CONFLUX

A Standard Framework for Reactor Neutrino Flux Calculation

Xianyi Zhang
On behalf of the CONFLUX project

9/20/2023

AAP 2023

LLNL-PRES-844089

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Motivation for an accessible prediction framework

Antineutrino spectra and their applications

Summary of the Technical Meeting

IAEA Headquarters, Vienna, Austria
23-26 April 2019

Outstanding issues:

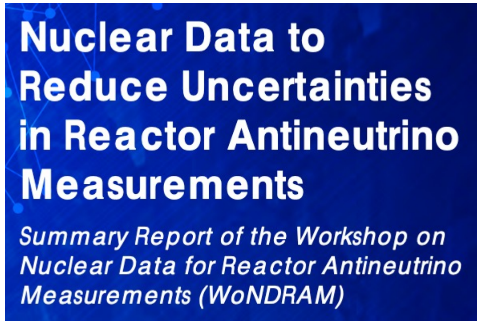
10. Up-to-date summation antineutrino models are not easily accessible for use by neutrino experimentalists.

They therefore recommend the creation of a working group (Antineutrino Flux Working Group) that maintains updated, fully documented antineutrino flux predictions and measurements for isotopes and reactors.

The scope of the working group will cover three specializations:

- standardized antineutrino data,
- standardized models,
- Antineutrino model input nuclear data and experiment.

WoNDRAM 2021 summary:



The development of an open software framework enabling uncertainty quantification for and standardized comparisons between direct neutrino measurements and conversion and summation calculations would greatly facilitate progress and reduce hurdles of participation for use case communities. The following recommendations would benefit all three discussed end user communities: nuclear data, reactor monitoring, and particle physics. *That broadened access and utility can be delivered to both the predictions and direct measurement communities by these tools further strengthens the recommendation for their development (recommendation 5).*

Motivation for an accessible prediction framework

Current Situation:

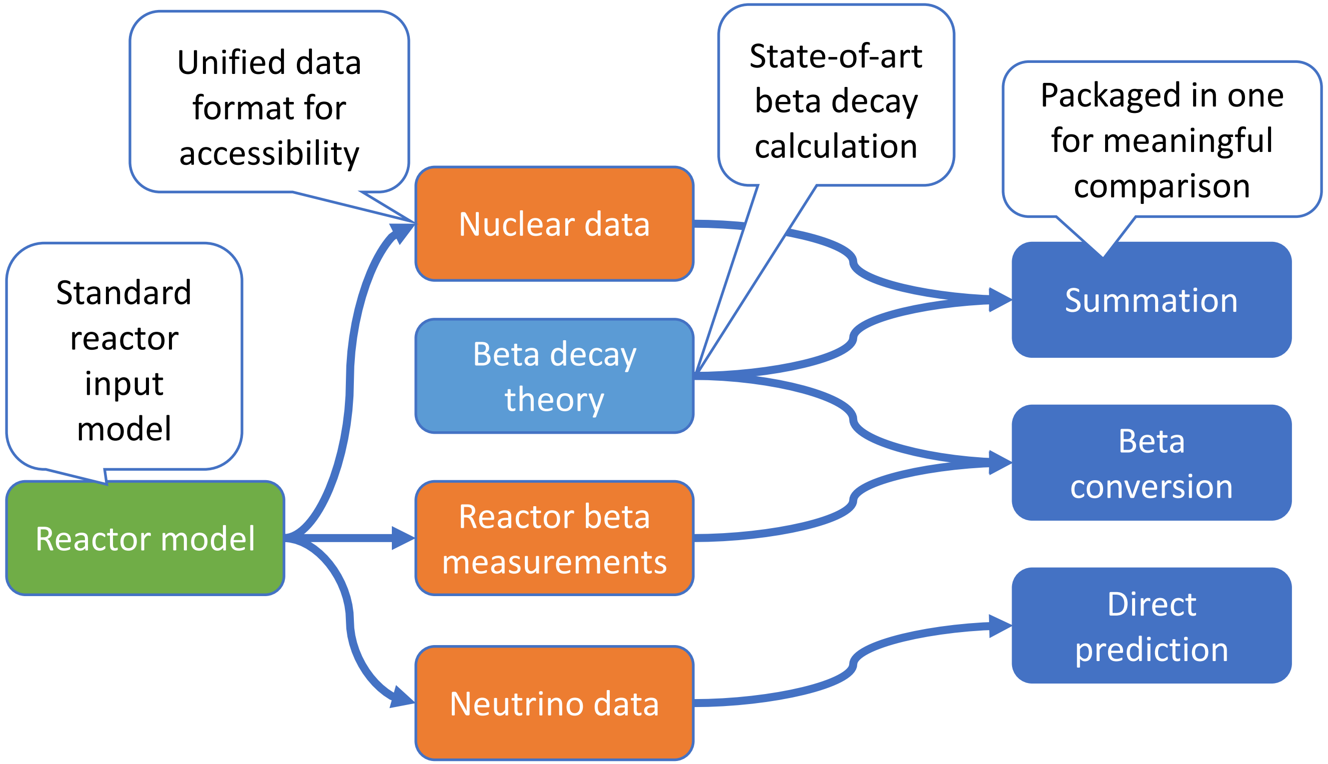
- Expert groups working independently on state-of-the-art predictions
- No neutrino community standard for data sharing (nuclear data, reactor parameters, flux models, documentation of model inputs, …)
- Steep learning curve for non-experts to contribute to the reactor flux prediction enterprise
- Since situation is rapidly developing, no widely-used state-of-the-art flux prediction to use for applications, sensitivity studies, …

Needs of an open-source prediction framework:

- Common tools and data used for different prediction methods
- Standardized uncertainty quantification
- Standardized comparison between predictions and data
- Widely accessible to particle and nuclear physicists
- Straightforward to update with new databases and measurements

