

NJOY Status



Jeremy Lloyd Conlin

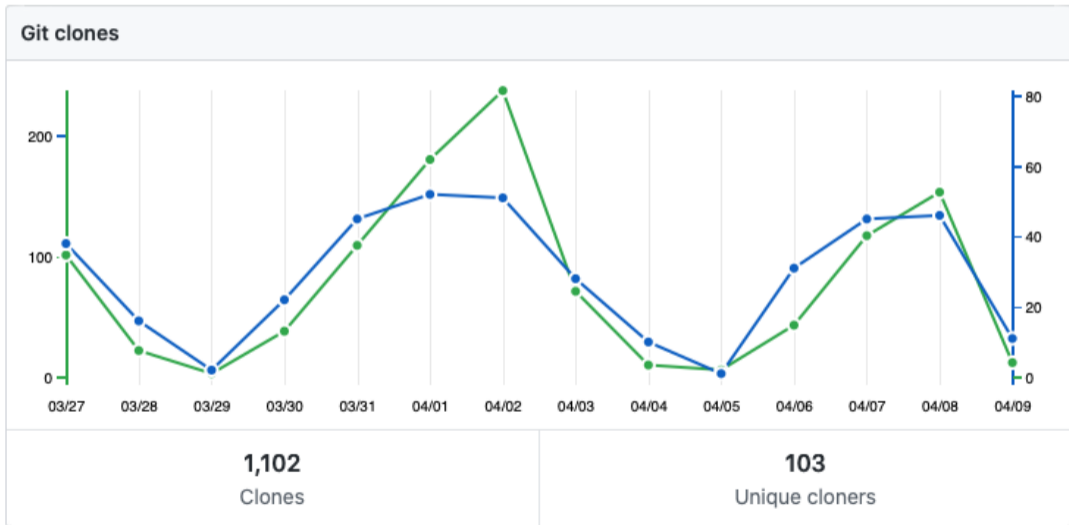
November 9–10, 2020



Managed by Triad National Security, LLC for the U.S. Department of Energy's NNSA

NJOY2016

NJOY2016



RECONR

RECONR

“The RECONR module is used to reconstruct resonance cross sections from resonance parameters and to reconstruct cross sections from ENDF nonlinear interpolation schemes.” — NJOY2016 manual pg. 43

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..and so much more

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..and so much more

- Resonance reconstruction
- Linearization of cross sections, photon production cross sections, etc.
- Unresolved resonance evaluation
- Unionization of energy grid
- Summation of cross sections, photon productions

Resonance Reconstruction

- Resolved and Unresolved regions
- Many different options and corner cases

Resolved Formalisms:

- Single- and Multi-Level Breit-Wigner (LRF=1,2)
- Reich-Moore (LRF=3)
- R-Matrix Limited (LRF=7)

Unresolved cases

- Energy-independent (CaseA)
- Energy-dependent fission widths (CaseB)
- All parameters are energy-dependent (CaseC)

The physics capabilities for resonance reconstruction are contained in our [resonanceReconstruction](#) component developed by Austin McCartney and Wim Haeck.

resonanceReconstruction **Component**

2017–2019 (A.P. McCartney and W. Haeck)

- Implementation of Breit-Wigter and Reich-Moore capabilities
- Implementation of R-Matrix Limited capabilities

FY2020 (W. Haeck and N. Gibson)

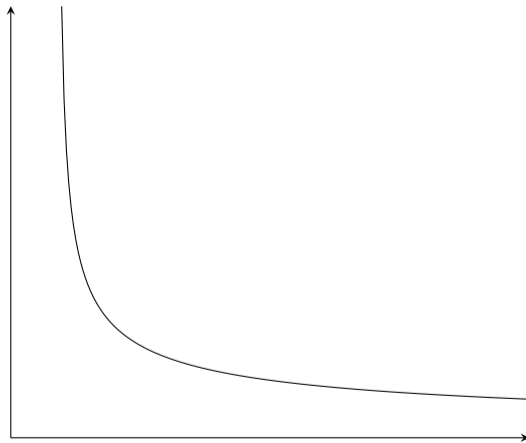
- Unresolved resonance reconstruction
- Polishing/debugging/improving of R-Matrix Limited capabilities
- Common interface between different formalisms

