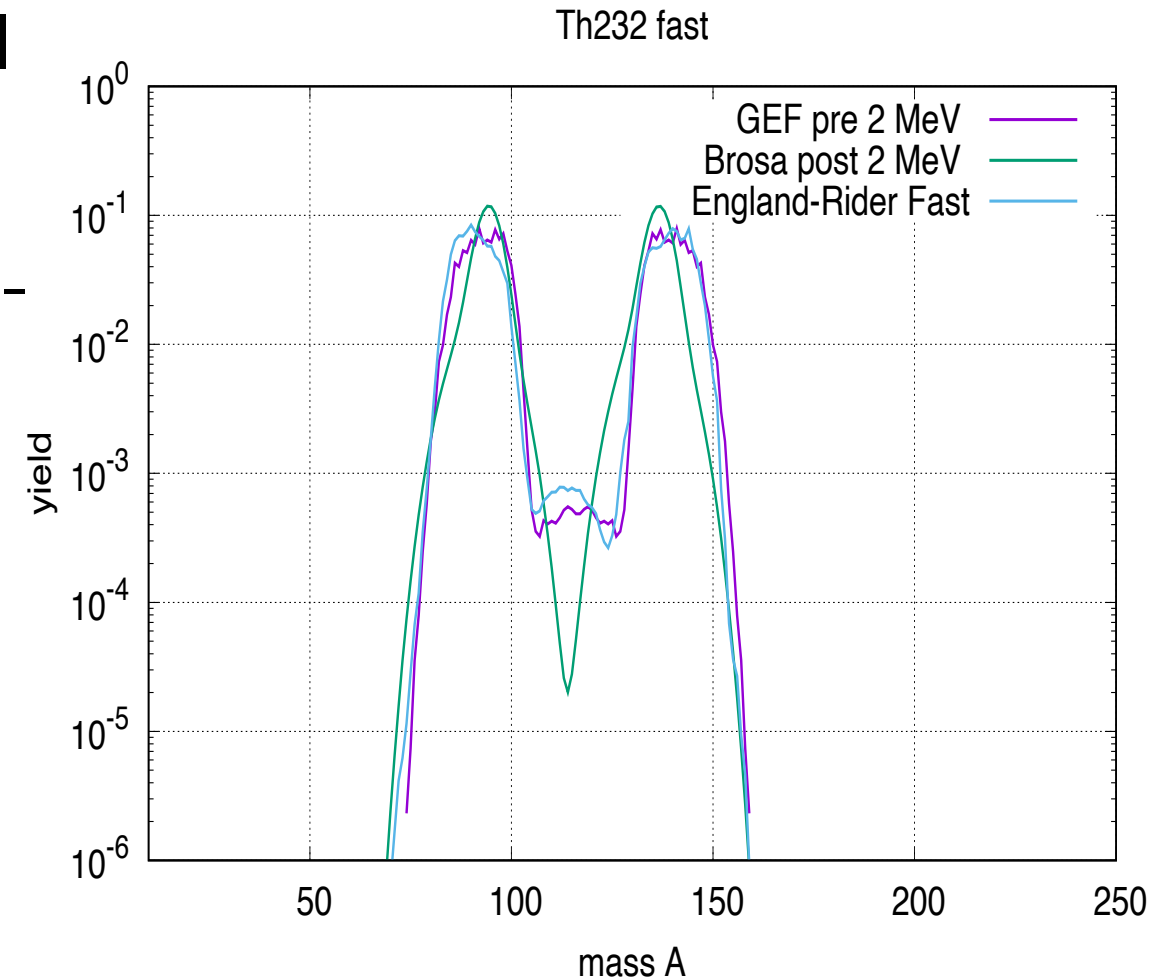
- No fission fragment libraries for charged particle and gamma induced reactions exist.
- By extending the data range to 150 MeV considerably increases the nuclides with fission channels.
- The fission fragment distributions exhibit a strong dependence to incident particle energy.
- A new approach needed to be taken.

# Fission fragment yield calculations (1)

- The TALYS2.0 code used for producing the TENDL libraries can be applied to perform fission fragment yield analyses with
  - BROSA model (fully functional with phenomenological model)
  - GEF model (insufficiently only first chance fission followed and requires evaporation of pre-evaporation fission fragment distributions).
- Modifications to TALYS2.0 developed:
  - by updating GEF model from 2016 version to 2023 version,
  - by building a library of fission fragment deexcitation information for 4200 possible pre-evaporation fission fragments for a list of excitation energies from 1-100 MeV.
  - expand TALYS2.0 by generating pre-evaporation fission fragment distributions from multi-chance fission branches and applying the deexcitation library for producing post-evaporation (final) fission fragment distributions.

# Generate Fission Fragment libraries

- Perform TALYS2.0 analyses for all CINDER radionuclides with fission channel for neutron-, charged-particle-, and gamma-initiated reactions (about 800 per sub-library) and for all energy groups.
- Perform TALS2.0 analyses for 90 spontaneous fission nuclides of the CINDER library by running cases of low-energy incident gammas.