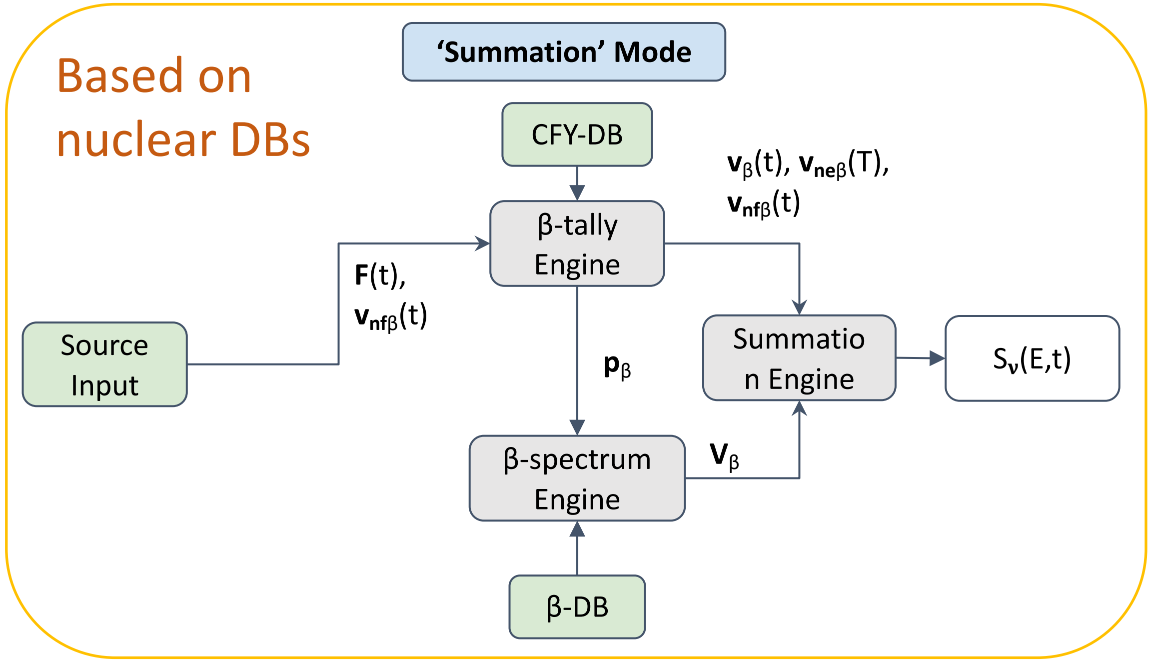
Calculation Of Neutrino FLUX

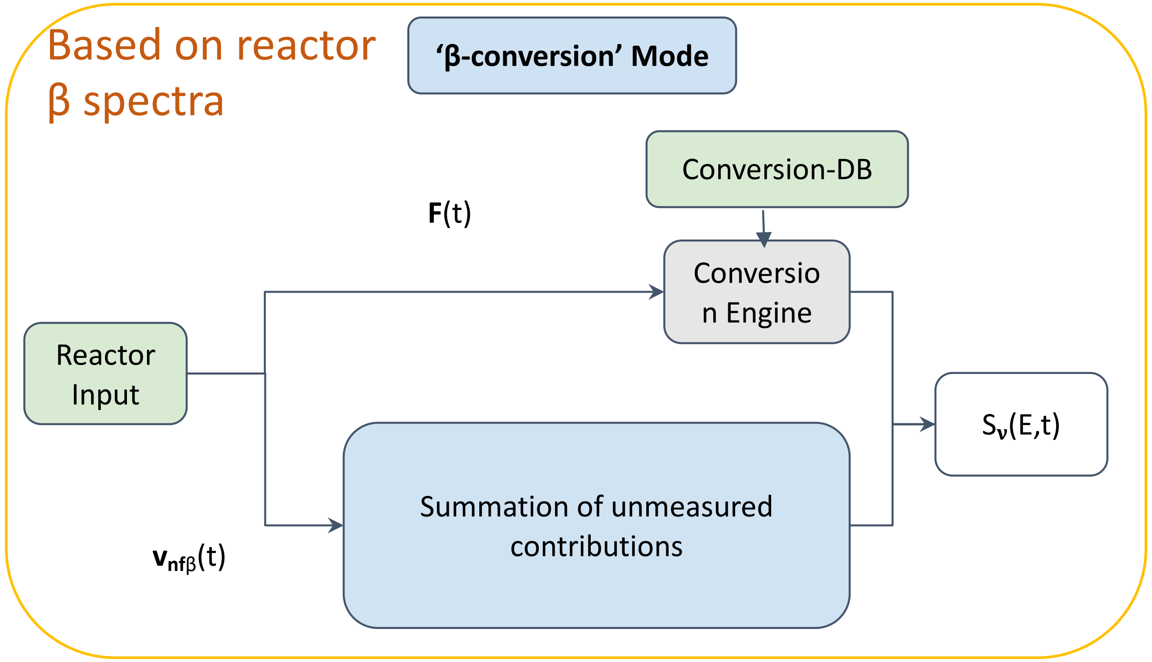
- Multi-institute project
- Modular software
  - Easy for customization
- Methods integrated in one software
  - Summation β spectra
  - Conversions of reactor β spectra
  - Neutrino data
- Ingredients
  - Parsed nuclear data for readability
  - Common, flexible beta theory engine
- Open source in Python



The CONFLUX Framework

- Prediction with three different modes: summation, conversion, and neutrino data
- Flexible user inputs
- Nuclear DBs (ENDF, ENSDF formats) are parsed into xml formats for accessibility





Flexible inputs of different modes

- User input: Time dependent reactor fission fragments or compositions
- **Summation:**
  - The β branches and fission yield parsed from databases such as ENSDF, ENDF, JEFF, JENDL
  - Parser of ENDF and ENSDF format included
  - Updated β decay measurement with TAGS
- **Conversion:**
  - β spectrum measurements of fission isotopes at ILL

