Testing of ENDF/B-VIII.0 in the GNDS format: update

CSEWG2018
NOV 5, 2018

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LLNL-PRES-757053

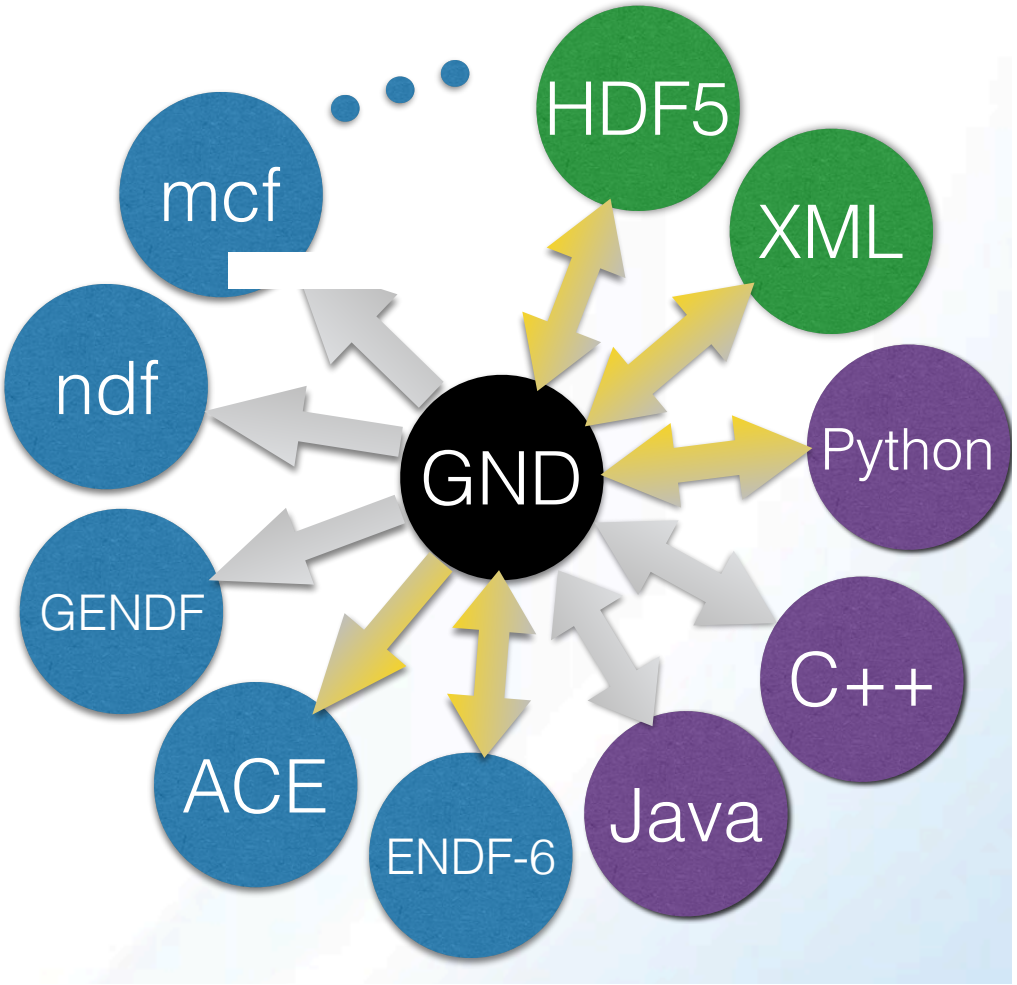
This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

Outline

- Translation from GNDS data to ACE format
- Integral testing with ENDF/B-VIII.0
- Status: LLNL pulsed spheres

Generalized Nuclear Data Structure

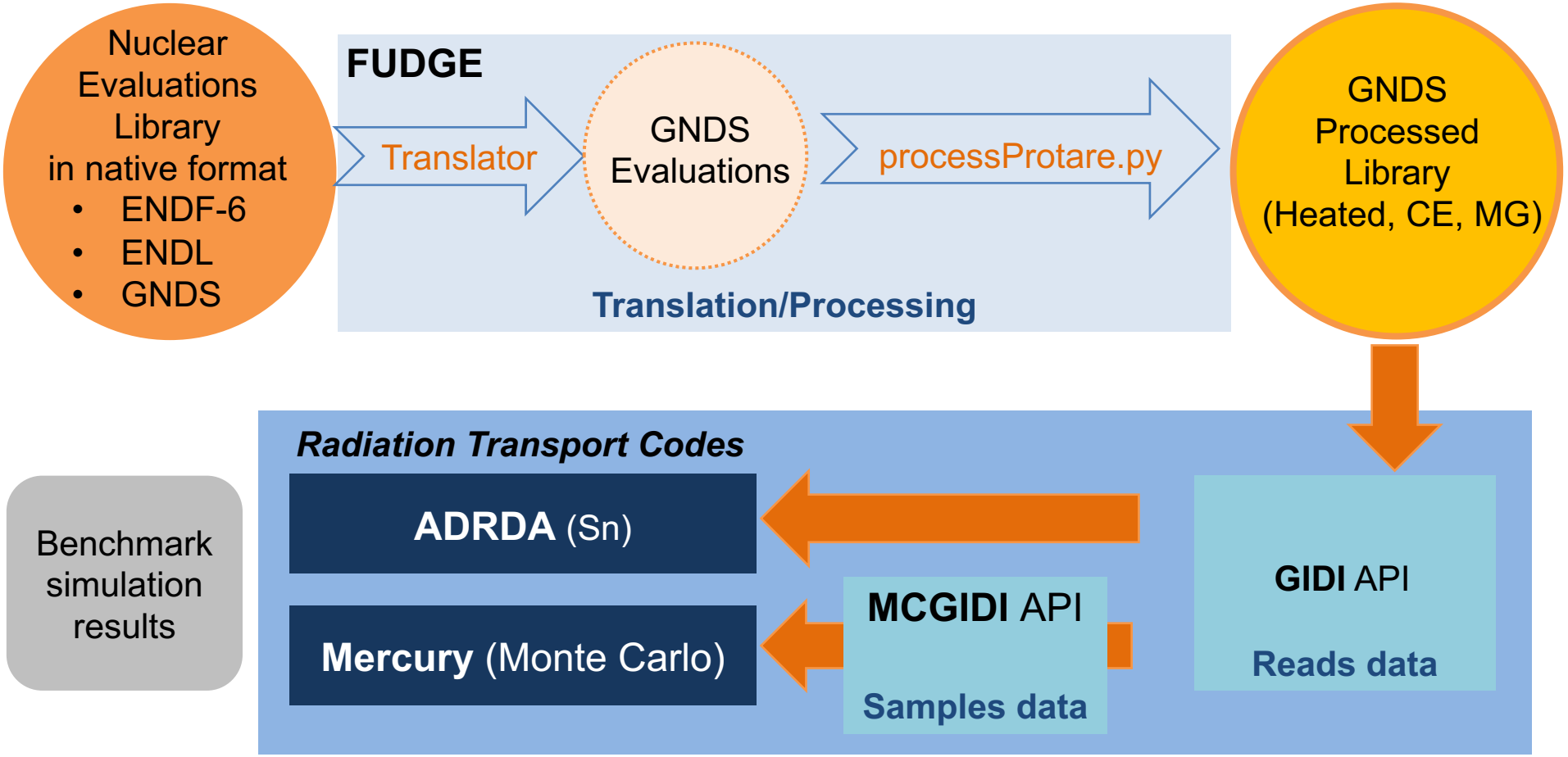
- Initially, LLNL wanted to replace its own ENDL format
- GNDS international effort under OECD/NEA/WPEC/SG38, SG43 (2017-2020) and EG-GNDS
- Adapted to both evaluated and processed data