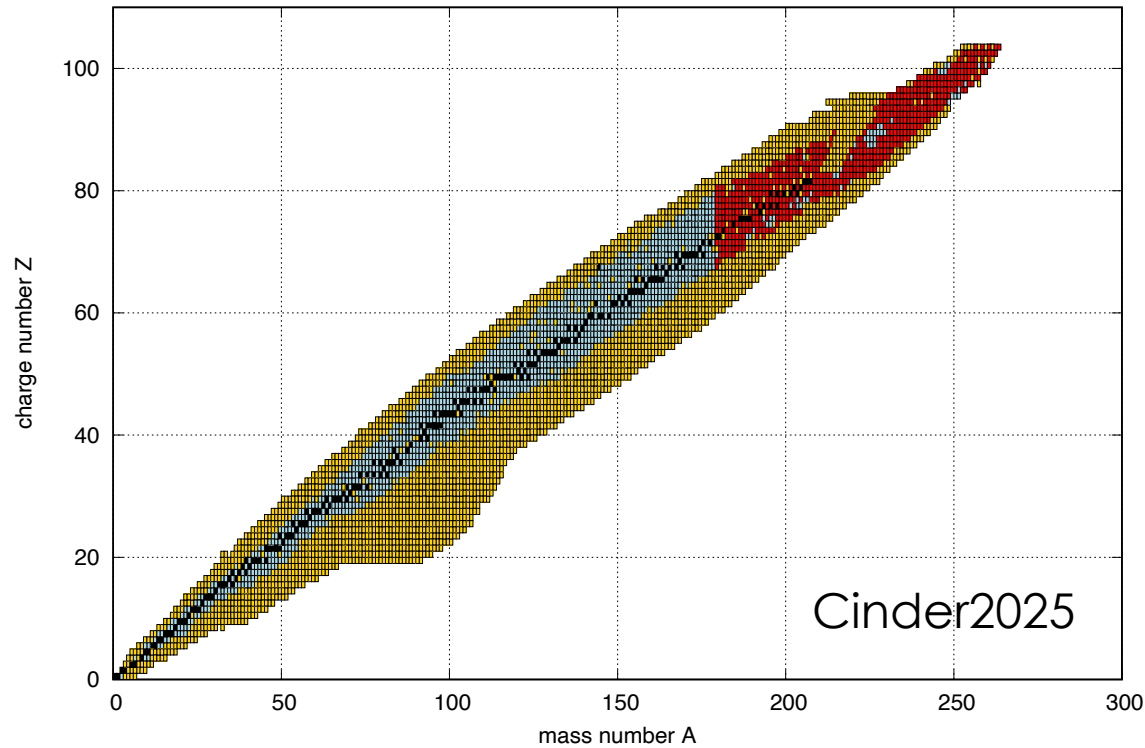


# The Creation of the CINDER Libraries

- The Library\_Maker\_Tool of the AARE package was updated to merge all the decay, cross section, and fission fragment yield data into independent sub-libraries for neutrons ... gammas.
- Upgrades applied for:
  - Merging explicit reaction channel and radionuclide production data to unified cross sections;
  - Adding energy-dependent fission fragment yield blocks to each fissile radionuclide, and a block of fission Q-values;
  - Adding the nuclide-specific spontaneous fission yield data;
  - Adding the mapping of reaction outcomes from TENDL and other sources to CINDER (impacted mostly metastable states).

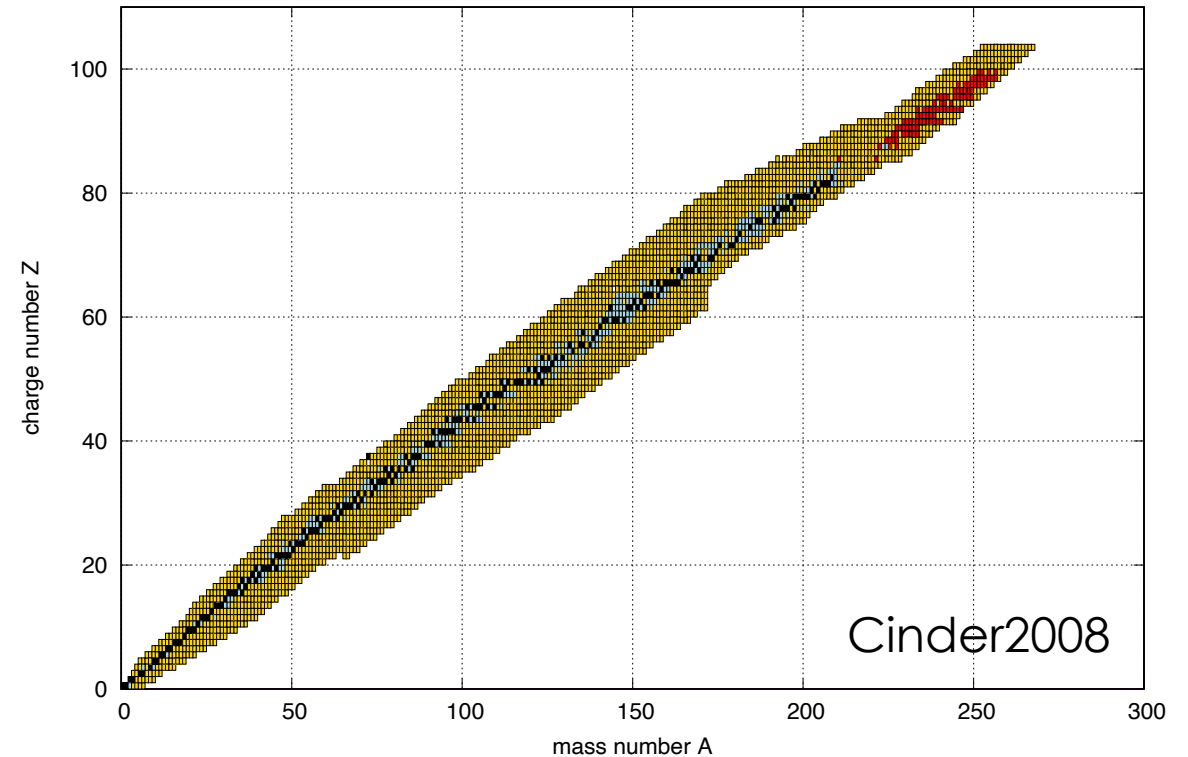
# Neutron library comparison: Cinder2025 vs Cinder2008

C25 Nuclide Map flagging Stables Cross-section and Fission Coverage



- 5711 nuclides
- 250 stable nuclides (black)
- 2752 nuclides with cross section (blue)
- 858 fission nuclides (red)