Beta spectrum DB


```xml
<betaDB>
  <isotope name="Nn1" isotope="10" Q="0.782347" HL="613.9 S    " Ex="0.0">
    <branch fraction="1.000" sigma_frac="0.000" end_point_E="0.782" sigma_E0="0.000" dJpi="0"/>
  </isotope>
  <isotope name="H3" isotope="10030" Q="0.0185906" HL="12.32 Y    " Ex="0.0">
    <branch fraction="1.000" sigma_frac="0.000" end_point_E="0.019" sigma_E0="0.000" dJpi="0"/>
  </isotope>
  <isotope name="He6" isotope="20060" Q="3.5078" HL="806.7 MS   " Ex="0.0">
    <branch fraction="1.000" sigma_frac="0.000" end_point_E="3.508" sigma_E0="0.001" dJpi="1"/>
  </isotope>
  <isotope name="He8" isotope="20080" Q="10.651" HL="119.1 MS   " Ex="0.0">
    <branch fraction="0.840" sigma_frac="0.010" end_point_E="9.671" sigma_E0="0.008" dJpi="1"/>
    <branch fraction="0.160" sigma_frac="0.000" end_point_E="7.571" sigma_E0="0.007" dJpi="1"/>
    <branch fraction="0.160" sigma_frac="0.000" end_point_E="5.501" sigma_E0="0.007" dJpi="1"/>
    <branch fraction="0.009" sigma_frac="0.001" end_point_E="0.981" sigma_E0="0.007" dJpi="1"/>
```


Beta tally DB


```xml
<?xml version="1.0" ?>
<nfy-092_U_235>
  <HEAD AWR="233.025" FissionZA="92235" LE="3" MT="IFP">
    <LIST Ei="0.0253" Ii="2" NFPi="1247">
      <CONT DY="1.3122e-19" FPS="0.0" Y="2.05032e-19" ZA="23066"/>
      <CONT DY="1.54228e-14" FPS="0.0" Y="2.40981e-14" ZA="24066"/>
      <CONT DY="0.0" FPS="0.0" Y="0.0" ZA="24067"/>
      <CONT DY="0.0" FPS="0.0" Y="0.0" ZA="24068"/>
      <CONT DY="1.34924e-18" FPS="0.0" Y="2.10819e-18" ZA="24069"/>
      <CONT DY="0.0" FPS="0.0" Y="0.0" ZA="24070"/>
      <CONT DY="4.60767e-12" FPS="0.0" Y="7.19949e-12" ZA="25066"/>
      <CONT DY="3.44296e-12" FPS="0.0" Y="5.37962e-12" ZA="25067"/>
      <CONT DY="4.2621e-13" FPS="0.0" Y="6.65953e-13" ZA="25068"/>
      <CONT DY="5.1387e-14" FPS="0.0" Y="8.02922e-14" ZA="25069"/>
```

Beta Spectrum Generator

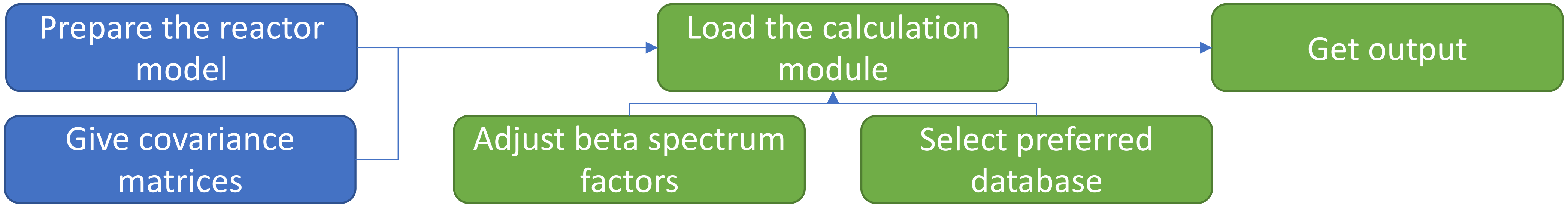
- A common β spectrum generator for the summation and conversion modes
- Use of state-of-art theoretical calculation with BSG[CPC 240 (2019) 152]
- Capable of making virtual beta spectra
- Theoretical corrections are important for low energy beta spectra. Customizable shape factors:
  - Forbidden transitions
  - Weak magnetism factor
  - …

Item	Effect	Formula	Magnitude
1	Phase space factor	$pW(W_0 - W)^2$	Unity or larger
2	Traditional Fermi function	F_0	
3	Finite size of the nucleus	L_0	10^{-1}-10^{-2}
4	Radiative corrections	R	
5	Shape factor	C	
6	Atomic exchange	X	
7	Atomic mismatch	r	
8	Atomic screening	S	10^{-3}-10^{-4}
9	Shake-up	See item 7	
10	Shake-off	See item 7	
11	Isovector correction	C_I	
12	Recoil Coulomb correction	Q	
13	Diffuse nuclear surface	U	
14	Nuclear deformation	D_{FS} & D_C	
15	Recoiling nucleus	R_N	
16	Molecular screening	ΔS_{Mol}	
17	Molecular exchange	Case by case	
18	Bound state β decay	Γ_b/Γ_c	Smaller than $1 \cdot 10^{-4}$
19	Neutrino mass	Negligible	