slide based on slide from D. Brown/F. Malvagi

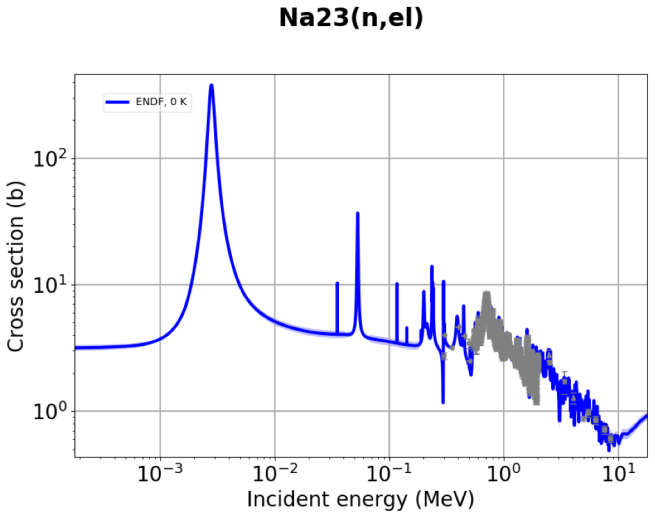
Motivation: *to easily share evaluated and processed data across institutions within a modern framework*

GNDS: from evaluated nuclear data to transport simulations

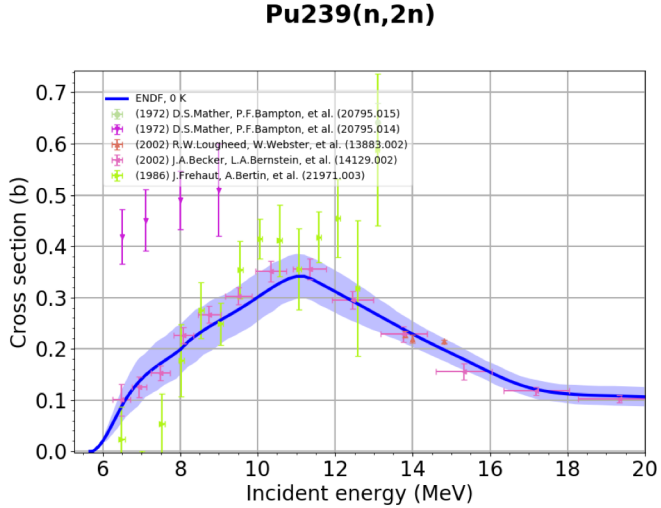


FUDGE: For Updating Data and Generating Evaluation

- FUDGE toolkit, now
  - Python 2.7 with extension in C and C++ to handle computationally expensive tasks *(->soon conversion t 3.6*)
  - Translate LLNL ENDL and ENDF-6 to GNDS, and GNDS to ENDF-6
  - Manage, manipulate, view, check and process GNDS data



- LLNL production code for managing and processing Nuclear Data
  - Point of contact: Caleb Mattoon



- **Open source**: released under BSD license

- Download fudge via **http://www.nndc.bnl.gov/endf/codes/FUDGE/index.html**

Status of Translation/Processing of ENDF to GNDS

- **Translation** of the following ENDF sub-libraries
  - Note that the definition for nfy and sfy is not finalized in GNDS

neutrons	protons	deuterons	tritons
helium3s	gammas	photoat	standards
electrons	decay	atomic_relax	thermal_scatt
nfy	*sfy*	alphas	