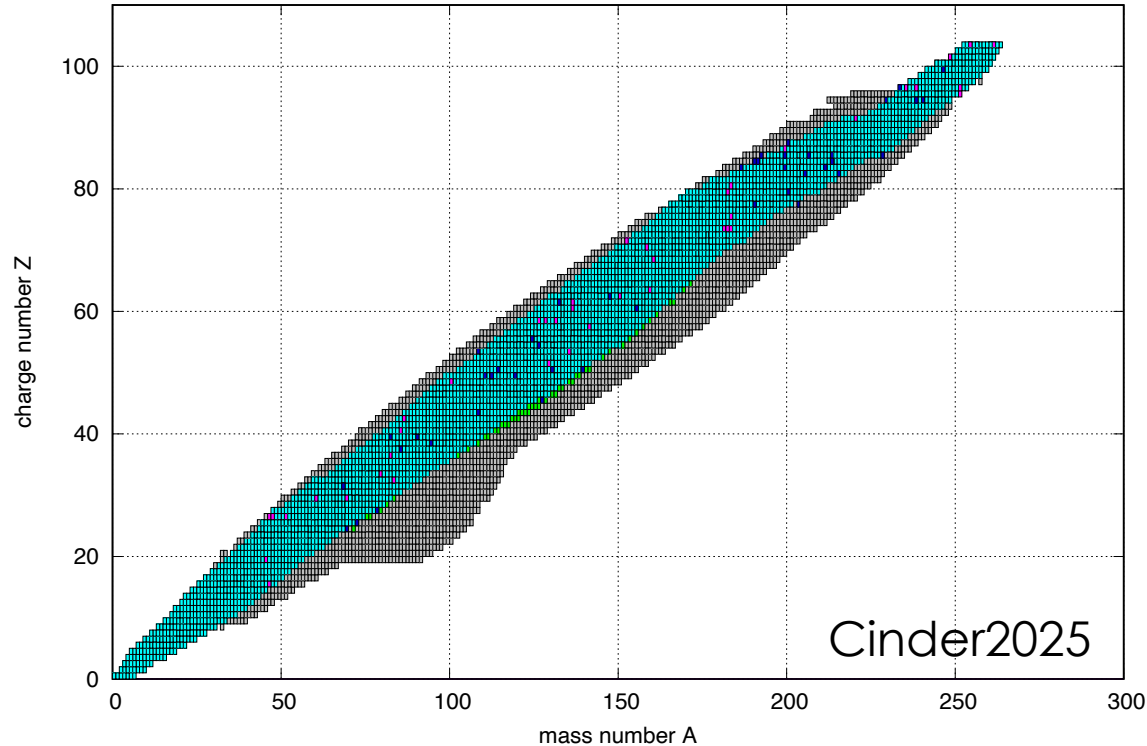
C08 Nuclide Map flagging Stables Cross-section and Fission Coverage



- 4084 nuclides
- 248 stable nuclides (black)
- 819 nuclides with cross section (blue)
- 103 fission nuclides (red)

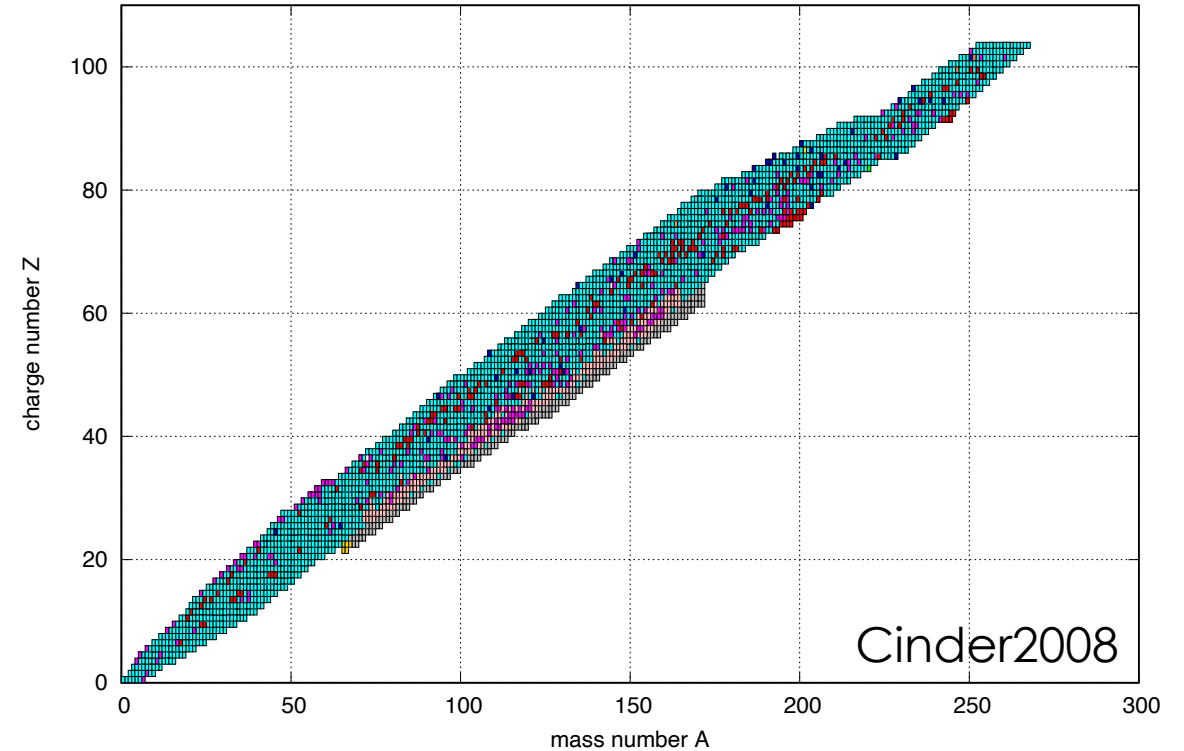
# Decay information sources: Cinder2025 vs Cinder2008

