LA-UR-12-20397

Advanced Monte Carlo for Reactor Physics Core Analysis

Forrest Brown [a], Brian Kiedrowski [a], David Brown [b], William Martin [c], David Griesheimer [d]

[a] *Los Alamos National Laboratory*
[b] *Brookhaven National Laboratory*
[c] *University of Michigan*
[d] *Bettis Atomic Power Laboratory*

Abstract

Advanced Monte Carlo for Reactor Physics Core Analysis

Workshop for PHYSOR-2012, Knoxville TN, 15 April 2012

Forrest Brown (LANL), Brian Kiedrowski (LANL), David Brown (BNL), William Martin (Michigan), David Griesheimer (BAPL)

Monte Carlo criticality calculations are performed routinely on large, complex models for reactor physics core analysis. This workshop provides an introduction to some of the key issues for code developers and reactor analysts, a description of the recent release of the ENDF/B-VII.1 nuclear data, and a review of current and future Monte Carlo code capabilities for mulltiphysics calculations. The workshop includes university and national laboratory perspectives. It should benefit both Monte Carlo practitioners and developers.

- Monte Carlo Methods & Advanced Computing – F. Brown, B. Kiedrowski
- Release of the ENDF/B-VII.1 Evaluated Nuclear Data File – D. Brown
- Multiphysics Reactor Calculations – W. Martin, D. Griesheimer

Agenda

Forrest Brown & Brian Kiedrowski (LANL)

- Monte Carlo methods & advanced computing
- Recent developments – OTF Doppler, population diagnostics, alternate eigenvalues, sensitivites

David Brown (BNL)

- Release of the ENDF/B-VII.1 Evaluated Nuclear Data File
- Advances in the 5 years since ENDF/B-VII.0
- Early examples of ENDF/B-VII.1 in applications

William Martin (Michigan), David Griesheimer (BAPL)

- Prospects for full-core Monte Carlo simulation including multiphysics feedback
- MC21 & multiphysics coupling

Monte Carlo Methods & Advanced Computing

Forrest Brown & Brian Kiedrowski

Monte Carlo Codes Group (XCP-3)

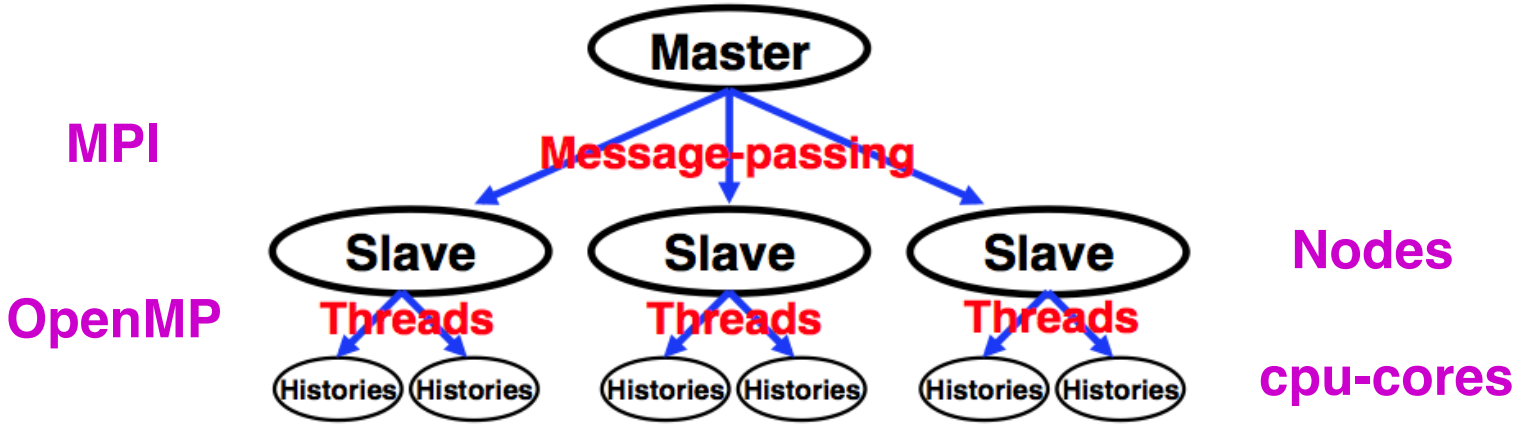
Topics

- Monte Carlo & Advanced Computers
- MCNP & Reactor Design
- On-The-Fly Doppler Broadening

- Population Size & Fission Source Coverage
- Alternate Eigenvalues for Criticality Searches
- Time Absorption Eigenvalues
- Continuous-Energy Nuclear Data Sensitivities
- Boundary Sensitivities

Monte Carlo
&
Advanced Computers

- **Monte Carlo is inherently parallel, on histories**
  - **MCNP**
    - Hierarchical parallelism, history-based
    - MPI to compute nodes, OpenMP threads for cores on node
  - **MPI**
    - Standard, portable, easy to implement in codes, private address space
    - Storage hog – can't share memory among MPI processes
  - **OpenMP threading**
    - Standard, portable, tricky to implement, shared address space
    - Can easily share common data – geometry, xsecs, tallies
    - Fully supported by only a few compilers (eg, Intel)