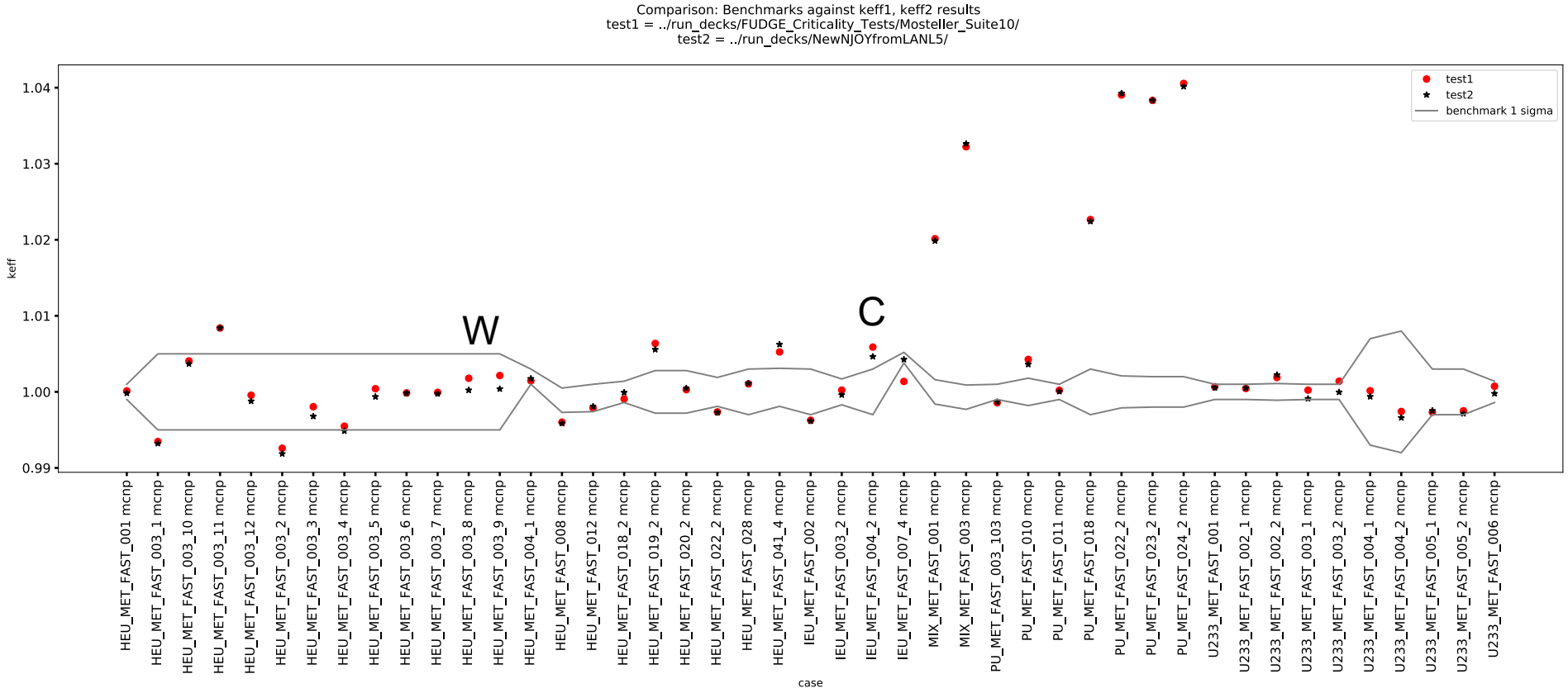
- FUDGE handles all properly formatted ENDF-6 formatted files
  - In ENDF/B-VII.1, VIII.0
  - *Except* for new data format for fission in ENDF/B-VIII.0
- **Processing** of the following ENDF sub-libraries

neutrons	protons	deuterons	tritons
gammas	helium3	photoat	alphas

- FUDGE can translate GNDS data to ACE format for use in MCNP

TO DO LIST (partial)
- Thermal scattering laws
- URR probability tables

FUDGE processing to ACE format



Fairly good agreement for 45 fast critical assemblies.
Differences for W, C, ^{238}U reflectors

GIDI & MCGIDI: General Interaction Data Interface

- GIDI version 3
  - C++ API to read GNDS files for transport codes
  - Can get data at any level in GNDS structure
  - Multi-group collapsing
    - For vectors and matrices
    - Transport correction
  - Calculates multi-group energy deposition
  - Complete for neutrons, photons and charged particles

- MCGIDI version 3: Monte Carlo GIDI
  - C++ API to store and sample for Monte Carlo transport codes
  - Uses GIDI to read data, then puts it into better form for optimal MC sampling
  - Handles point-wise cross sections and pdf/cdf distributions
  - Supports GPUs
  - Will sample a reaction for a protare and outgoing distribution
  - Angular biasing
  - multi-group support for cross sections
- Currently working on:
  - point-wise energy deposition
  - fixed-grid support for cross sections, deposition energy, etc.

- **Open Source** will be released *soon* under BSD license
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Testing ENDF/B libraries in GNDS format

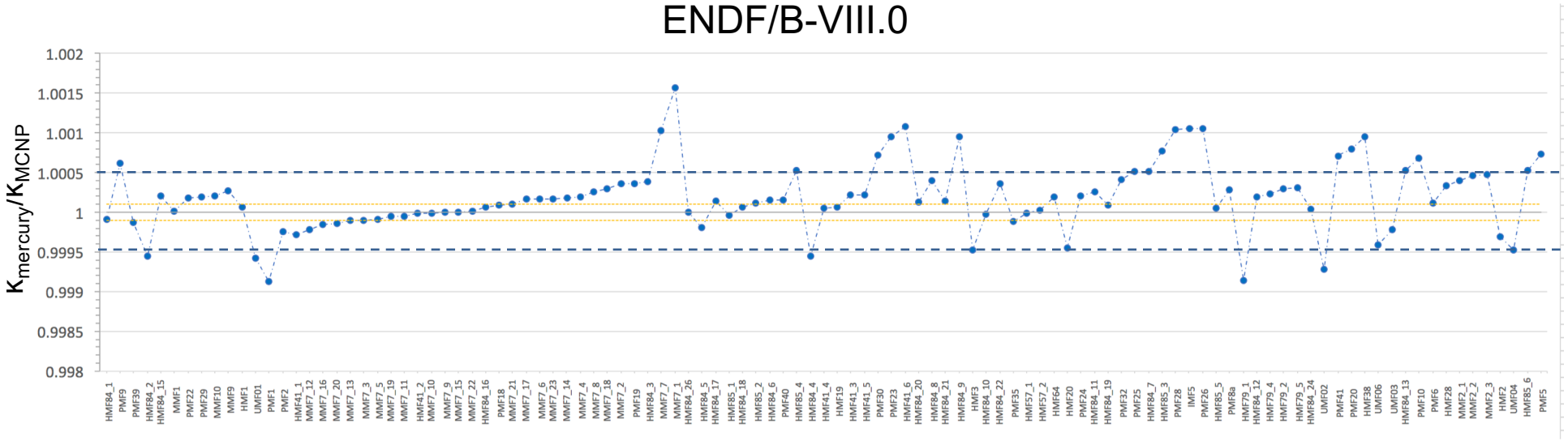
- Two ENDF libraries were translated and processed with FUDGE into GNDS format
  - ENDF/B-VII.1
  - ENDF/B-VIII.0
- V&V with LLNL Codes