Future Work

- Look into g++ compile-time problem
- Replace Coulomb wave function implementation
- Python bindings and documentation

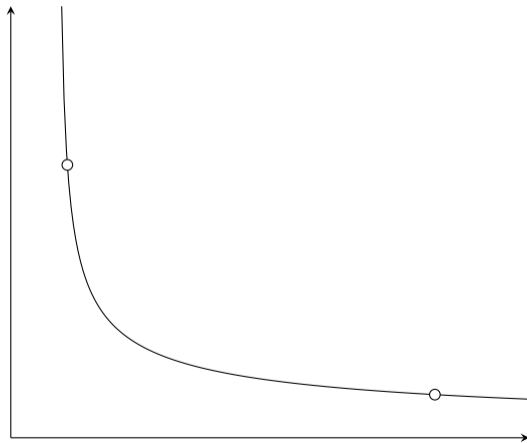
Linearization

$$1/\sqrt{x}$$



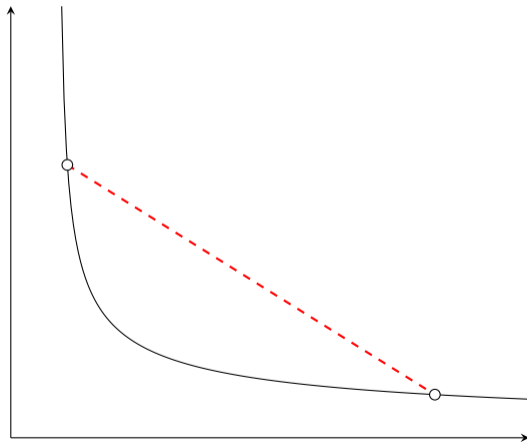
Linearization

$$1/\sqrt{x}$$



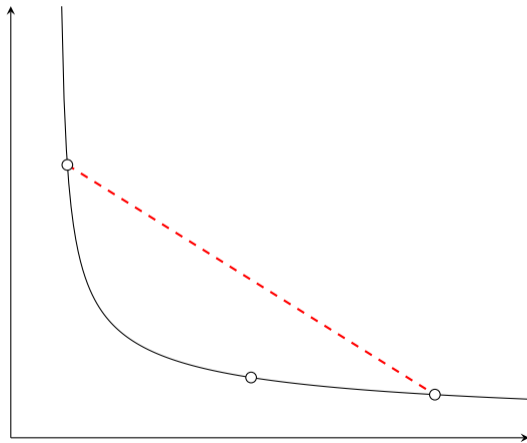
Linearization

$$1/\sqrt{x}$$



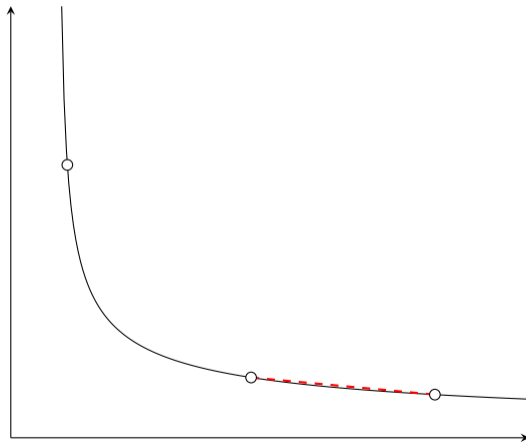
Linearization

$$1/\sqrt{x}$$



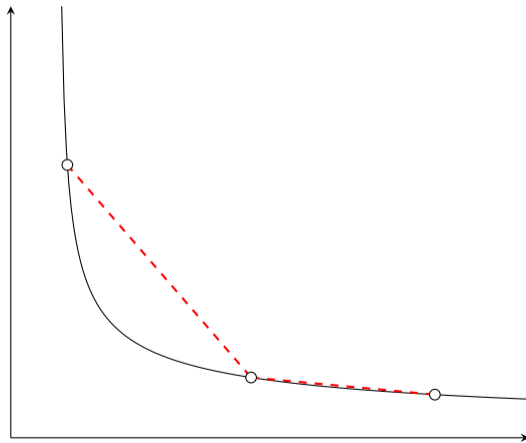
Linearization

$$1/\sqrt{x}$$



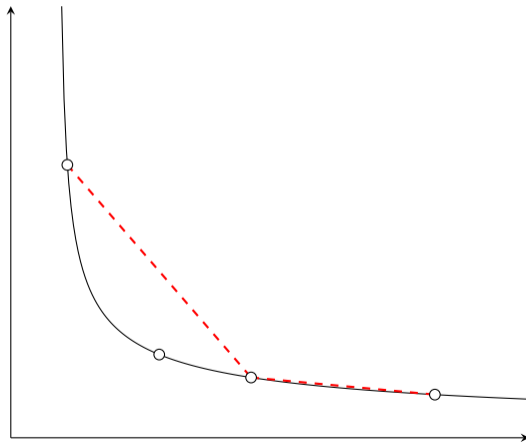
Linearization

$$1/\sqrt{x}$$



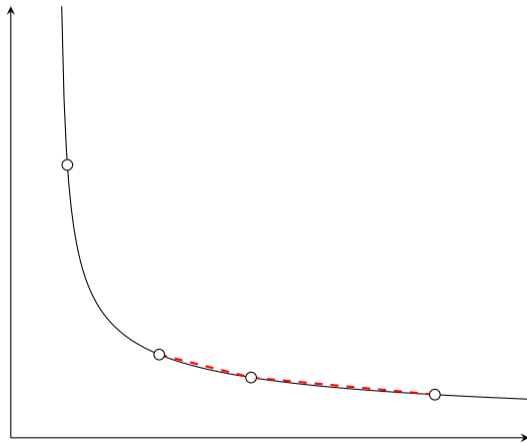
Linearization

$$1/\sqrt{x}$$



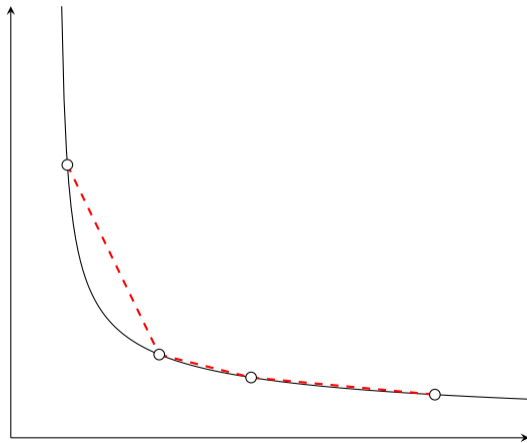