C25 Nuclide Map showing Decay Data References



3742	ENDF/B-8.0	(cyan)
59	JEFF33	(magenta)
1	JENDL5	(red)
80	NDS	(blue)
52	ENSDF	(green)
1768	Moeller 2019	(grey)

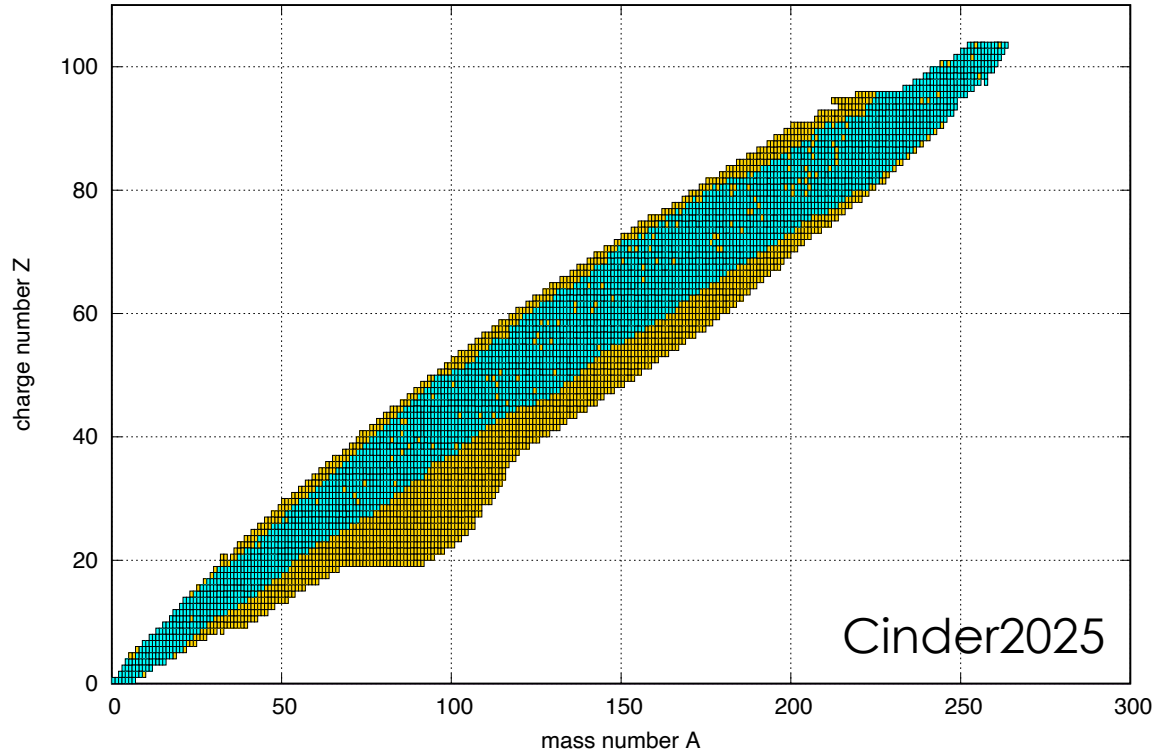
C08 Nuclide Map showing Decay Data References



2864	ENDF/B-7.0	(cyan)
421	JEFF31	(magenta)
278	EAF	(red)
219	ENDF/B-6.0	(pink)
106	NDS	(blue)
9	XDL	(coral)
181	Moeller 1997	(grey)

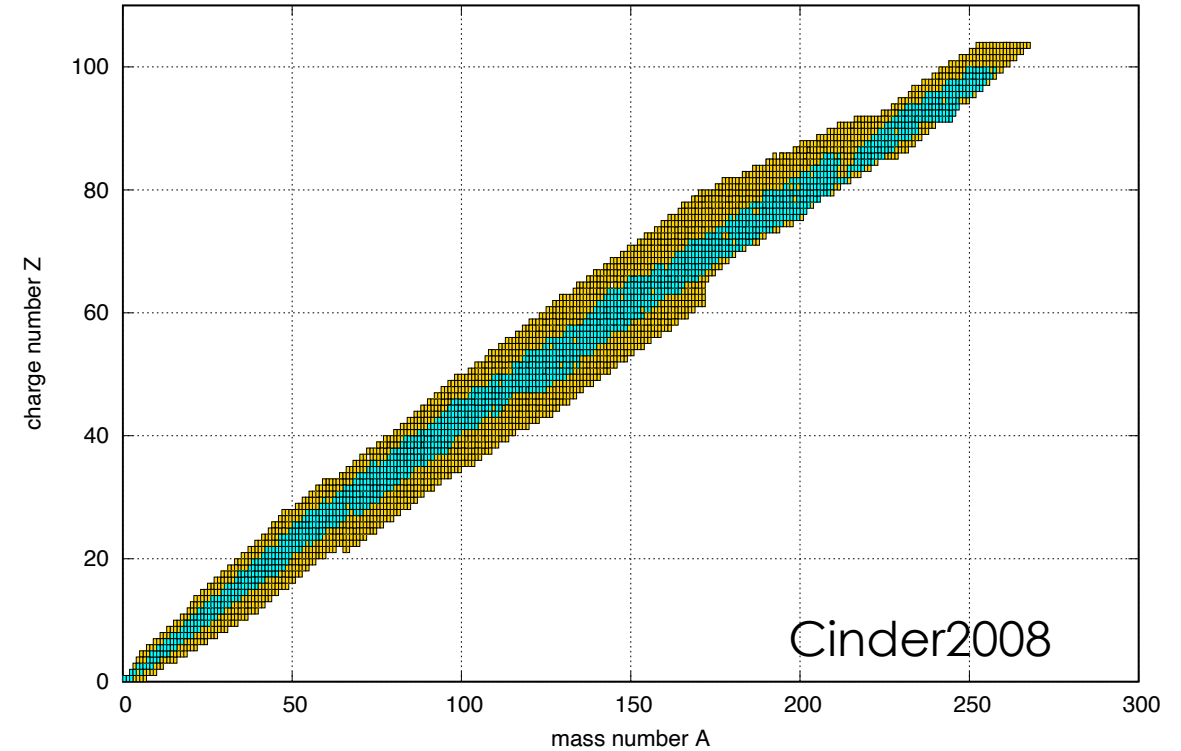
# Nuclide production coverage: Cinder2025 vs Cinder2008