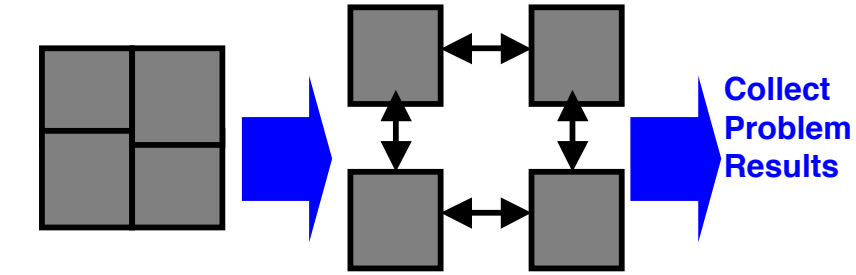


- **Challenges**
  - **Today's models are very large**
    - Detailed geometry, CSG or meshes with Ms of regions
    - Large, detailed continuous-energy xsec data
    - Huge number of tallies – regions, isotopes, reactions, depletion
    - Multiphysics coupling – very many temperatures & densities
    - Problem memory requirements > memory on compute node
  - **Data management for multiphysics**
    - Match-up temperatures, number densities, heat production, ..., for Ms of regions between MC, depletion, CFD, mechanical, ...
    - Old-fashioned method (read/write from disk files) does not work well on today's large parallel clusters
  - **Heterogeneous computing**
    - GPUs & Many-core, vs traditional cpus
    - Requires extensive recoding
    - Huge bottleneck – data motion among heterogeneous processors
    - Scaling to Ms of cpu-cores

Memory size issues

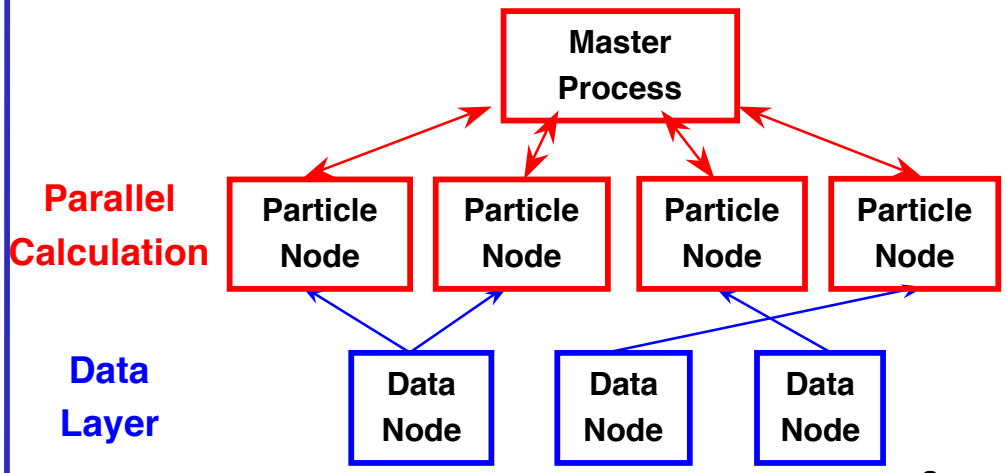
Spatial domain decomposition

- Partition problem (spatially) into blocks, store only data needed for block
- Move particles (and their state) among blocks as needed
- Solves memory issue, but creates difficulties for tallies, code complexity, load balancing, and communications overhead
- To date, most codes and R&D have focused on domain decomposition



Data decomposition

- Spread out data among nodes, use remote memory puts/gets to access
- Particles stay on node, move data to particles as needed
- Solves memory issue, but creates difficulties for communications overhead



Data management for multiphysics

- **Match-up temperatures, number densities, heat production, ..., for Ms of regions between MC, depletion, CFD, mechanical, ...**
  - Old-fashioned method (read/write from disk files) does not work well on today's large parallel cluster
  - Possible solutions
    - Data & dataset manager software
    - Framework, with methods for storing, retrieving, interchanging datasets
- **See Martin-Griesheimer talks**

Heterogeneous computing

- **GPUs**
  - Methods from 1980s vector MC apply (well-known, extensive recoding)
  - Need double-precision + SECDED, slower than PR peak speeds
  - Major difficulty: managing data flow between cpu & gpu
    - Could be handled similar to old fashioned disk i/o
    - Buffering, with asynchronous read-ahead / write-behind

- **MICs - many integrated cores**
  - 100s or 1000s of cores per processor
  - Need to re-examine threading locks & thread-private storage
  - No major obstacles

- **Challenges**
  - Huge bottleneck – data motion among heterogeneous processors
  - Scaling to Ms of cpu-cores

MCNP
&
Reactor Design

MCNP & Reactor Design (1)

- MCNP5 is widely used & well respected – detailed geometry, detailed continuous-energy physics, long V&V history, etc.
- MCNP6 promises all of that & much more.
- There is a huge difference between a research-oriented benchmarking MC code & a production tool for serious reactor design
- What does MCNP need for reactor design applications, including multiphysics?
- Some proposals follow. Email us regarding others.
  (Send $$$ or beer if you really want something...)