Code	Code Type	Run mode	Data Format/API	Benchmark tests	Cross-sections
Mercury	Monte Carlo	Batch	GNDS/ GIDI/ MCGIDI	Criticality: 123 fast assemblies Reaction ratios: 3 assemblies 16 Pulsed spheres	Continuous Energy
Ardra	Deterministic Sn	Interactive	GNDS/ GIDI	Criticality:79 assemblies	Multigroup: 230 groups

- Results were compared to MCNP6 - ENDF/B-VII.1 and VIII.0 results (2017)

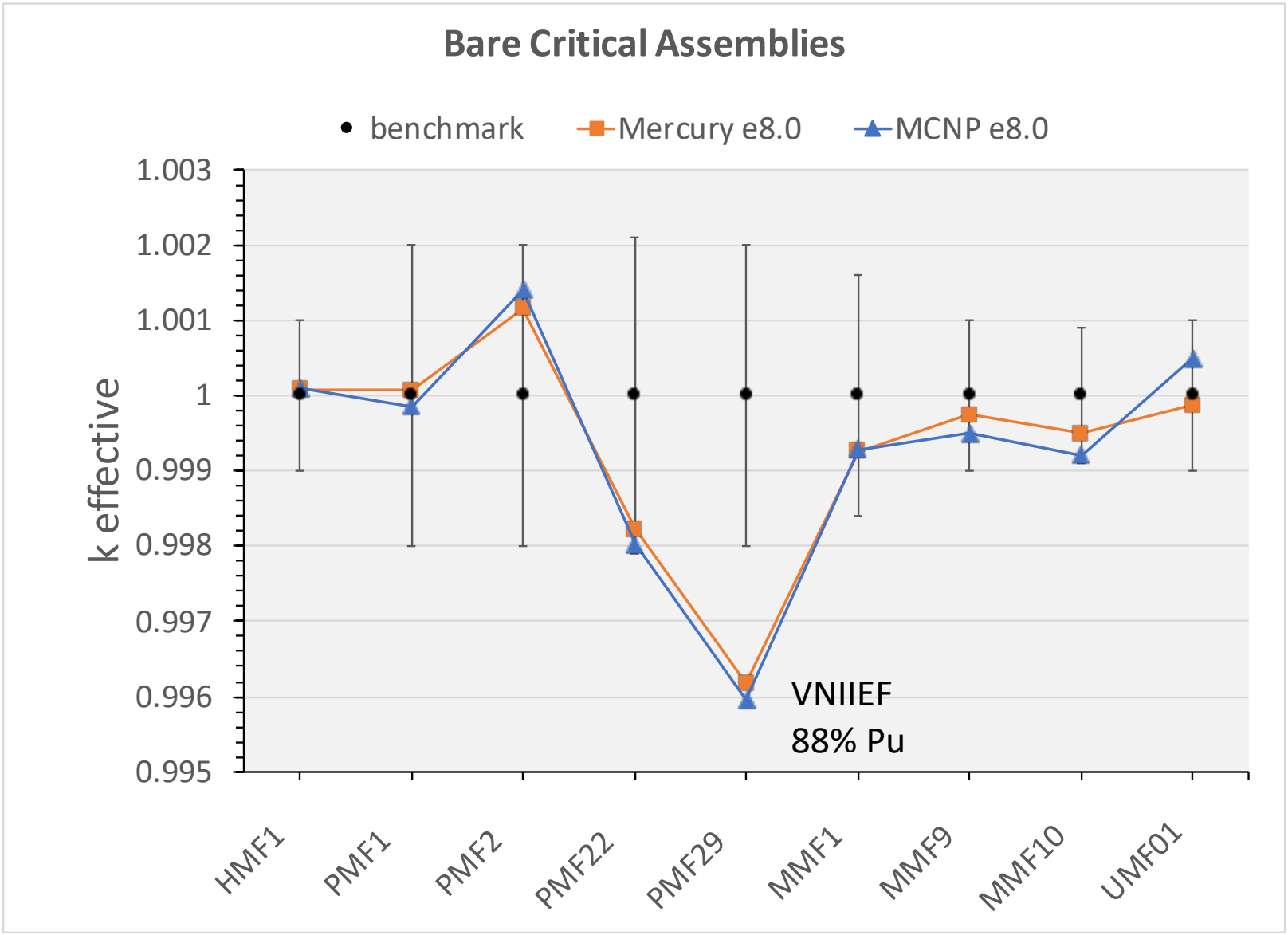
Criticality

- 107 fast benchmarks

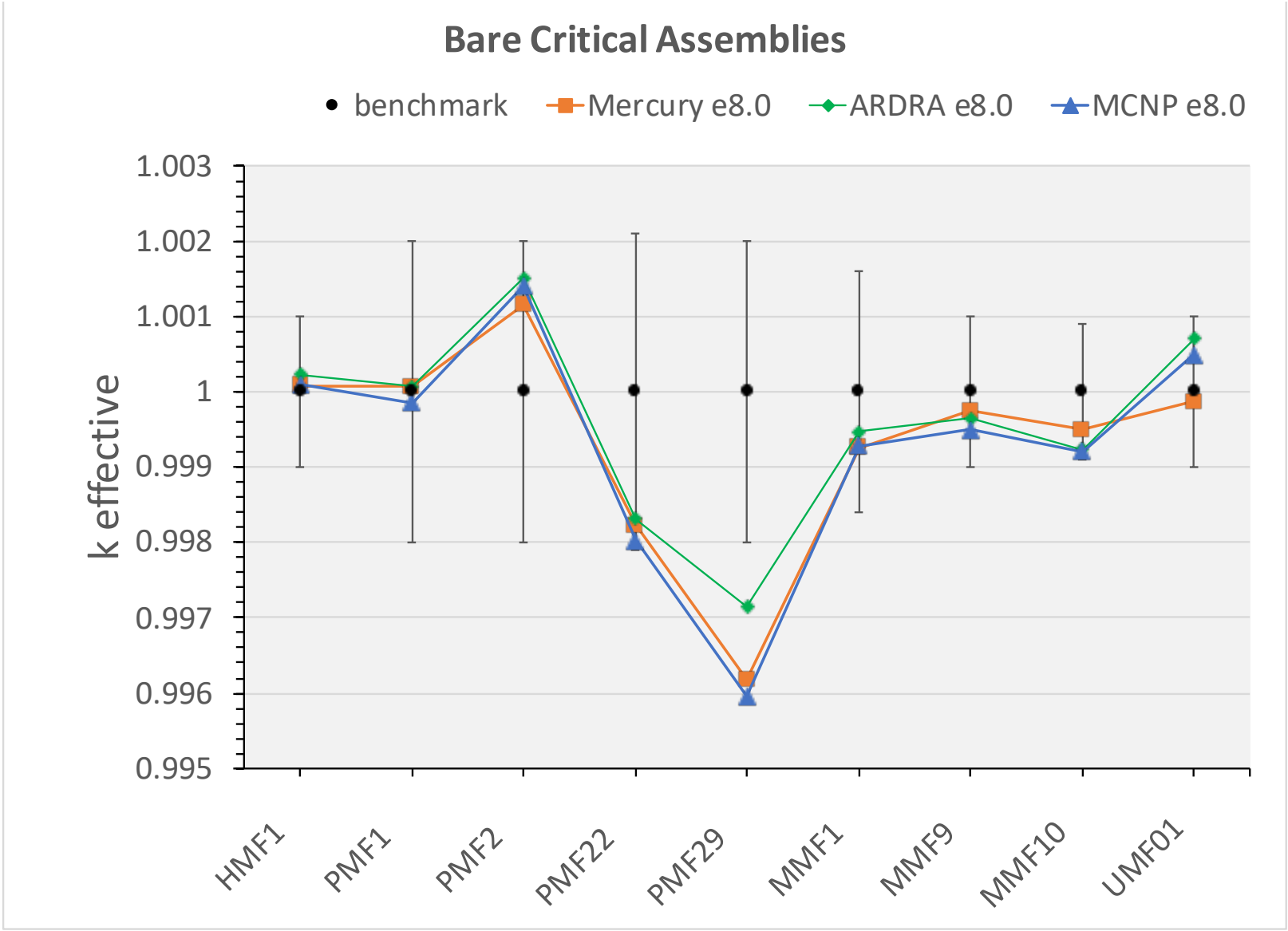


Mercury/GNDS' k_{eff} are within 5e-4 of ENDF's for 80/107 fast critical assemblies

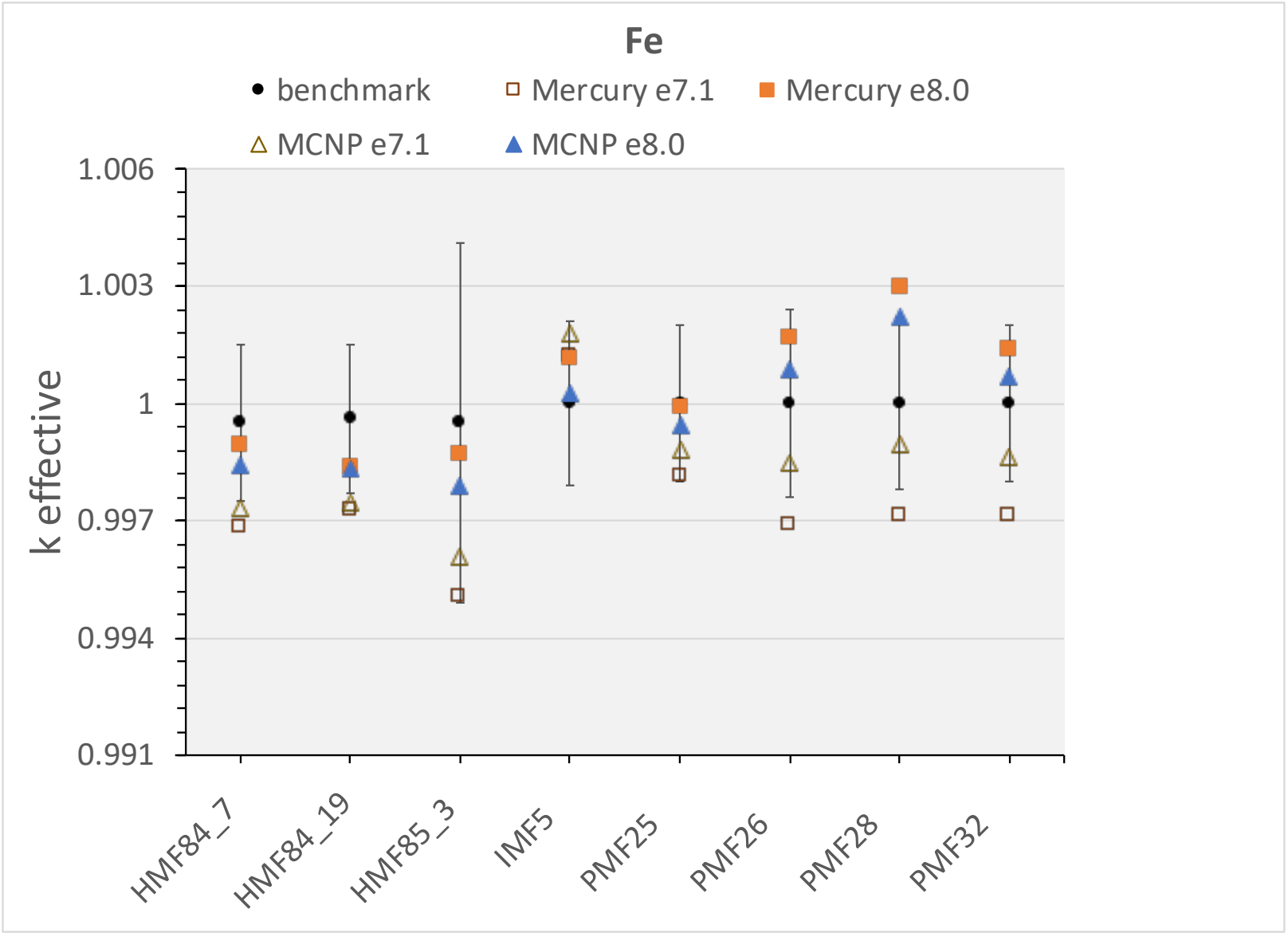
Bare assemblies: Godiva, Jezebel, Jezebel240,…