C25 Nuclide Map showing Reaction Product Coverage



3647 nuclides produced by reactions

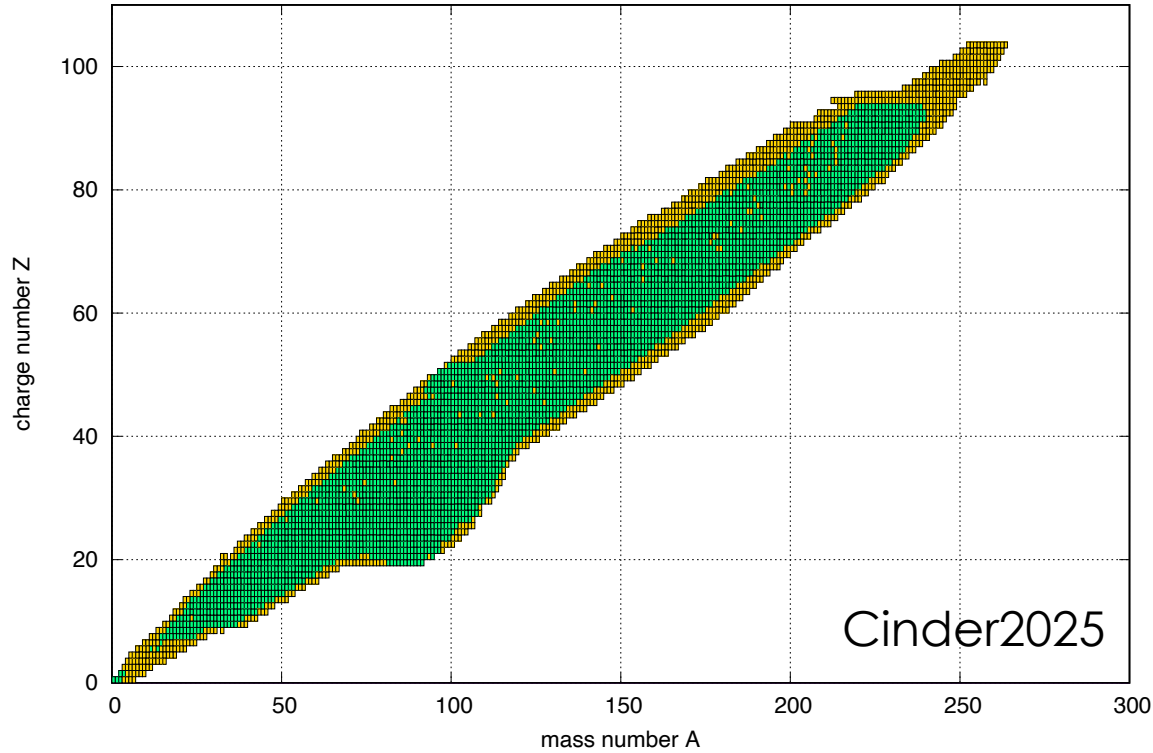
C08 Nuclide Map showing Reaction Product Coverage



1808 nuclides produced by reactions

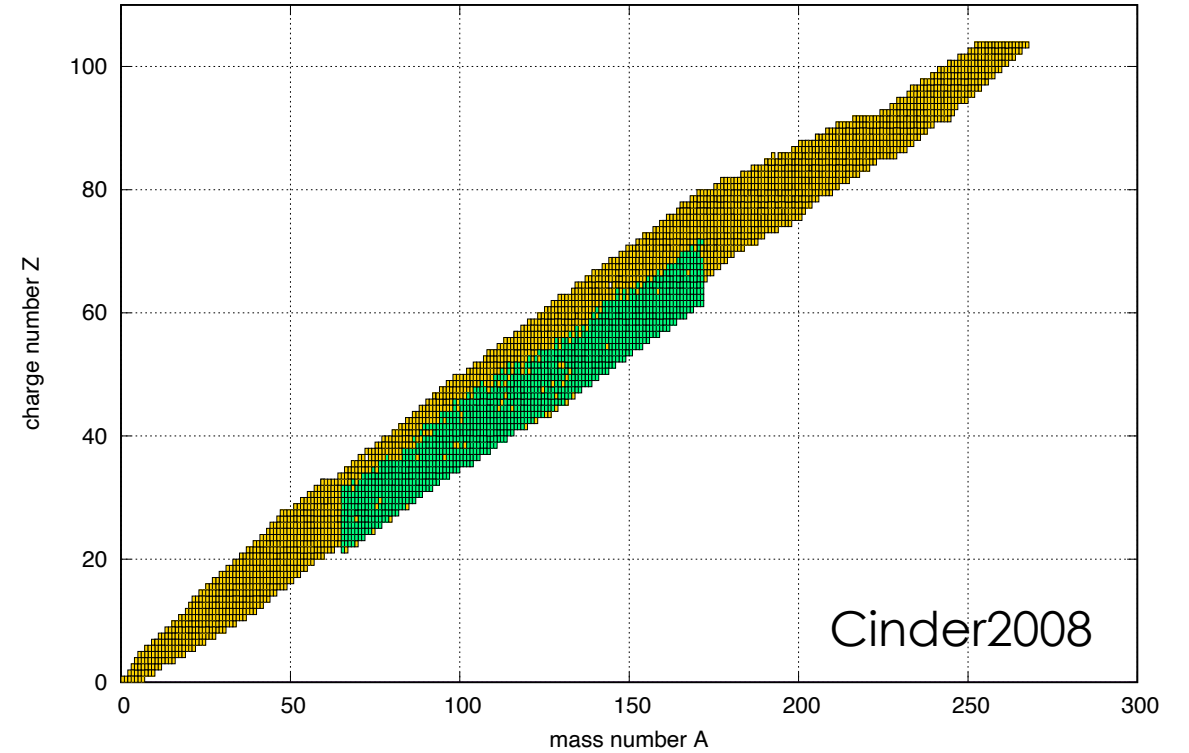
# Fission fragment coverage: Cinder2025 vs Cinder2008