- **Criticality searches**
  - Rod height & other geometry changes
  - Soluble boron
  - Buckling

- **Self-consistent equilibrium Xenon**
  - For depletion, power shape & Xenon distributions must be consistent
  - Improves robustness & stability, permits longer timesteps
  - Can adjust Xenon spatially during Keff iterations (mildly nonlinear)

- **Temperature distributions**
  - Need to permit mesh or continuous temperature maps
  - Independent of cell-based geometry

- **Resonance scattering free-gas treatment at epithermal energies**
  - Demonstrated, needs production implementation

- **Sensible units**
  - Degrees K for temperatures (not MeV)
  - Seconds for time (not shakes)

- **Features for tallies**
  - Combinations of several tallies
  - Ratios of tallies
  - Kernel density estimators (KDE)

- **Features for easy generation of multigroup cross-sections**
  - Could use MCNP to generate few-group xsecs, to use in nodal codes
  - Tallies for group-to-group scattering

- **Library of standard materials**
  - Standard, common material definitions
  - Permit mixing of materials

- **More robust tracking**
  - Background material to handle gaps in geometry
  - Fixup for gaps/overlaps
  - Improved “locate” operation, using ray-trace instead of cell-search

- **Improved problem setup**
  - More user-friendly input
  - Input setup does not use parallel threads
  - Many input setup & checking routines scale as N^2 or N^3, need rework

- **Improved output**
  - Reduce huge amount of unwanted, unneeded output

- **Standard file formats for problem input (or linkage), & standard file formats for problem tally results (or linkage)**
  - Including complete descriptions of all file formats

MCNP & Reactor Design (5)

- **Reactor depletion, using built-in CINDER**
  - Branch calculations for depletion
  - Standard output files for each timestep
  - Easier control over depletion chains & isotopes
  - Improved predictor-corrector scheme
  - Equilibrium Xenon
  - Etc.
- **Automated weight-window generation**
  - Eliminate need for multiple runs, with manual editing, etc.
- **Improved parallel processing efficiency for large reactor caclulations**
- **Simpler, automated setup for TRISO fuel particles**
- **Sensitivity/uncertainty (or perturbation) techniques that include all types of continuous-energy scattering**
- **Delayed-neutrons in alpha-eigenvalue calculations**

On-The-Fly Neutron Doppler Broadening for MCNP

Forrest Brown (LANL), William Martin (Michigan),
Gokhan Yesilyurt (ANL), Scott Wilderman (Michigan)

US DOE NE-UP Project

Introduction

Doppler Broadening

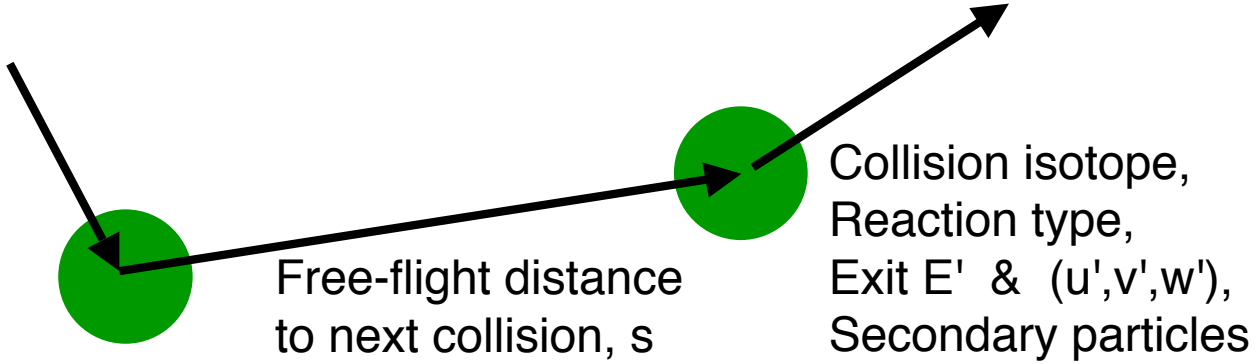
Temperature Variation in Monte Carlo Codes

- **Low neutron energies:**
  - **S(α,β) interaction data** is used in modeling collision physics
    - 2002 data: 10^{-5} eV - **4.46 eV** neutron energies (15 nuclides)
    - 2012 data: 10^{-5} eV - **9.15 eV** neutron energies (20 nuclides)
  - S(α,β) data accounts for target nucleus chemical binding, molecular binding, crystal structure, thermal motion, etc.
  - Nuclides without S(α,β) data: use free-gas model (see below)
- **High neutron energies:**
  - Target nucleus **thermal motion neglected**
  - Typical: $E_{neutron} > 400\ kT$ for A>1
- **Epithermal neutron energies:**
  - **Target nucleus thermal motion important**
  - **Free-gas model -- nuclides have Maxwell-Boltzmann energy distribution at temperature T, isotropic direction**

$$f(E_{nuc}) = \frac{2}{\sqrt{\pi}} \cdot \frac{1}{kT} \cdot \left(\frac{E_{nuc}}{kT}\right)^{1/2} e^{-E_{nuc}/kT}$$