CPC 240 (2019) 152

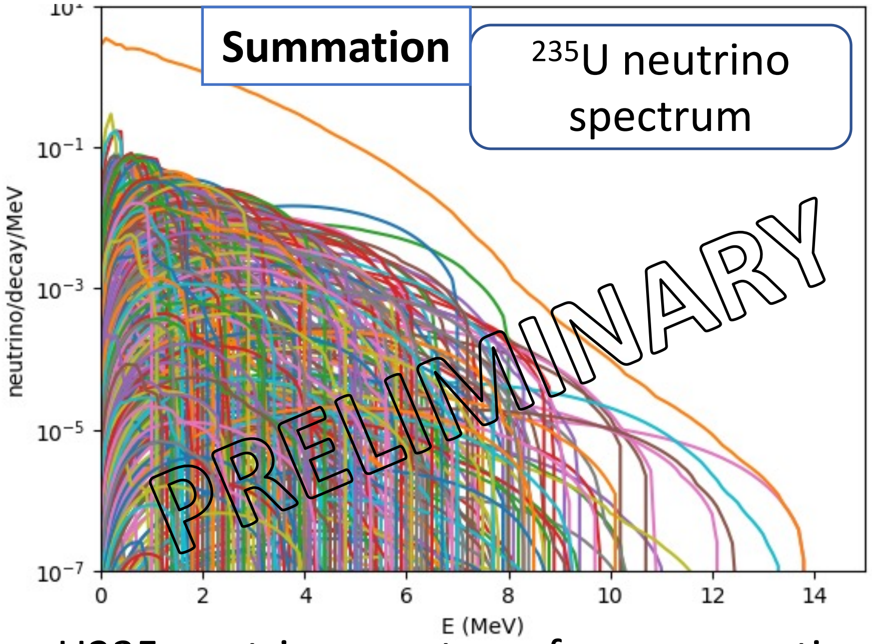
Simplified calculation workflow

- Codes are formatted for PIP installation to be used as Python modules
  - Beta spectrum generator
  - Nuclear DB parsers
  - Summing and converting methods
- Documentation and manuals will be available online
- Database parsers and calculation methods can be applied generally to ENDF DB format for future DB update
- Examples are provided for most common applications

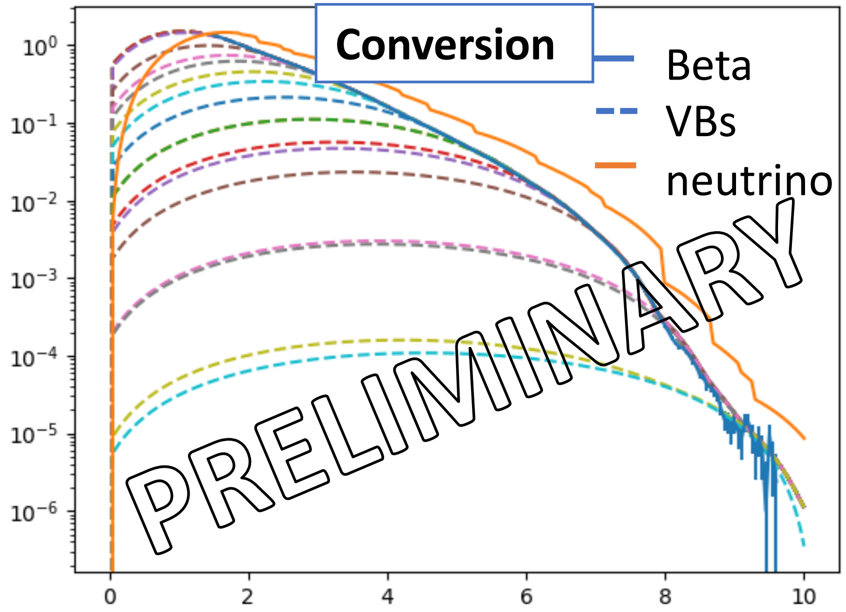


Default calculation conditions

- Summation mode uses ENSDF beta decay info and fission yield from JEFF
  - Databases with similar formats to ENDF can be directed plugged in
- Conversion mode set to repeat the Huber model through virtual spectra fitting



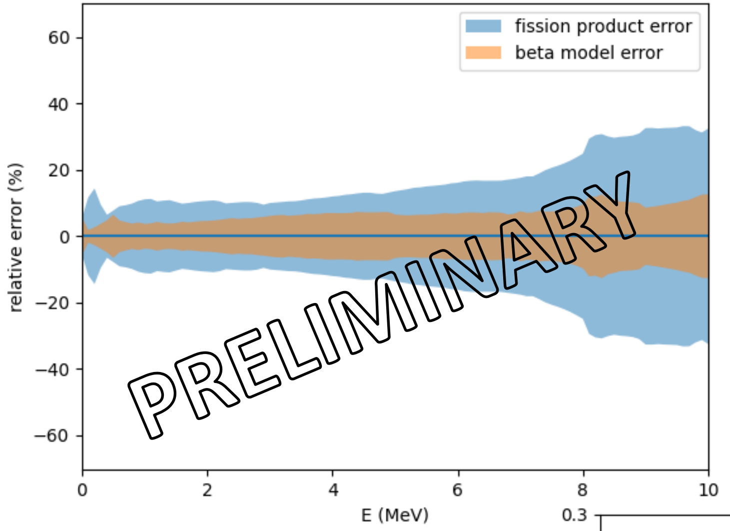
U235 neutrino spectrum from summation mode



U235 beta spectrum fitted with virtual branches

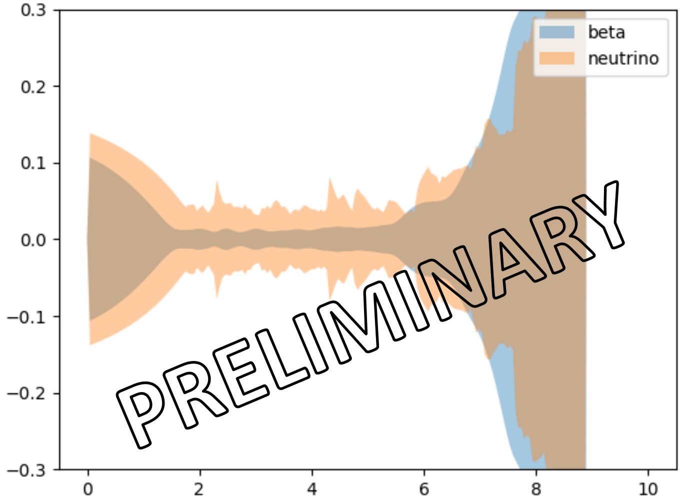
Uncertainty calculation

- Uncertainties in the summation mode:
  - Beta spectra – E_0, correction factors
  - Beta branching – correlated branching fraction, ground state feeding correlation
  - Correlated fission products
  - Reactor model uncertainty
- Uncertainties in the conversion mode:
  - Uncertainty of referred beta data
  - Uncertainty of converted neutrino spectrum – effective atom number, shape factors