C25 Nuclide Map showing Fission Fragment Coverage



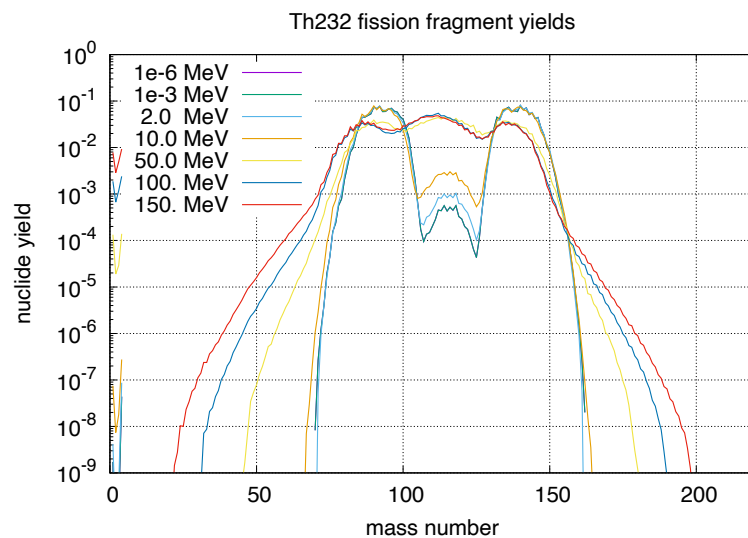
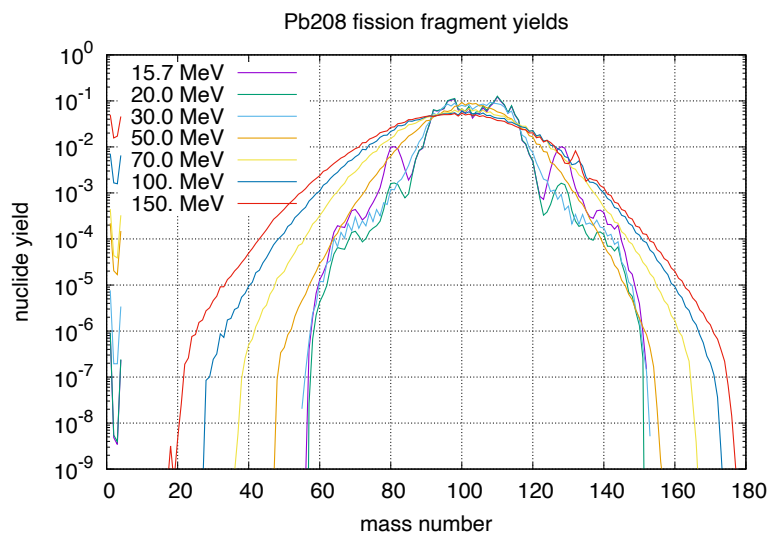
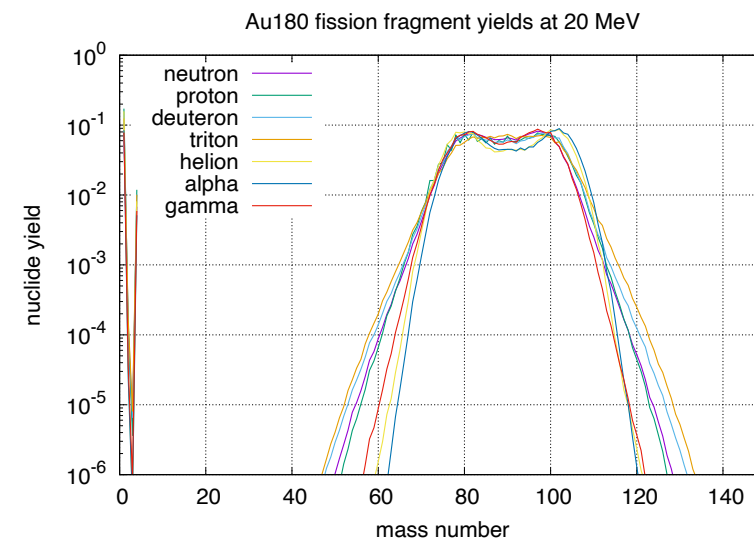
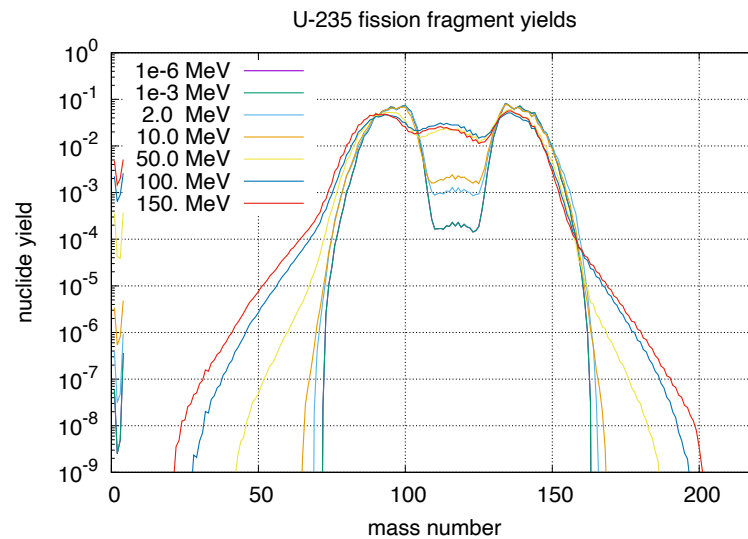
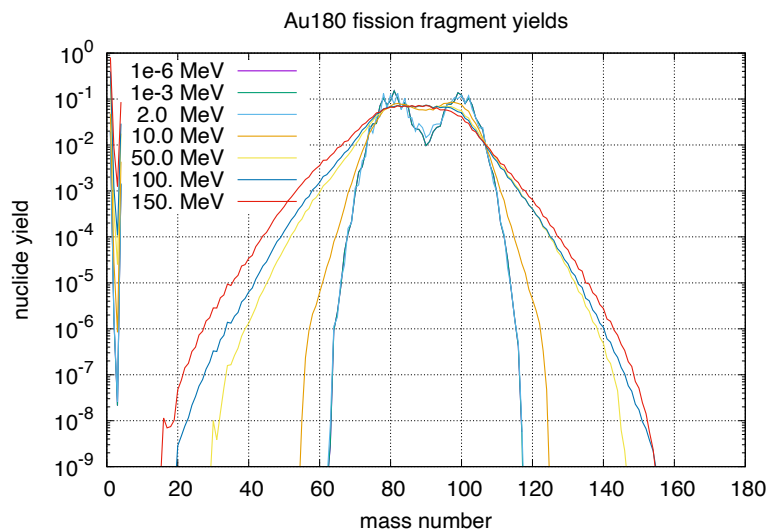
4205 nuclides produced by fission