Gamma(kT, 3/2),
mean = 1.5 kT
mode = .5 kT

Doppler Broadening



- **Detailed kinematics of collisions must include nucleus E & Ω**
- **For free-flight, selection of collision isotope, & tallies of overall reactions: must use effective cross-sections, averaged over (E, Ω) distribution of nuclides at temperature T**

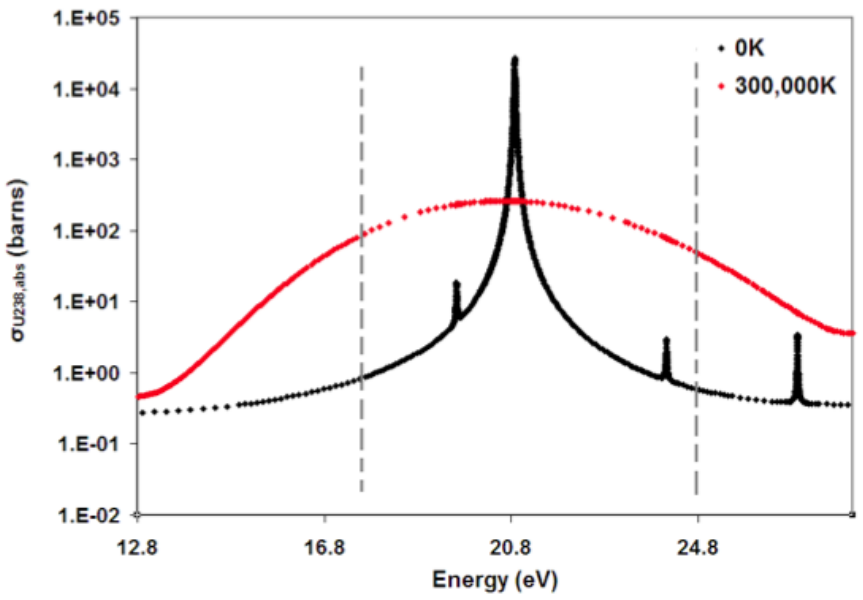
$$\sigma_{eff}(v)=\int \frac{|\vec{v}-\vec{V}|}{v}\sigma(|\vec{v}-\vec{V}|)P(\vec{V})d\vec{V}, \qquad P(\vec{V})=\left(\frac{M}{2\pi kT}\right)^{3/2} e^{-\left(M/2kT\right)V^2}$$

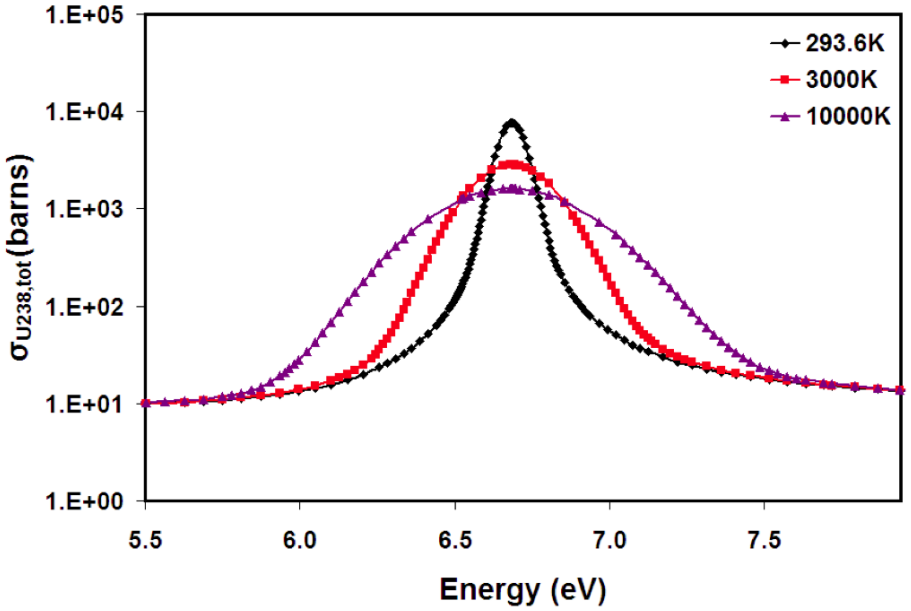
Doppler broadening equation v = neutron, V=nucleus