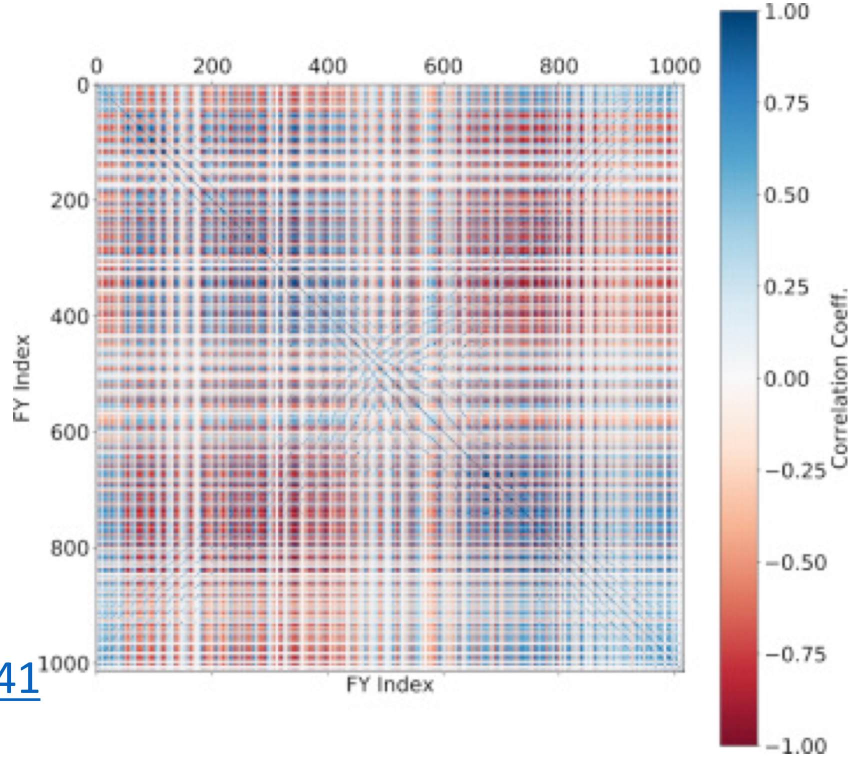
Relative uncertainties from beta model and fission yields

Relative uncertainties of 235 beta conversion through MC sampling



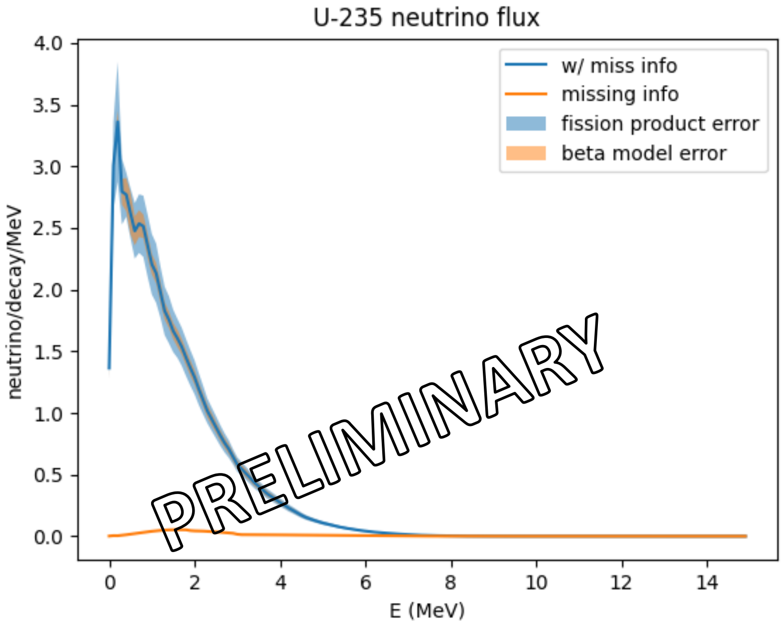
Processing correlated uncertainty

- User can provide correlation/covariance matrices in csv for summation uncertainty study
  - Fission fragments
  - Beta branching



Example correlation matrix [j.adt.2021.101441](j.adt.2021.101441)

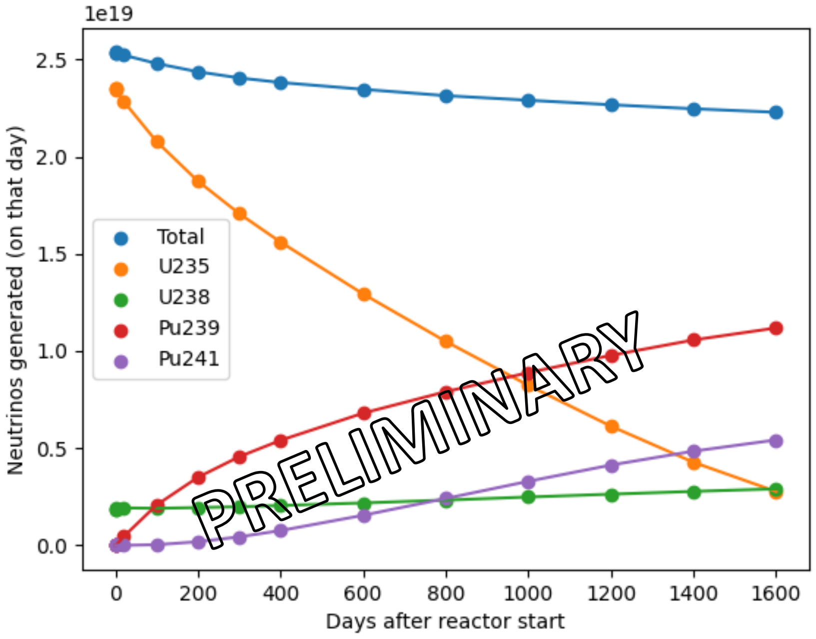
235 summation example with correlated uncertainty