C08 Nuclide Map showing Fission Fragment Coverage

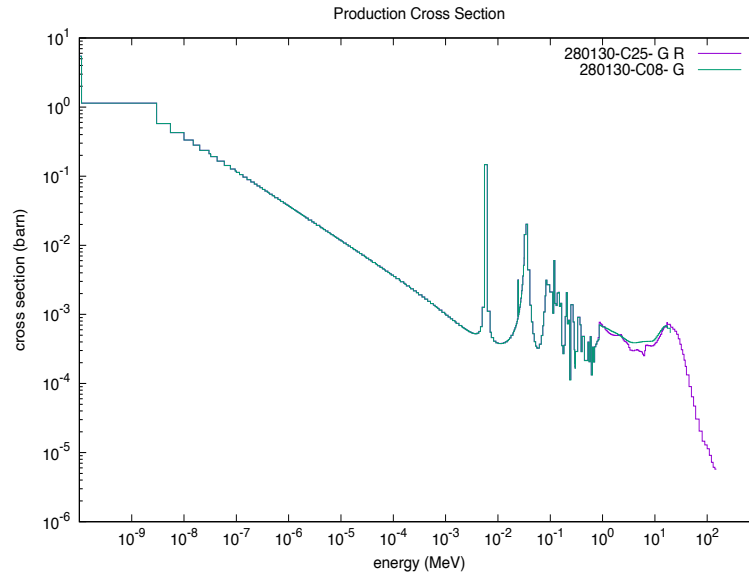
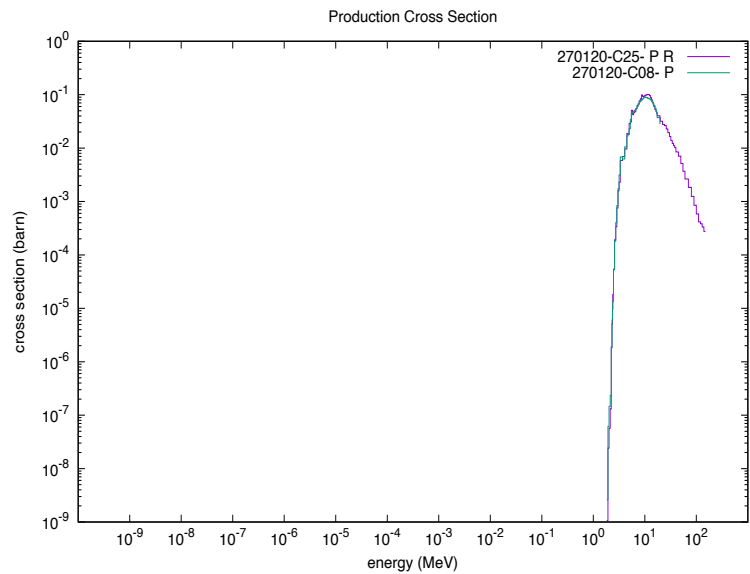
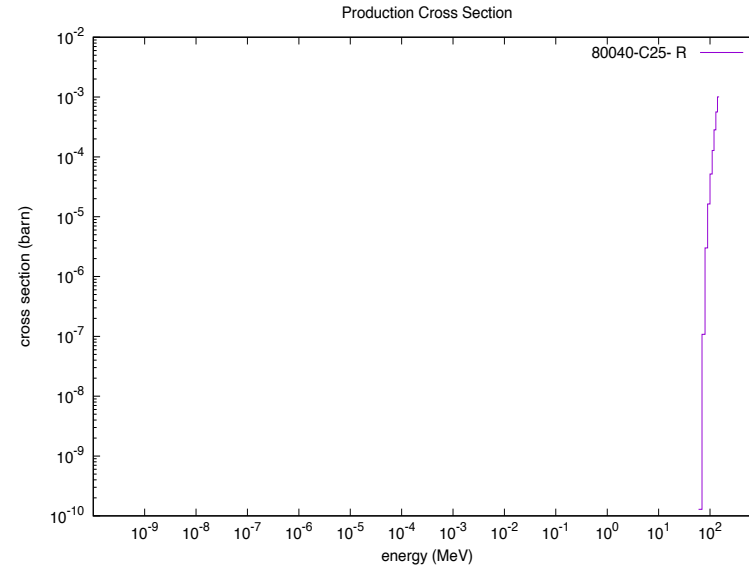
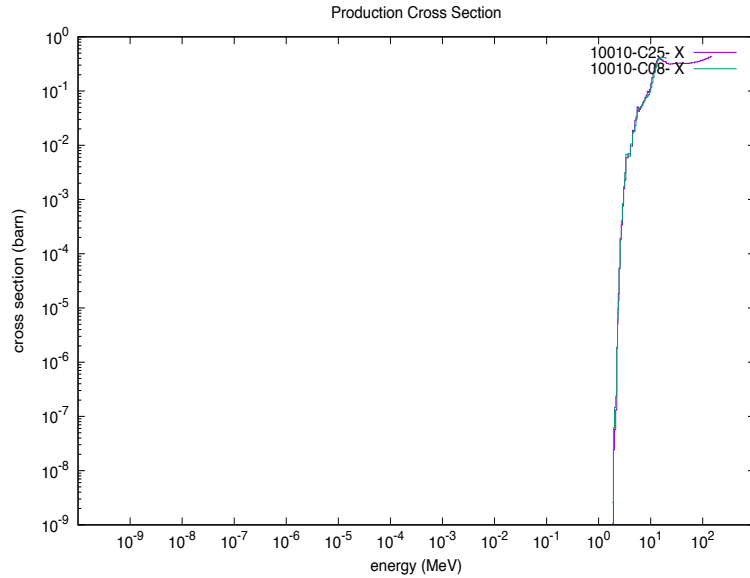