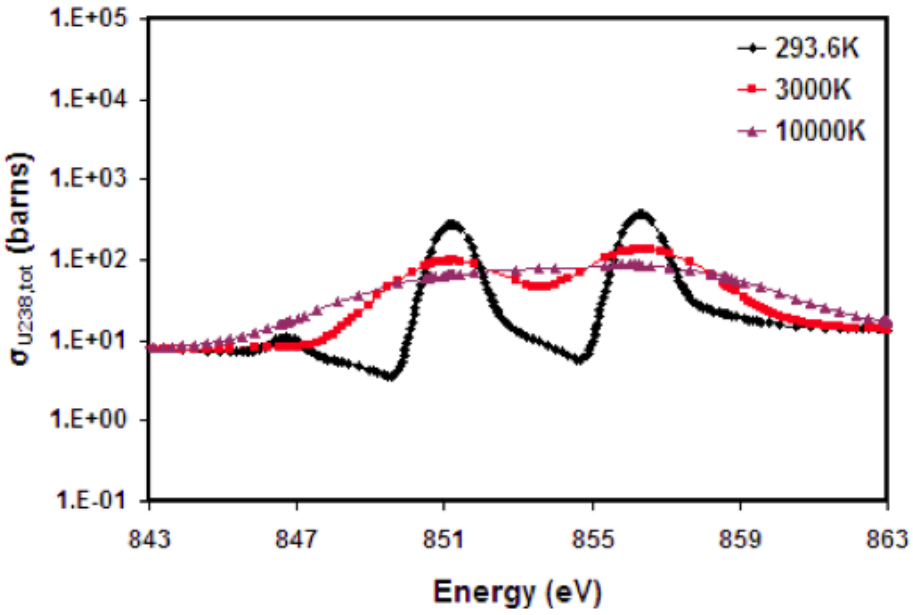
This is a convolution of the cross-section with the target energy or speed distribution. Smears out & smoothes the cross-section, reduces peak values.