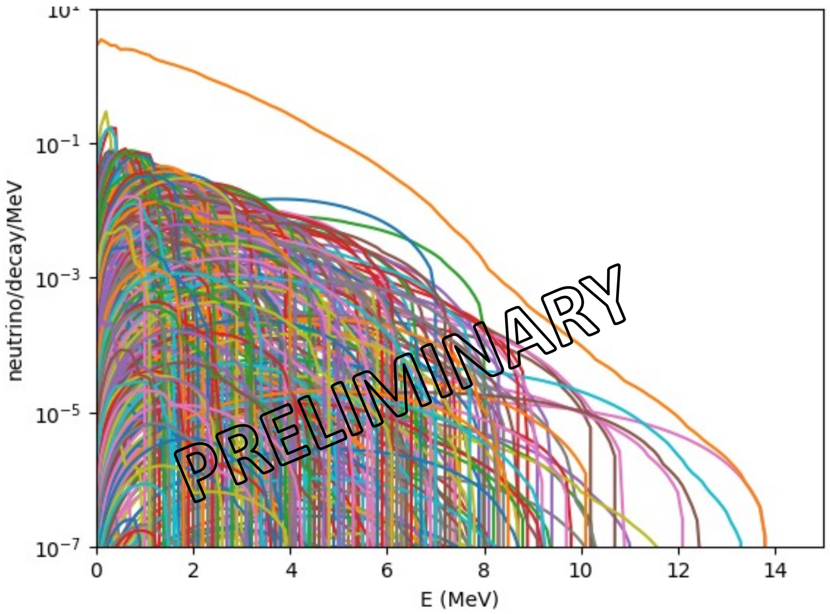
Time dependent reactor neutrino modelling

- CONFLUX reactor models with time dependent
  - Fission fragments
  - Beta decaying components (summation only)
  - Reactor simulation results, e.g., MCNP simulation (summation only)

Neutrino flux evolution of a LEU reactor



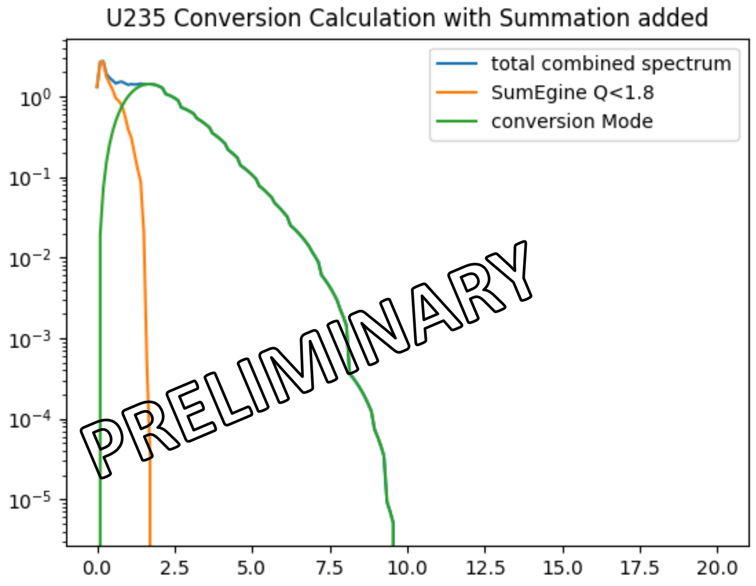
Summed spectra of individual beta-unstable sources

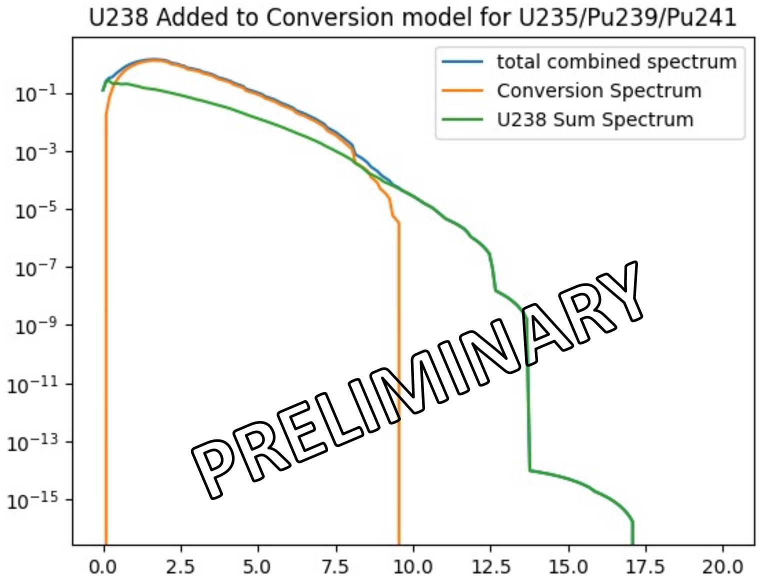


Combined prediction with different modes

- Result of two modes can be combined
  - Due to common datasets and methods used
  - Minimum work to compare results for different modes, data or methods

Combination of summation and conversion in different energy range
and different fissile isotopes