1325 nuclides produced by fission

# Fission fragment distributions

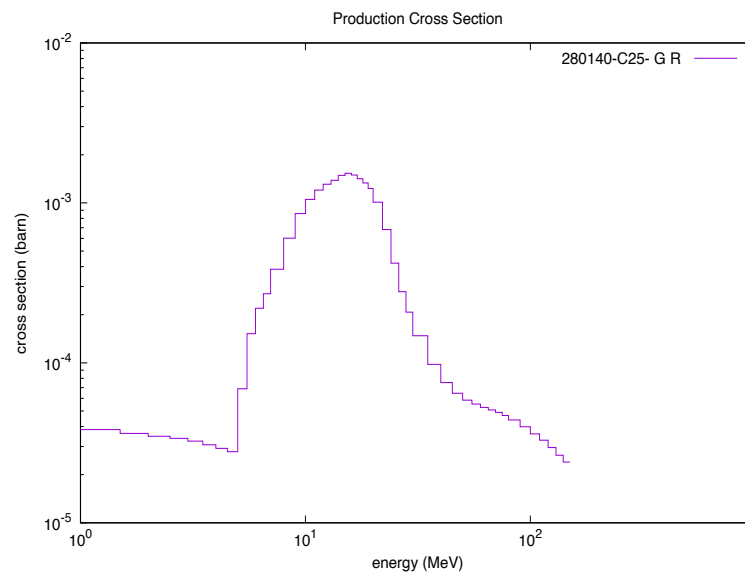
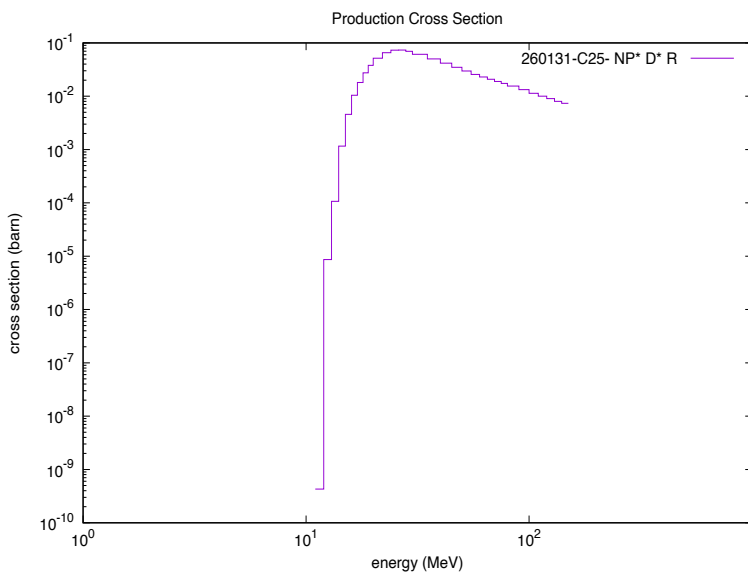
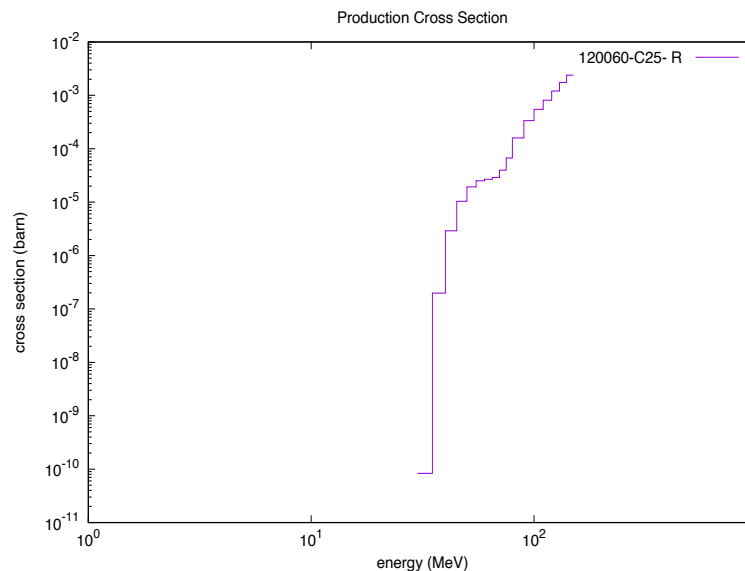
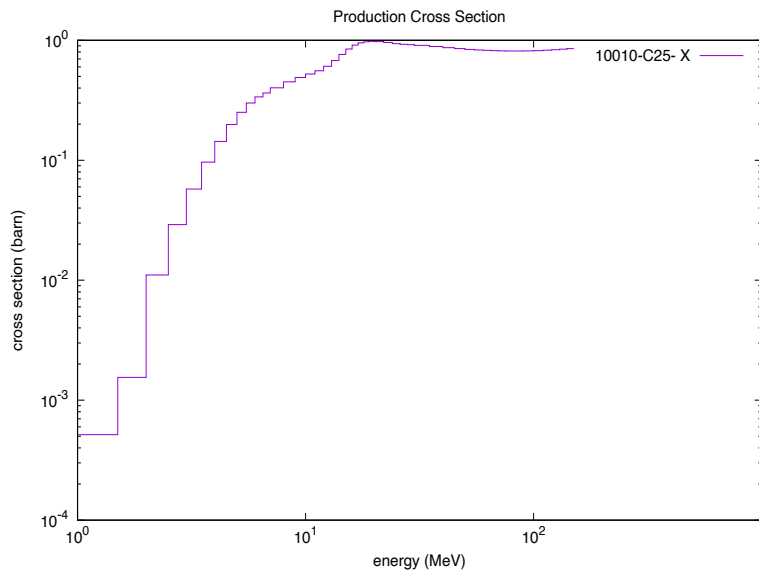


# Cinder2008 vs Cinder2025 XS comparison: neutron -> Al27



- For stable nuclides best parameter nuclide structure data set exist in TALYS
- The cross sections compare well using these input data
- Higher upper energy opens many more channels:  
15 Cinder08  
vs 107 Cinder25

# Cinder2025 Cross sections: proton $\rightarrow$ Al27



- 96 nuclide production data sets exit for protons on aluminum

# Summary

- New activation libraries consisting of decay, production cross section, and fission yield data were generated extending the cross section energy to 150 MeV, and extending projectiles from neutrons to light ions and gammas to adapt activation and residual dose analyses to the upgrades of MCNP6.
- LANL is developing an upgraded CINDER code, CINDER2025, which was used for first tests of the neutron library.