Linearization

$$1/\sqrt{x}$$



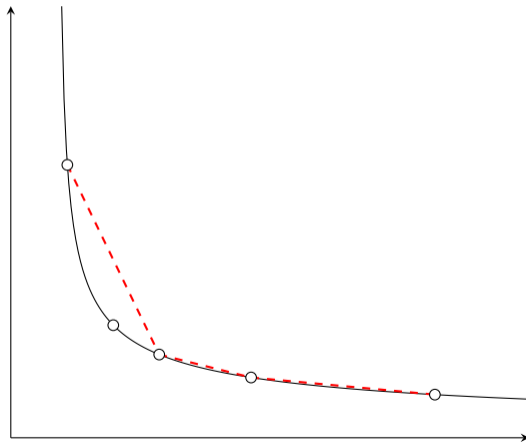
Linearization

$$1/\sqrt{x}$$



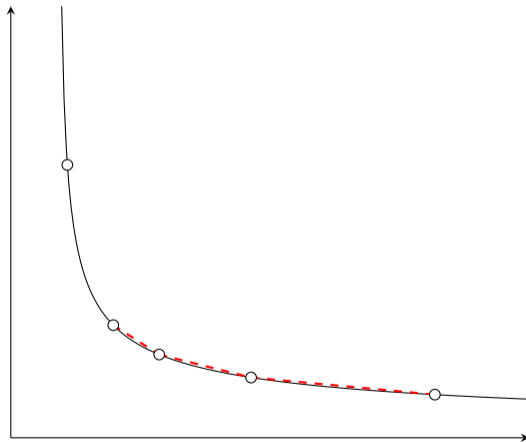
Linearization

$$1/\sqrt{x}$$



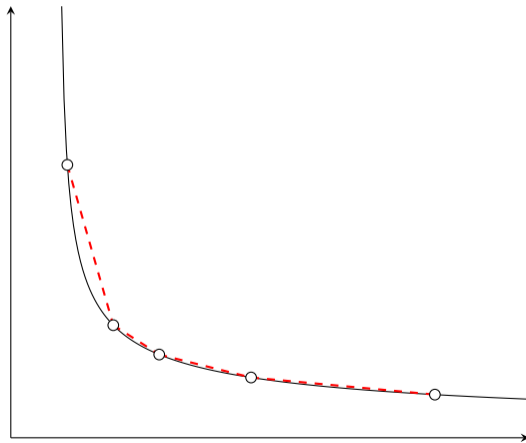
Linearization

$$1/\sqrt{x}$$



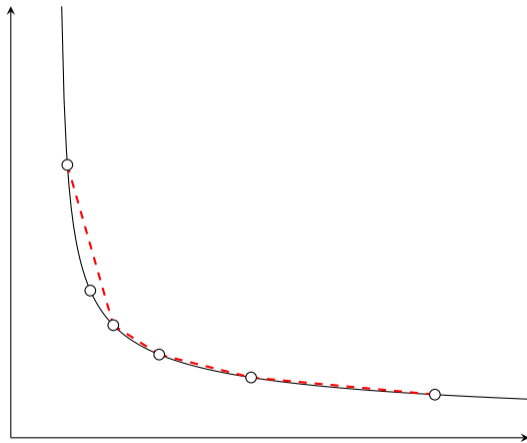
Linearization

$$1/\sqrt{x}$$



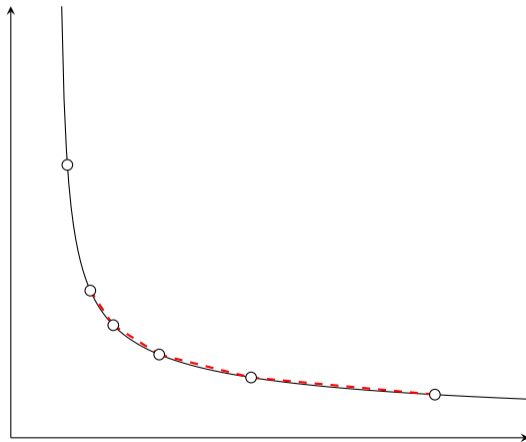
Linearization

$$1/\sqrt{x}$$



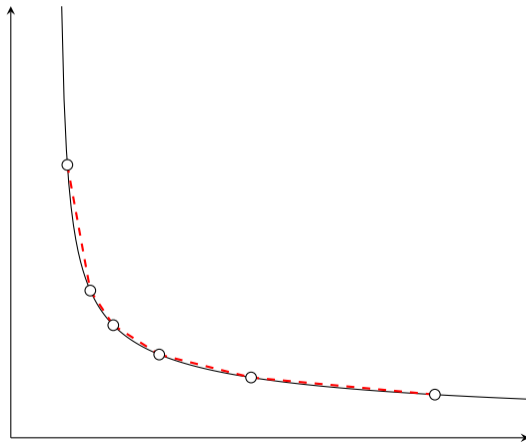
Linearization

$$1/\sqrt{x}$$



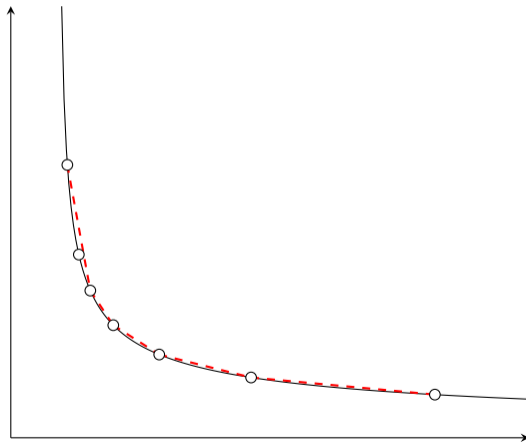
Linearization

$$1/\sqrt{x}$$



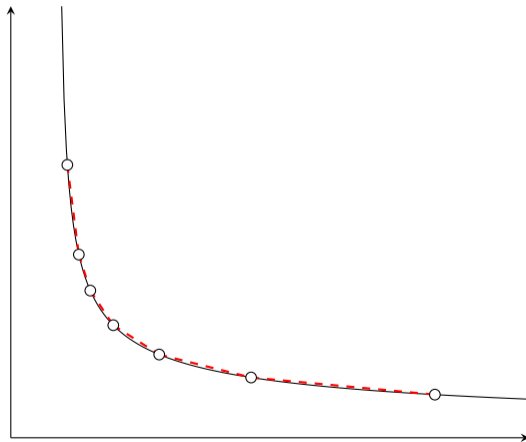
Linearization

$$1/\sqrt{x}$$



Linearization

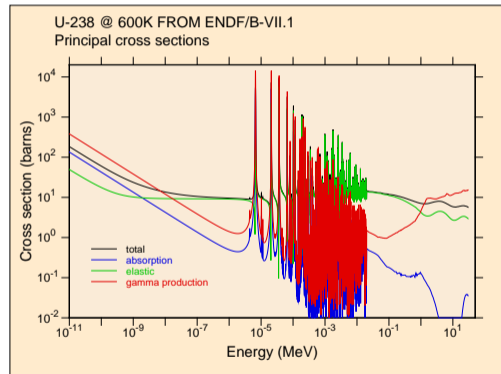
$$1/\sqrt{x}$$