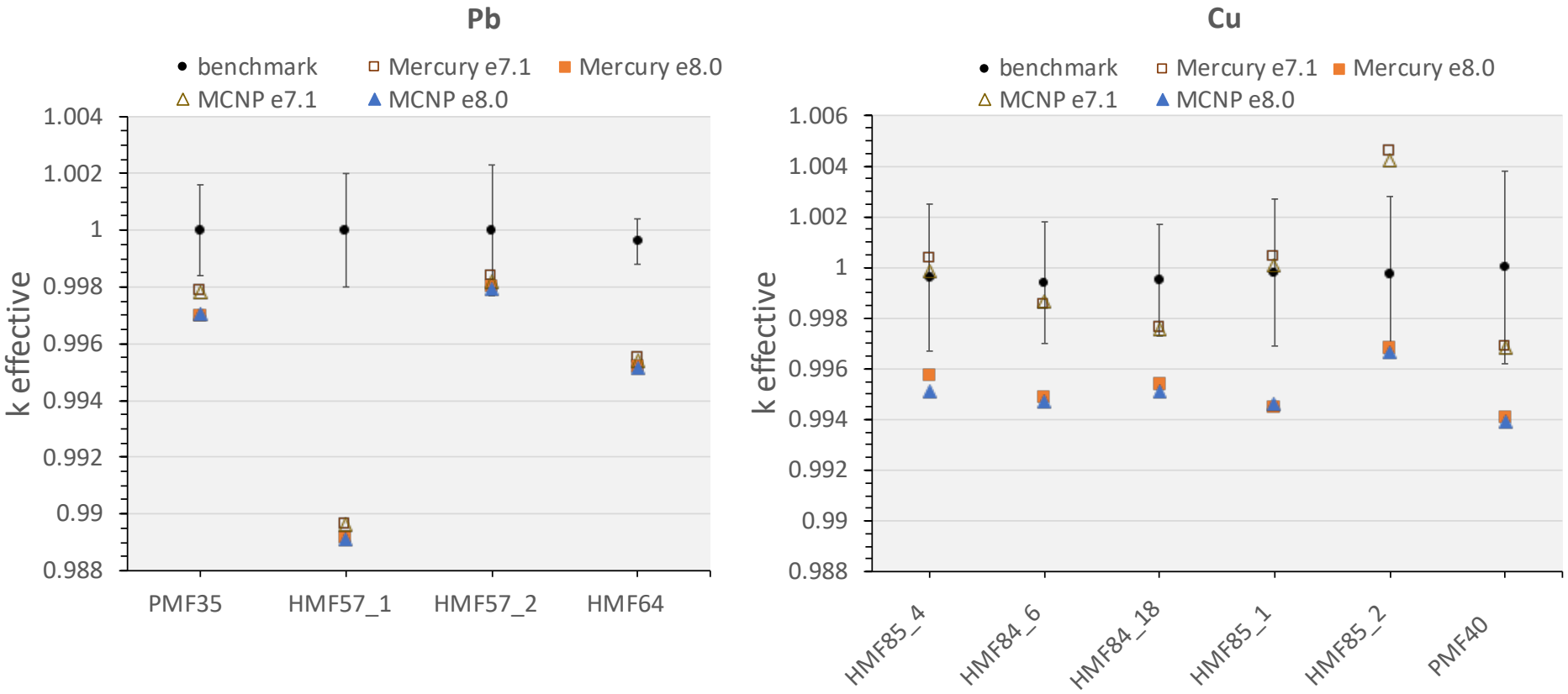
…Adding Ardra results



Fe

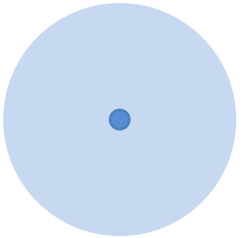

Fe
benchmark
Mercury e7.1
Mercury e8.0
MCNP e7.1
MCNP e8.0
k effective
1.006
1.003
1
0.997
0.994
0.991
HMF84_7
HMF84_19
HMF85_3
IMF5
PMF25
PMF26
PMF28
PMF32

Pb and Cu


Pb
benchmark
Mercury e7.1
Mercury e8.0
MCNP e7.1
MCNP e8.0
k effective
1.004
1.002
1
0.998
0.996
0.994
0.992
0.99
0.988
PMF35
HMF57_1
HMF57_2
HMF64
Cu
benchmark
Mercury e7.1
Mercury e8.0
MCNP e7.1
MCNP e8.0
k effective
1.006
1.004
1.002
1
0.998
0.996
0.994
0.992
0.99
0.988
HMF85_4
HMF84_6
HMF84_18
HMF85_1
HMF85_2
PMF40