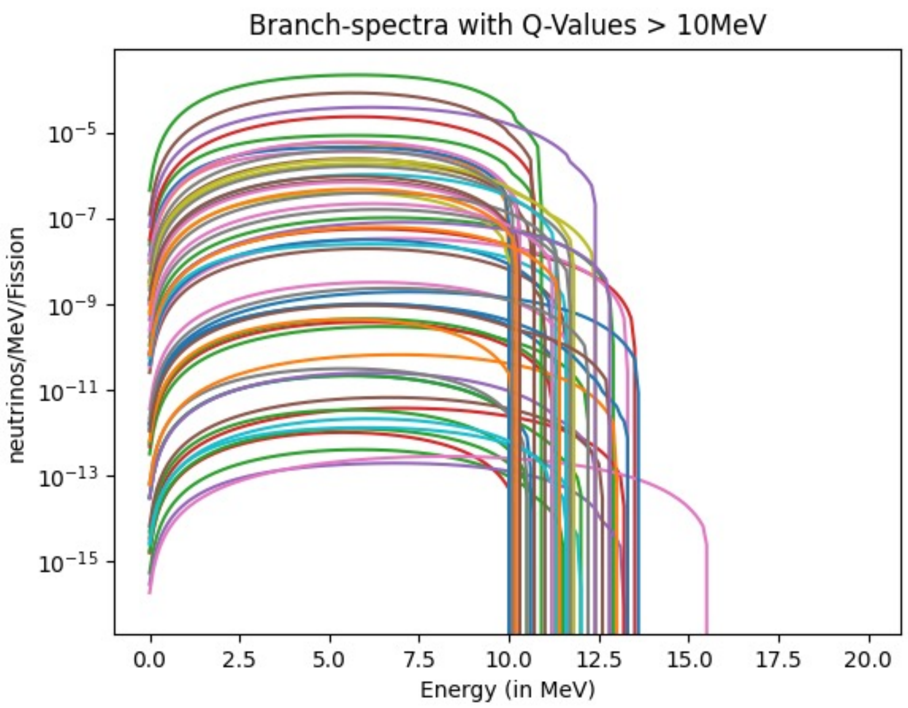




Calculation output with selected conditions

- Calculation output with selected condition (e.g., specified energy range, specified uncertainty contribution)
- Important to pinpoint isotopes contributing to deficits

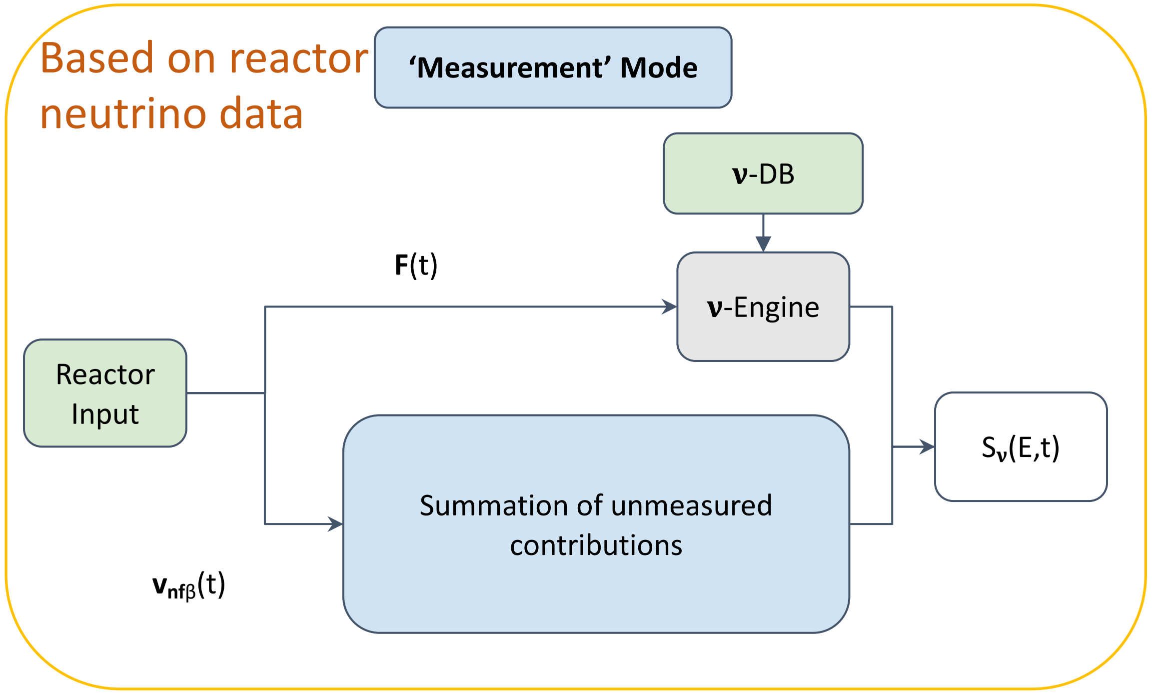
Fission products contributing > 10 MeV region



Isotope	percent-contribution	Q-Value
Br-90	$5.6 * 10^{-3}$	10.959 MeV
As-86	$5.5 * 10^{-3}$	11.541 MeV
Rb-100	$3.5 * 10^{-3}$	13.574 MeV
Rb-96	$2.1 * 10^{-3}$	11.571 MeV
As-84	$1.3 * 10^{-3}$	10.094 MeV
In-130	$9.7 * 10^{-4}$	10.249 MeV
Rb-97	$3.8 * 10^{-4}$	10.432 MeV
Br-92	$2.7 * 10^{-4}$	12.537 MeV
Cd-131	$1.4 * 10^{-4}$	12.87 MeV
Ga-80	$1.2 * 10^{-4}$	10.38 MeV
Ga-84	$1.1 * 10^{-4}$	13.69 MeV
Ga-82	$6.3 * 10^{-5}$	12.484 MeV
In-132	$6.2 * 10^{-5}$	14.14 MeV
Rb-98	$4.0 * 10^{-5}$	12.054 MeV
Br-93	$3.1 * 10^{-5}$	11.09 MeV