Summation of Cross Sections

Cross section summation is somewhat complicated

- Total cross section is sum of:
 - elastic scattering
 - “non-elastic” scattering
- non-elastic is sum of:
 - $(n, 2n)$,
 - fission,
 - (n, p) , (n, d) , (n, t) ,
 - and many more



Linearized cross sections on a unionized energy grid makes summation *much* easier.

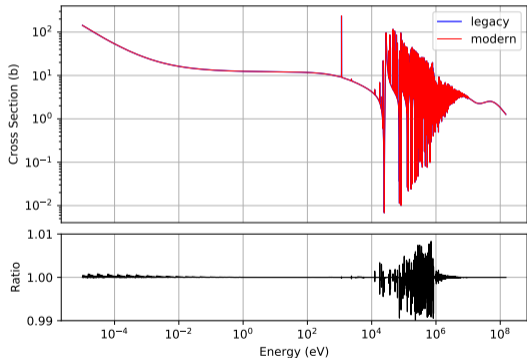
RECONR

1. Collect evaluation data
2. Linearization of cross sections
3. Resonance reconstruction—and linearization
4. Processing of unresolved resonances
5. Unionization of energy grid
6. Summation
 - Reconstructed resonances with “background” cross sections
 - Photon production cross sections
 - Redundant cross sections
 - Unresolved cross sections with background (sometimes)
7. Write processed data
 - Output should be the same format as the input

Comparison to Legacy RECONR

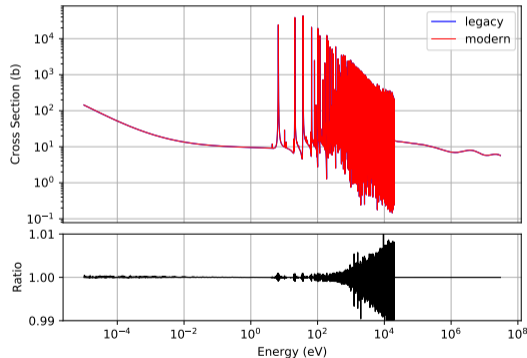
Fe-56

fe056



U-238

u238



Comparison to Legacy RECONR

- Run NJOY through:
 - Modern RECONR
 - BROADR
 - HEATR
 - GASPR
 - THERMR
 - PURR
 - ACER
- 976 MCNP benchmark calculations
- Compare k_{eff} results

$n\text{-}\sigma$	Gaussian	Benchmarks
$1\text{-}\sigma$	68.2 %	60.55 %
$2\text{-}\sigma$	95.45 %	89.75 %
$3\text{-}\sigma$	99.73 %	96.72 %
$3+\text{-}\sigma$	–	3.28 %

Updated Build System

NJOY21 1.2.0 introduces a new/improved build system for NJOY21.