Reaction ratios

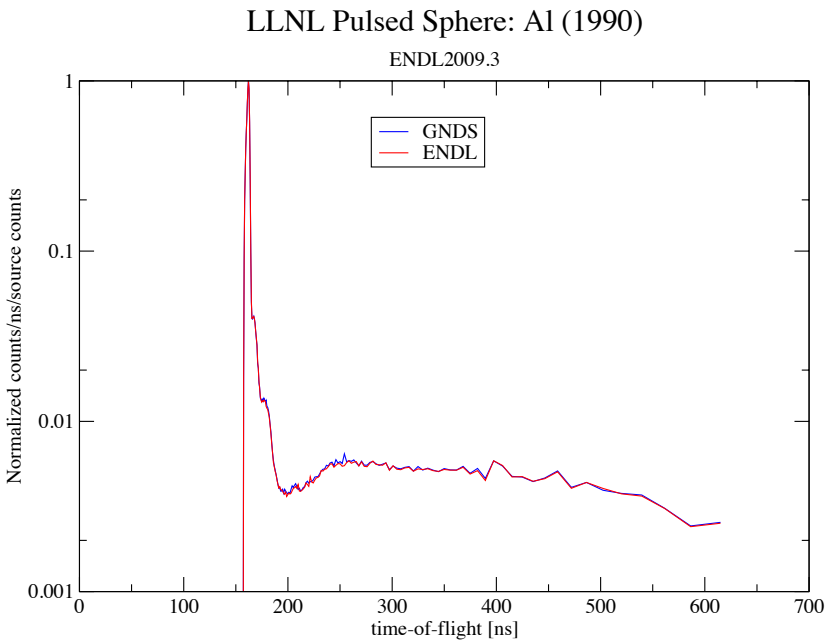
- ENDF/B-VIII.0 library
- Mercury/GNDS – MCNP6.2/ACE
- Reaction rates are normalized by $^{235}U(n,f)$

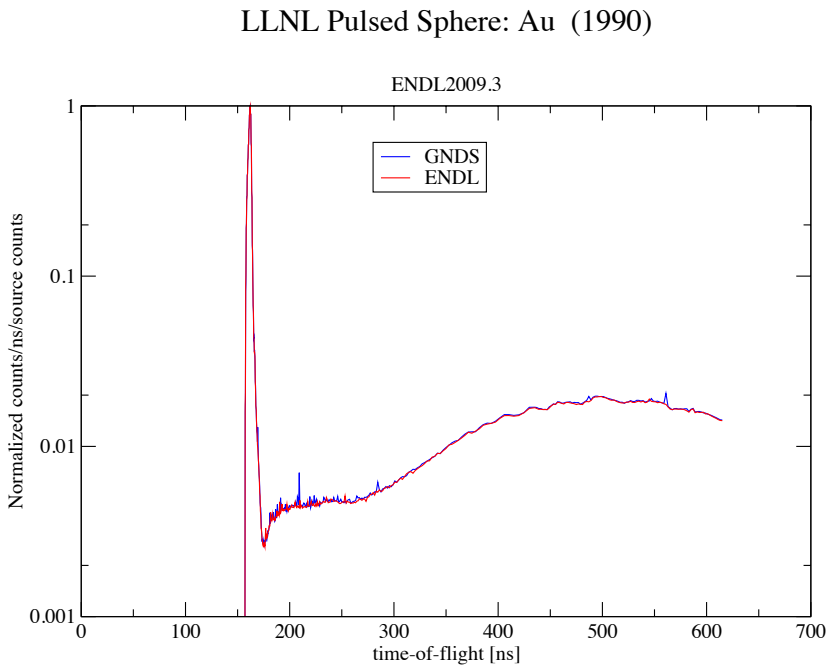


Benchmark	Reaction Ratio	$^{233}U(n,f)$	$^{238}U(n,f)$	$^{237}Np(n,f)$	$^{239}Pu(n,f)$	Simulated k_{eff}
Godiva	Mercury	1.5793	0.1583	0.8314	1.3844	1.00016 +/-0.00010
	MCNP	1.5793	0.1583	0.8318	1.3846	1.00009 +/-0.00008
	Mercury/MCNP	*1.0000*	*1.0001*	*0.9995*	*0.9998*	
Jezebel	Mercury	1.5660	0.2120	0.9772	1.4275	0.99986 +/-0.00010
	MCNP	1.5560	0.2121	0.9770	1.4273	1.00073 +/-0.00008
	Mercury/MCNP	*1.0064*	*0.9997*	*1.0002*	*1.0001*	
Flattop25	Mercury	1.5776	0.1450	0.7737	1.3621	1.00115 +/-0.00010
	MCNP	1.5664	0.1451	0.7735	1.3622	1.00082 +/-0.00009
	Mercury/MCNP	*1.0072*	*0.9990*	*1.0003*	*0.9999*	

We are still investigating possible sources of differences for U233(n,f) in Jezebel and Flattop25.