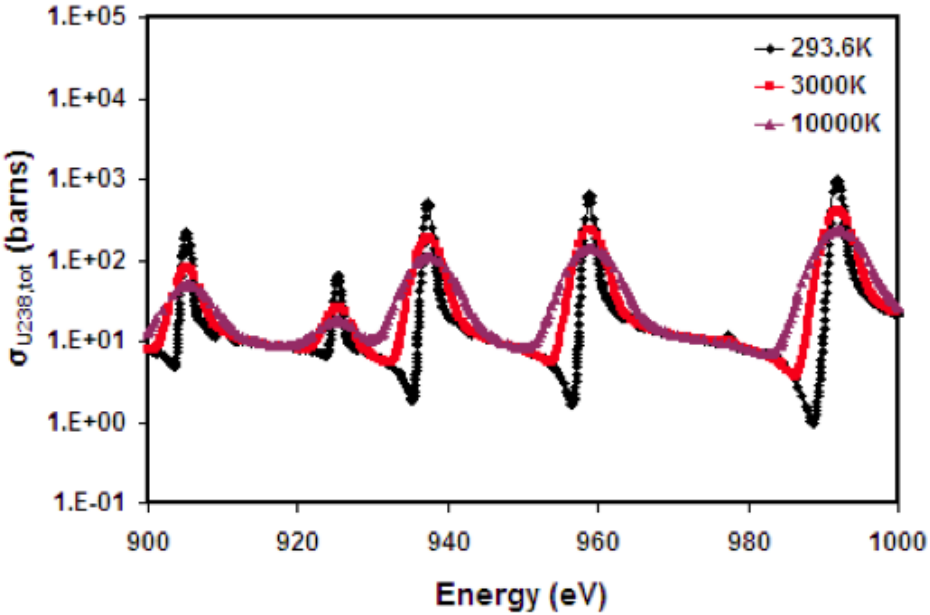
^{238}U Doppler Broadening Examples

Monte Carlo Codes
XCP-3, LANL



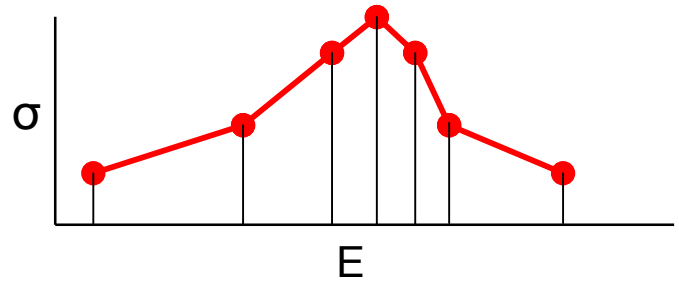






Doppler Broadening - Numerics

- **ENDF/B nuclear data is represented by piecewise-linear tabulation of σ(E)**



Typically, a linearization tolerance of 0.1% is used

- **Doppler Broadened Neutron Cross-sections**

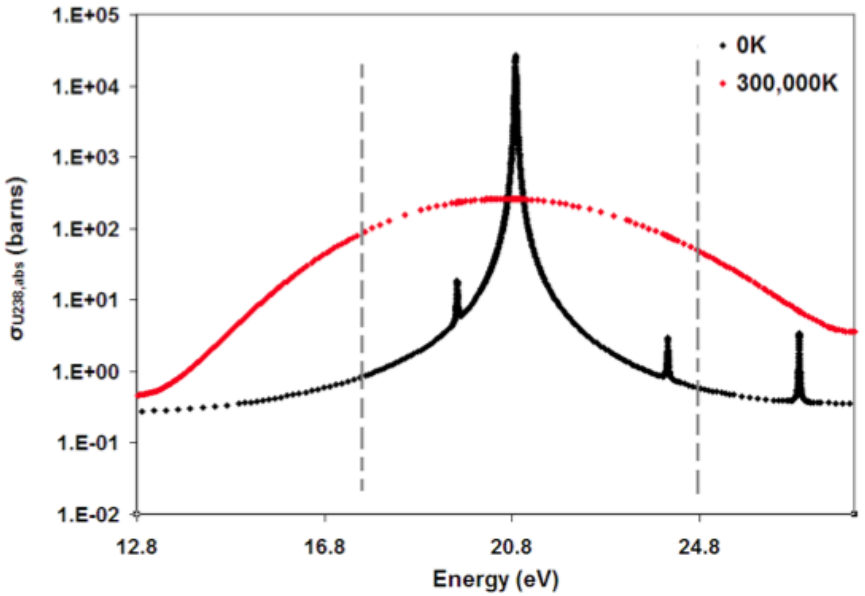
$$\sigma_{eff}(v) = \int_V \frac{|\vec{v}-\vec{V}|}{v}\,\sigma(|\vec{v}-\vec{V}|)P(\vec{V})\,d\vec{V}, \qquad P(\vec{V}) = \left(\frac{M}{2\pi kT}\right)^{3/2} e^{-\left(M/2kT\right)V^2}$$

  - Red Cullen (NSE, 1976) showed how to **exactly** perform this convolution of Maxwell Boltzmann PDF with piecewise-linear σ(E), called **sigma1 method**
  - **NJOY** code is similar & adaptively chooses energy points to meet 0.1% accuracy in σ_{eff} at T
  - σ_{eff}(E) has different E-mesh at different T's
  - **Very compute-intensive, typically performed prior to Monte Carlo in preparing nuclear data libraries**

Doppler Broadening with Adaptive Energy Grid

Monte Carlo Codes
XCP-3, LANL

Temperature Range (K)	Field of Study
77 - 293.6	Cold Neutron Physics
293.6 – 550	Benchmarking Calculations
550 – 1600	Reactor Operation
1600 – 3200	Accident Conditions



NJOY – adaptive E grid for ^{238}U Doppler broadening (ENDF/B-VI)

	Fractional Tolerance							
	0.1%	*0.3%*	*0.5%*	*1.0%*	*2.0%*	*3.0%*	*4.0%*	*5.0%*
T (K)	**Number of Energy Grid Points**							
0	193131	122935	100646	76856	57347	49659	44955	41676
77	103600	70240	59900	50049	43716	41408	40250	39514
293.6	85247	60192	52352	44810	39965	38089	37104	36494
500	77676	55786	49097	42506	38188	36509	35565	35006
1000	67437	50226	44773	39625	35957	34593	33810	33282
1500	62302	47227	42557	38000	34881	33616	32956	32490
2000	58735	45153	41098	36957	34109	32999	32384	31918
2500	56248	43774	39933	36177	33586	32543	31948	31560
3000	54282	42707	39051	35557	33208	32192	31661	31314

What if there are 1000s of T's ?

Six approaches:

1. Traditional NJOY+MC (exact)

- NJOY data at specific problem T's
- Each MC region in MC uses specific pre-broadened data
- **Exact, very cumbersome, very large amount of xsec data**

2. Traditional NJOY+MC (approx.)

- Like (1), but round off T's to nearest 10-20°
- **Aproximate, very cumbersome, very large amount of xsec data**

3. Stochastic Mixing (approx)

- NJOY data at a few bounding T's
- Set up MC input with a mix of hot & cold data for each nuclide, such that average T for the mix matches region T
- Run MC, will sometimes get "hot" data, sometimes "cold", average is OK
- **Approximate, cumbersome, very large amount of xsec data**

(OTF = On-The-Fly)

4. OTF Sigma1 (Monk)

- Use only 1 set of NJOY datafiles
- During MC, use **sigma1** method to broaden data as needed
- **Exact, but very expensive, ~10x increase in computer time**