- Still uses CMake.
- Dependencies are handled using the CMake native `FetchContent` feature.
- Can get version by checkout out specific git tag.
 - Eliminates need for awkward signature file.

New/Simplified Build Instructions

Download the latest version of the code

```
git clone --branch v1.2.0 https://github.com/njoy/NJOY21.git
```

```
cd NJOY21
```

Configure the build process

```
mkdir bin
```

```
cd bin
```

Build NJOY21

```
make
```

Test NJOY21

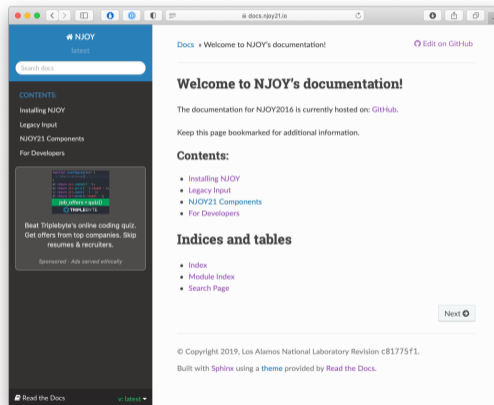
```
make test
```

Documentation

Updated Documentation

<https://docs.njoy21.io>

- Will continue to update as capabilities are added.
- [NJOY2016 manual](#) still valid



The screenshot shows a web browser window with the address bar displaying 'docs.njoy21.io'. The page has a blue header with the NJOY logo and 'latest' text. Below the header is a search bar labeled 'Search docs'. The left sidebar contains a 'CONTENTS:' section with links for 'Installing NJOY', 'Legacy Input', 'NJOY21 Components', and 'For Developers'. A Triplebyte advertisement is visible at the bottom of the sidebar, featuring a code snippet and the text 'Beat Triplebyte's online coding quiz. Get offers from top companies. Skip resumes & recruiters. Sponsored - Ads served ethically'. The main content area has a breadcrumb 'Docs » Welcome to NJOY's documentation!' and a link to 'Edit on GitHub'. The main heading is 'Welcome to NJOY's documentation!'. Below this, it states 'The documentation for NJOY2016 is currently hosted on: GitHub.' and 'Keep this page bookmarked for additional information.' There are two sections: 'Contents:' with a bulleted list of links, and 'Indices and tables' with a bulleted list of links.

docs.njoy21.io

NJOY
latest

Search docs

CONTENTS:

- Installing NJOY
- Legacy Input
- NJOY21 Components
- For Developers

function countSpaces(str) {
 // ...
 return str.indexOf(' ');
}
a) return str.indexOf(' ');
b) return str.toUpperCase().length - 1;
c) return str.toLowerCase().length - 1;
d) return str.length - 1;

job_offers = quiz()
TRIPLEBYTE

Beat Triplebyte's online coding quiz.
Get offers from top companies. Skip
resumes & recruiters.

Sponsored - Ads served ethically

Docs » Welcome to NJOY's documentation! [Edit on GitHub](#)

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Contents:

- [Installing NJOY](#)
- [Legacy Input](#)
- [NJOY21 Components](#)
- [For Developers](#)

Indices and tables

- [Index](#)
- [Module Index](#)
- [Search Page](#)

NJOY21 1.3.0

- Modern RECONR
- Modern LEAPR
- Modern THERMR

Expected December 2020.

Conclusion

- NJOY2016 continues to receive bug fix attention by Wim Haeck
 - Lots of people have downloaded (hopefully used) NJOY during quarantine
- Modern RECONR
 - Graphical comparison shows little differences with Legacy NJOY
 - Still some differences with coulomb wave functions used in R-Matrix Limited
 - Algorithms are independent of data source.
- Much improved build system
- Release coming December 2020