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Title: The Development of a New Cinder

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The Development of a New Cinder

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Introduction

What is Cinder?

Cinder is a tool that computes nuclide inventories after irradiation and decay.

Cinder computes the following ODE:

$$\frac{dN_i(t)}{dt} = \left(R_{j\to i}(t) + \lambda_{j\to i}\right) N_j(t) - \sum_j \left(R_{i\to j}(t) + \lambda_{i\to j}\right) N_i(t) + S_i(t)$$

Where:

- $N_i(t)$ is the atom density of nuclide i
- $R_{i\to j}$ is the transmutation rate from i to j
- $\lambda_{i\to j}$ is the decay constant from i to j
- $S_i(t)$ is the source of nuclide i

Cinder assumes R and S are constant over a time step.

A version of Cinder is embedded into MCNP and is used for the `BURN` and `ACT` cards.

The History of Cinder

1962 Tal England first writes CINDER at Bettis.

1975 CINDER-7 is released after Tal England moved to Los Alamos.

1993 CINDER'90 first mentioned to be used with LAHET and MCNP.

2008 *k*-eigenvalue depletion (`BURN`) added to MCNPX using CINDER'90. CINDER2008 started development.

2011 Last LANL version of CINDER (2008B9) released.

2015 Oak Ridge forks CINDER2008 to start AARE.

What Was the Problem?

The CINDER'90 coding caught our attention as being a good candidate for modernization:

- Code complexity was very high
- The capability was trivially isolated
- There was a new version of the base code (C90 $\rightarrow$ C08)
- There was a great deal of recent new methods research
- There were many unresolved bug reports and reported concerns

The last point meant that simply fixing the code would be costly.

The Path to a New Cinder

1. Modernize CINDER2008 $\rightarrow$ Cinder 2024
   - 1.1 Update the coding style to a modern one [Done]
   - 1.2 Rewrite data structures for thread safety [Done]
   - 1.3 Replace the main algorithm with CRAM48 for higher accuracy [Done]
   - 1.4 Perform significant bugfixes [When Found]
   - 1.5 Add testing and validation [In Progress]
   - 1.6 Create an HDF5 data format with reading/writing utilities [80% Done]
   - 1.7 Generate a new data library [Exploratory]
2. Replace MCNP-Cinder linkages
   - 2.1 Rewrite `ACT` linkage [40% Done]
   - 2.2 Rewrite `BURN` linkage [Exploratory]

The Cinder Algorithm

The Previous Algorithm

Versions of Cinder between C'90 and C2008 use a direct solve, assuming one nuclide has a non-zero starting quantity [1]:

$$N_{p,m}(t) = \left\{\prod_{k=1}^{m-1} \gamma_k\right\} \left(\bar{Y}_1 \left[\sum_{j=1}^{m} \frac{1 - e^{-\beta_j t}}{\beta_j \prod_{i=1, i\neq j}^{m} (\beta_i - \beta_j)}\right] + N_1(0) \left[\sum_{j=1}^{m} \frac{e^{-\beta_j t}}{\beta_j \prod_{i=1, i\neq j}^{m} (\beta_i - \beta_j)}\right] \right)$$

Where γ are the gain terms, β are the loss terms, and m is the chain length.

The issue is, if the chain loops (irradiation), $\beta_i - \beta_j$ can be zero. Options:

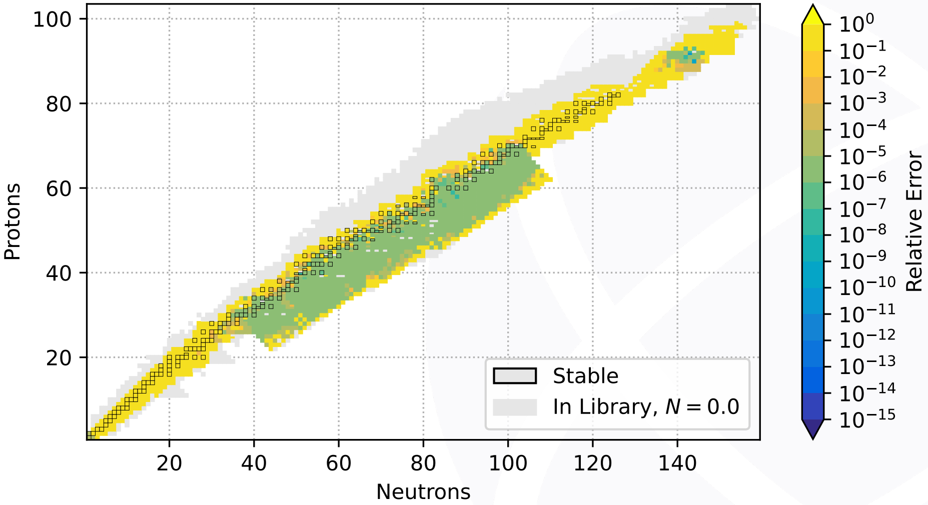
- CINDER'90 increments each β every time it is passed.
- CINDER2008 uses a limit equation derived as a series near $t = 0$.

Algorithm Testing

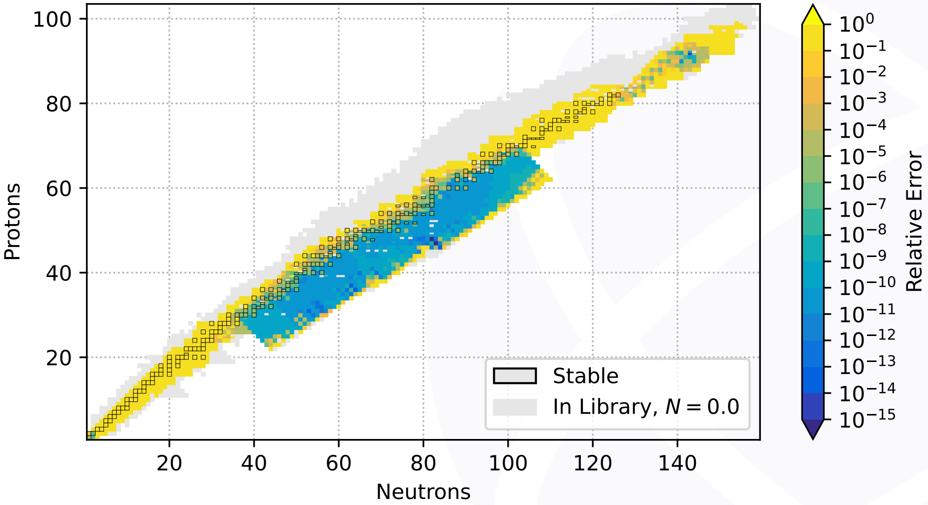
- Started with pure ^{235}U
- Irradiated with flux set to the same value in each group
- Integrated to 1 MWd/kgHM, 100 days
- Used C’90 decay chain (as it is compatible with all versions)
- All runs performed in double-precision
- Reference solution is scaling-and-squaring matrix exponent in 1024-bit arithmetic

Note, this test assumes the data is “correct.”

CINDER'90 Algorithm Test



CINDER2008 Algorithm Test



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Chebyshev Rational Approximation Method (CRAM)

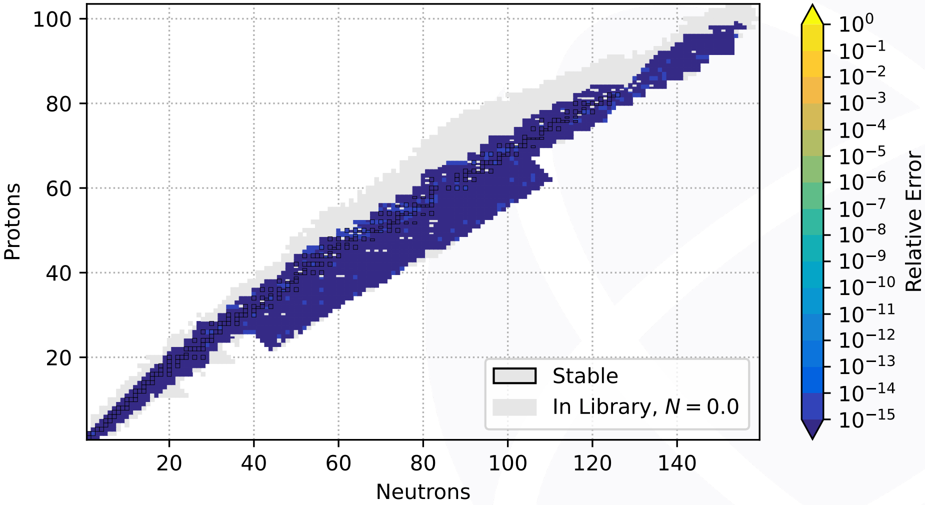
Instead, the algorithm was replaced with CRAM order 48 in the IPF form [2]:

$$
\begin{aligned}
y_0 &= N(0) \\
y_i &= 2\Re\left(\tilde{\alpha}_i\left(At - \theta_i I\right)^{-1} y_{i-1}\right) + y_{i-1} \\
N(t) &= \alpha_0 y_n
\end{aligned}
$$

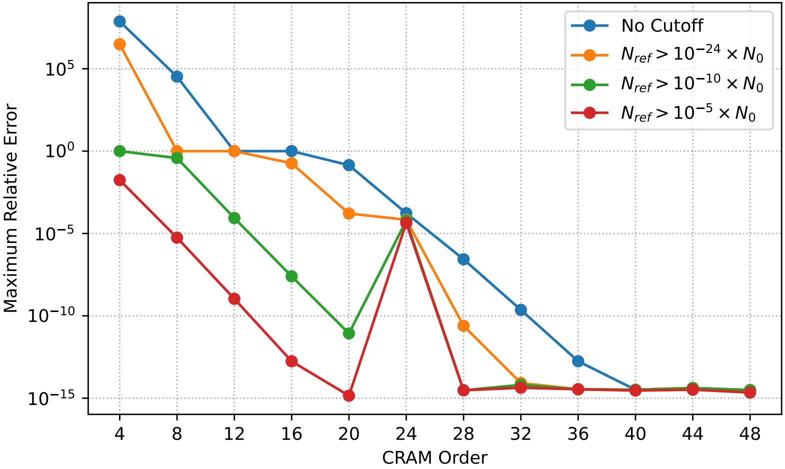
The algorithm is *very* sensitive to the numerical stability of the matrix solver used for the $\left(At - \theta_i I\right)^{-1} y_{i-1}$ step.

Once tuned, order 48 is extremely accurate.

New Cinder Algorithm Test



New Cinder Algorithm Test – Order



Published order-24 coefficients seem problematic.

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The Data

New Data Support

CINDER2008 was somewhat limited in what physics it could support:

- Only neutron-induced reactions.
- Fission is categorical ("thermal", "fast", "fusion"), not energy-dependent.
- Reactions were stored A$\rightarrow$B instead of by reaction channel.
- Particle emission for γ, n only. No neutron data present.

Cinder 2024 removes these restrictions:

- If data exists, supports n, γ, p, ^{2}H, ^{3}H, ^{3}He, ^{4}He reactions.
- Fission can be multigroup.
- Data stored by reaction channel, with branches.
- Particle emission for γ, n, β (in progress), α, p, $\bar{\nu}_e$ / ν_e (if data exists).

Completely new HDF5 data format written to support this.

New Library

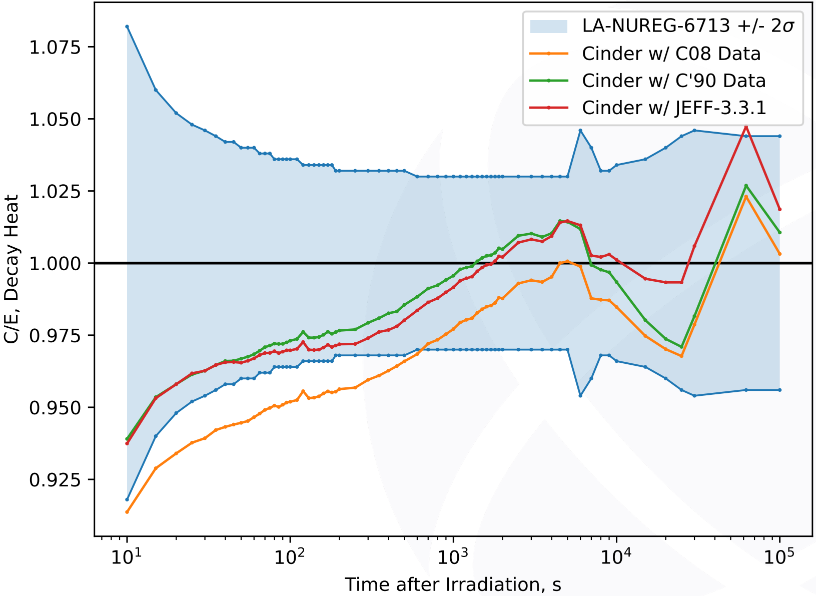
Early investigations begun. Examining data sources for:

- Decay chain completeness.
- Emission spectra completeness.
- Consistency in decay heat.
- Quality of reaction data.

So far, JEFF-3.3 decay chain appears more consistent than the ENDF/B-VIII.0 or JENDL-5 decay chains.

In talks with the theory division at LANL about models for filling gaps.

Library Comparisons [3]



The ACT Linkage

ACT Linkage

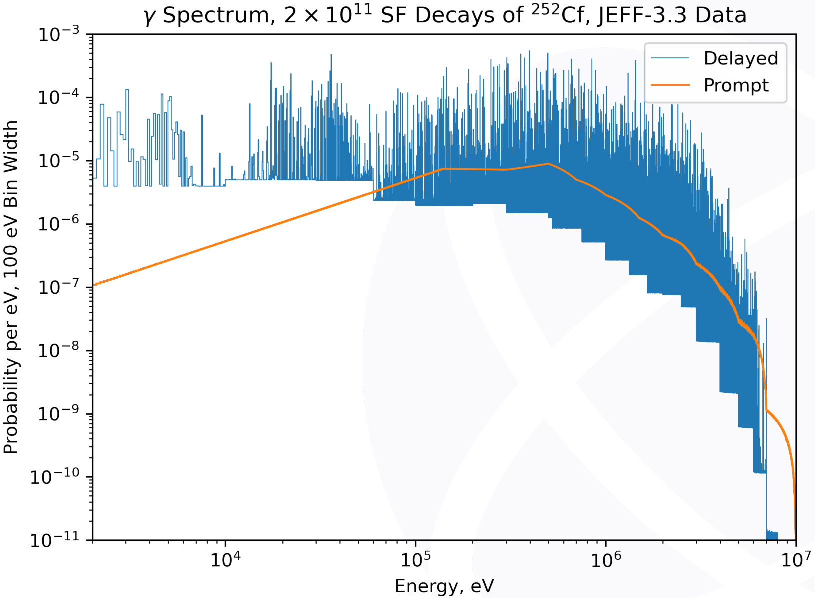
Previous method:

1. Run Cinder with 1 initial nuclide for 99 or 234 time steps
2. Construct emission line CDF
3. Directly sample CDF

While this approach has some neat features, it is often too slow and requires too much memory for practical use. Instead:

1. Start with 1 nuclide
2. Sample decay emission
3. Sample decay mode
4. Repeat until all residuals are stable

Preliminary ACT Results – ^{252}Cf SF Photons – Spectrum



Preliminary ACT Results – ^{252}Cf SF Photons – Performance

MCNP is using C'90 data, Cinder is using JEFF-3.3 data.

	MCNP-ACT		New-ACT
	`thresh=0.95`	`thresh=1.0`	
Time per Fission	112 μs	950 μs	1.38 μs
Memory	2.2 GB	2.2 GB	73.5 MB

New-ACT is equivalent to `thresh=1.0`. No lines missing.

If more nuclides are simulated, MCNP-ACT may run out of cache space, further harming performance.

Future Work and Conclusions

Conclusions

There is still a great amount of work to be completed:

- Generating a new library
- Writing new `BURN` bindings
- Figuring out better approaches to decay heat
- Performing integral testing and V&V

These changes are tentatively planned to be added to MCNP version 6.4.

Bibliography

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