5. OTF Using Delta-Track (Serpent)

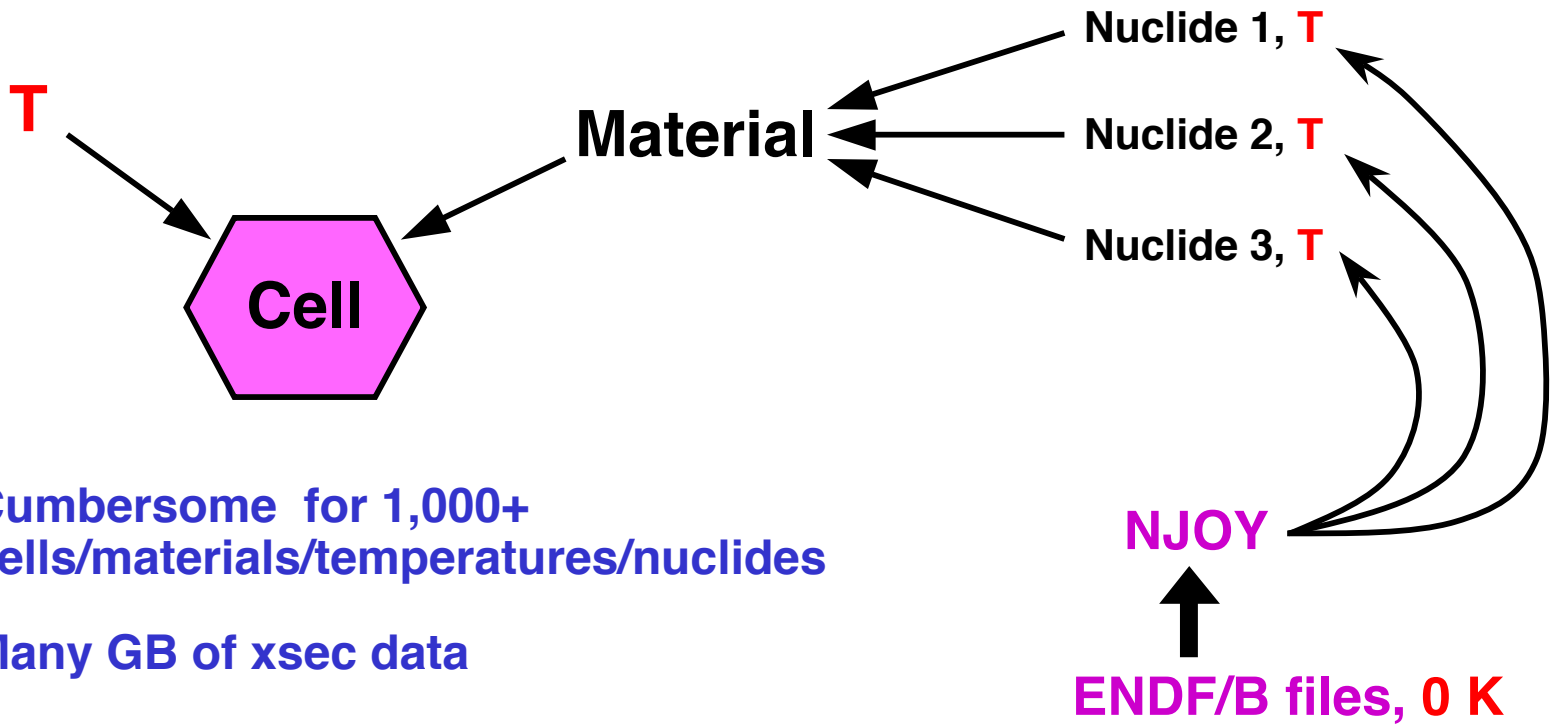
- Use only 1 set of NJOY datafiles
- During MC, use delta-tracking rejection method to broaden data as needed
- **Cannot do pathlength MC estimators or flux at a point estimators**
- **Exact, but complex & expensive, ~4x increase in computer time**

6. OTF Temp. Fitted Data (MCNP)

- Use only 1 set of NJOY datafiles
- Prior to MC, generate OTF datasets to handle temperature variation
- During MC, Doppler broaden as needed using fitting data
- **Exact, extra data for T-fits, ~1.1x increase in computer time**

(1)+(2) Traditional NJOY+MC

- **Conventional MCNP problem specification:**
  - **Temperatures** are assigned to **cells** (geometry regions)
  - **Materials** are assigned to **cells**
  - **Doppler broadening** for temperature T is performed on **nuclides**
  - **Materials** are composed of **nuclides**



  - **Cumbersome for 1,000+ cells/materials/temperatures/nuclides**
  - **Many GB of xsec data**

(1) Exact, number of datasets = number of T's

(2) Approx., match cell T to closest material with nuclides at T'

(3) Stochastic Mixing

- Often loosely called "stochastic interpolation" or "interpolation"
- This is simply mixing, not interpolation

- MCNP input example:
  - **Want this at 500 K:** m1000 92235 -.93 92238 -.07
  - **Have these datasets from NJOY:**

    92235.**91**c at **300 K**, 92238.**91**c at **300 K**
    92235.**92**c at **600 K**, 92238.**92**c at **600 K**

  - **For mixing linear in T, mix 2/3 of 300 K data + 1/3 of 600 K data**

    m1000 92235.91c -.62 92238.91c -.0466667
    92235.92c -.31 92238.92c -.0233333

- Cumbersome for 1,000+ cells/materials/temperatures/nuclides (could be scripted…..)
- Many GB of xsec data, 2x nuclides, complex input

(4) OTF Sigma1

- Recently implemented in **MONK**
- Numerical sigma1 method OTF during neutron tracking
- Increases overall runtime by ~10x
- See **Davies** paper from ICNC-2011