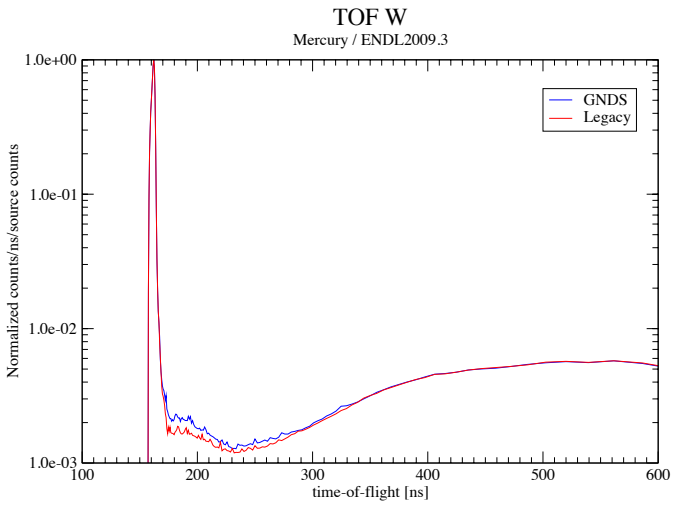
TOF experiment – LLNL pulsed spheres

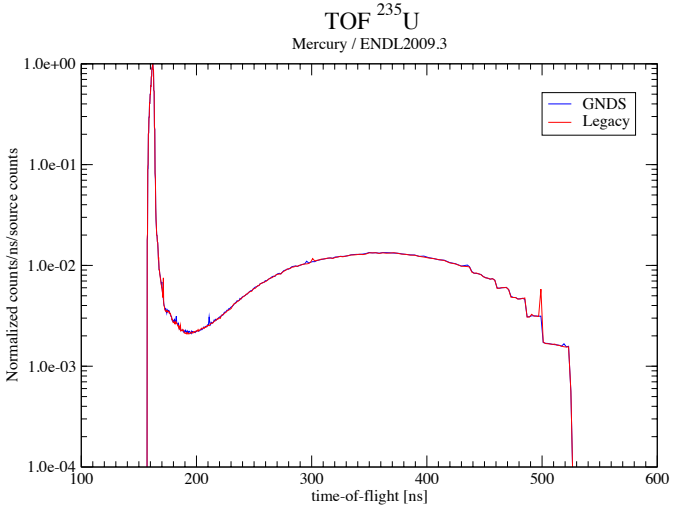


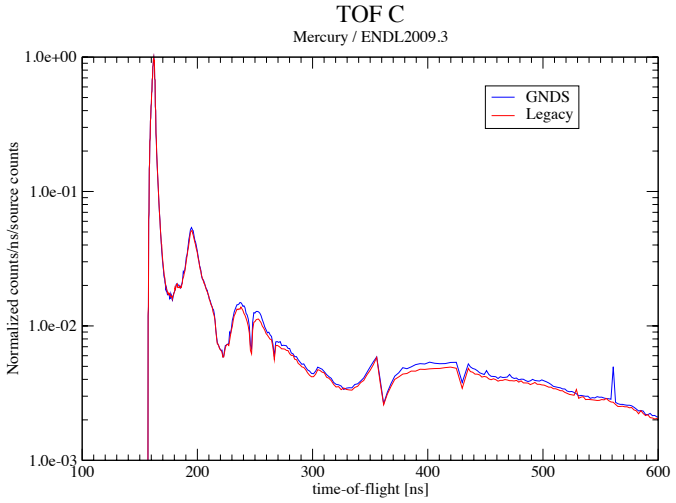


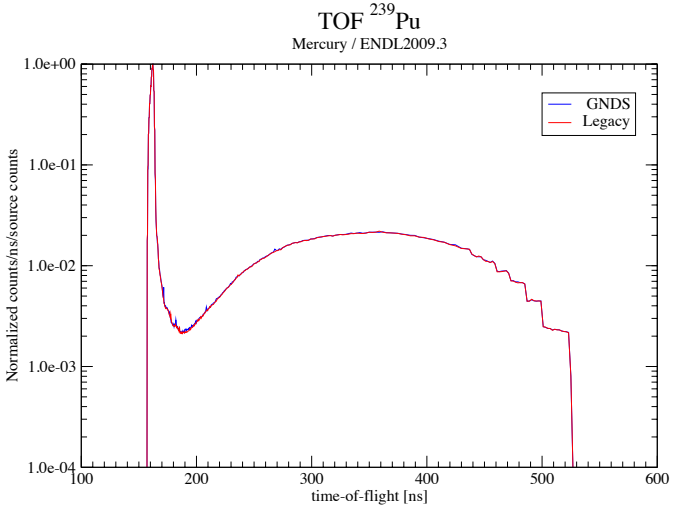
We have implemented angular biasing in MCGIDI and tested with LLNL's library in GNDS for 16 LLNL pulsed spheres.
Different models - Testing ENDF/B-VIII.0 in GNDS format is next

TOF experiment – LLNL pulsed spheres



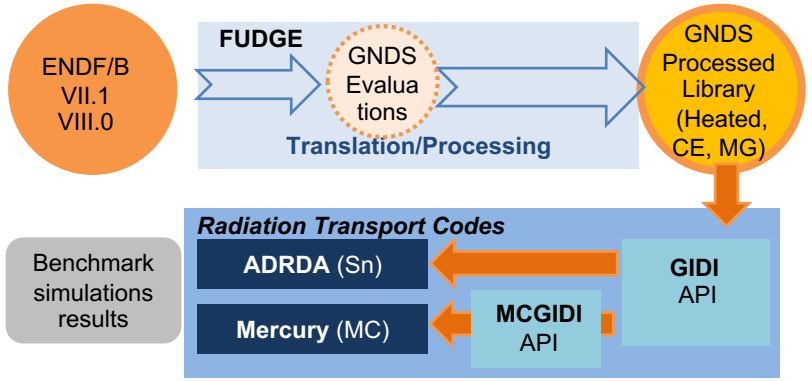






Summary

- LLNL implemented the GNDS format for evaluated and processed nuclear data
- FUDGE Processing
  - significantly faster compared to previous tools
  - Recently added: GNDS to ACE translator (n sub-library, outgoing n)
- GIDI/MCGIDI APIs
  - Recently added: multi group (group collapsing) ; angular biasing model (MCNP)



- The process was tested on ENDF/B-VIII.0 and VII.1 libraries and compared to MCNP6 results published in ENDF/B-VIII.0 release paper

Future work

- FUDGE Processing
  - **Unresolved resonance region probability tables**
  - Neutron thermal scattering laws
  - Multi-band (Sn and Monte Carlo)
  - GNDS to NDI, etc.

- GIDI / MCGIDI
  - **Unresolved resonance region probability tables**
  - Neutron thermal scattering laws
  - Hybrid angular biasing model (more memory, better statistics)

- CODES: ARDRA & Mercury
  - Multi-band

- Kiwi - creates realizations for Uncertainty Quantification
  - Include Kiwi in FUDGE
  - Update for GNDS data