Coming soon

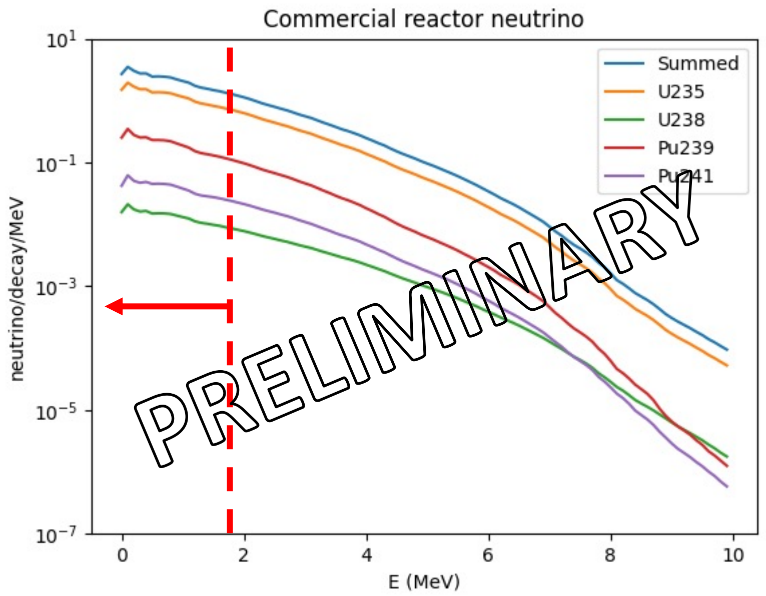
- Code testing in progress
  - Demonstrating beta-calculation result in with established beta decay measurements and calculations
  - Sanity checking the calculation result with published calculations
  - Synthetic data are used to check the quality of fitting and uncertainty calculations
- Building the direct prediction mode with existing neutrino data
  - Standardize neutrino data as an input



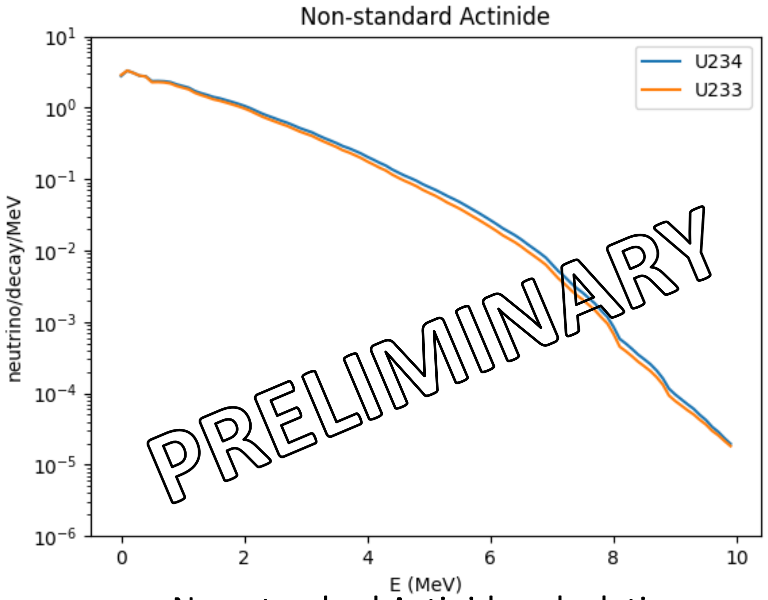
Potential Scientific Output

- **Neutrino spectra and flux prediction from different reactor types:**
  - BSM neutrino measurements
  - Reactor CEvNS
- **Contribute to the nuclear data community**
  - Direct cross-database comparisons
  - Search for deviations to prioritize beta decay measurements to be revisited
- **Studies on the reactor simulation for near field reactor survey**

…



Reactor neutrino flux calculation below IBD



Non-standard Actinide calculation

Summary

- CONFLUX is a framework of reactor neutrino flux prediction to meet the need for a standardized simple calculation software
- The software contains three modes with upgradable databases and customizable methods
- Analyzers can use flexible, time dependent reactor inputs and corrections
- The framework is being tested before publication
- CONFLUX is a tool can be utilized to provide a wide range of scientific output for the nuclear and particle physics communities

CONFLUX

ILLINOIS INSTITUTE OF TECHNOLOGY

X. Zhang, N. Bowden, P. Huber, L. Hayen, S. Bogetic,
B. Littlejohn, A. Irani, B. Cogswell

Thank you!

Backup – needs from nuclear data

- Decay information of missing branches:
  - Roughly 6% of beta decay branches missing.
  - Unknown impact in the below IBD range.
- Result of pandemonium effect:
  - Biased branching fractions.
- Correlated uncertainty:
  - Correlation among fission yields needs to be accounted.
  - Program needs to calculate correlated uncertainty.

Backup – examples of inputs

Input:

- Time dependent reactor model with fission fractions (all three modes):

  {{“time_0”, “power_0”, {“235_Thermal”, [frac, d_frac]}, {“238_fast”, [frac, d_frac]}, {...}, ...},

  …

  {“time_n”, “power_n”, {“235_ Thermal”, [frac, d_frac]}, {“238 _fast”, [frac, d_frac]}, {...}, ...}}

- Time dependent radioactive source model with simulated beta branches (summation mode only):

  {{“time_0”, “power_0”, {“beta_branch_0”, [frac, d_frac]}, {“beta_branch_1”, [frac, d_frac]}, …},

  …

  {“time_n”, “power_n”, {“beta_branch_0”, [frac, d_frac]}, {“beta_branch_1”, [frac, d_frac]}, …}}