(5) OTF Delta-tracking

- Currently being tested in **Serpent**
- Very elegant & innovative, very promising
- Increases overall runtime by ~2-4x, may improve
- Does not fit with many conventional MC schemes:
  - No pathlength estimators
  - No point-detector (flux at a point) tallies
  - No reaction rate tallies (at present)
  - Requires radical revisions to codes such as MCNP
- See **Viitanen & Leppanen** paper from PHYSOR-2012

(6) OTF for MCNP -- rest of talk

OTF Doppler Broadening in MCNP

OTF Methodology
Union Energy Mesh
Temperature Fitting
OTF Doppler in MCNP
Testing
Work-in-Progress

On-The-Fly Neutron Doppler Broadening

- **OTF Methodology (for each nuclide)**
  - **Create union energy grid for a range of temperatures**
  - **Create fits for $\sigma_{eff}(T,E)$, for range of temperatures, on union E-grid**
  - **MCNP – evaluate $\sigma_{eff}(T,E)$ OTF during simulation**

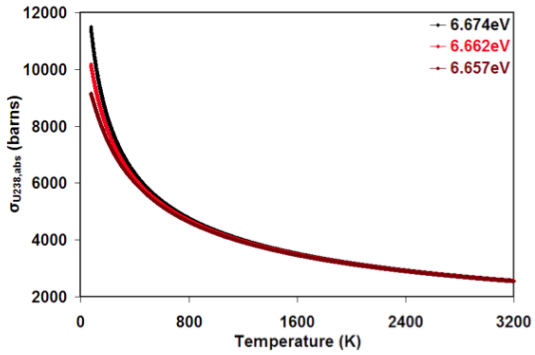
- **Comments**
  - **Target application, for now: reactors**
  - **Relies on NJOY methodology**
    - Supplements & extends NJOY
    - Methodology consistent with NJOY
  - **Fitting σ vs temperature (at each E)**
    - High precision, least squares with singular value decomposition
    - Adaptive (for each E, MT, & nuclide)
    - Explicit, direct error checking for fits - fit error < linearization tolerance
    - Threaded parallel, broadening routines called millions of times
    - Over temperature, maintains accuracy consistent with NJOY

OTF Methodology – Union Energy Grid

- **For 1 nuclide, determine:**
  - **MT numbers** for reactions to be broadened
  - **Energy range** for broadening, E_{min} - E_{max}
    - Up to start of unresolved data, or high-threshold reactions (whichever smaller)
  - **Temperature range** T_{min} – T_{max} & interval ΔT for tolerance testing (input)
  - **Base set of $\sigma_x(e)$'s** from NJOY at T_{base}
    - "x" = any MT reaction that needs broadening
    - ACE data file from NJOY: Yesilyurt: T_{base}=0 K, Brown: T_{base}=293.6 K
  - **Energy grid** from NJOY at T_{min}

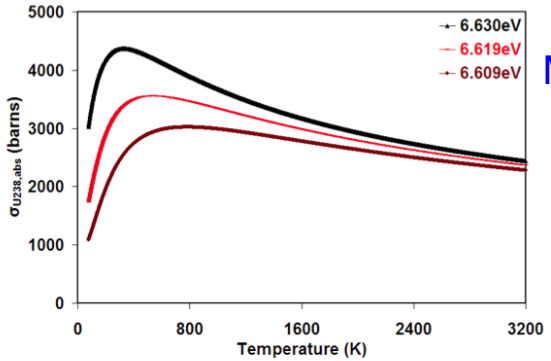
- **For 1 nuclide & a set of T's in range, at each T:**
  - **Adaptively add E points so that 0.1% linear tolerance is maintained**
    - Exact Doppler broadening from T_{base} to T, using sigma1 method
    - Check **all** broadened MT reaction data for each E interval
    - Subdivide E interval until 0.1% linearization tolerance met for all MT's
    - Add E points as needed, do not remove E points
  - Compute-intensive – millions of calls to sigma1 routine, parallel threads
  - Typically expands number of E points by **~10%**, for 293-3200 K range
  - **Result:** **union E-grid for nuclide, 0.1% linear tolerance over entire T range**

OTF Methodology – Fitting vs T (1)



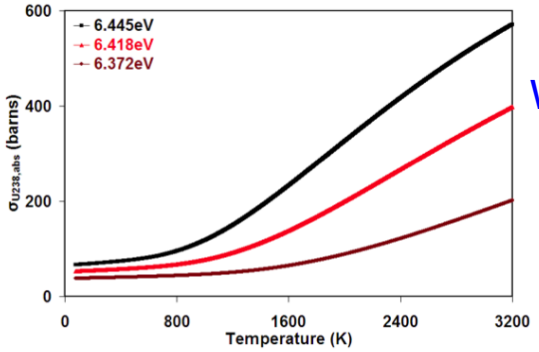
Near resonance peaks:

$$\sigma_{T,C,F}(T) \sim \sum_{k=0}^{\infty} \frac{d_k}{T^{k/2}}$$



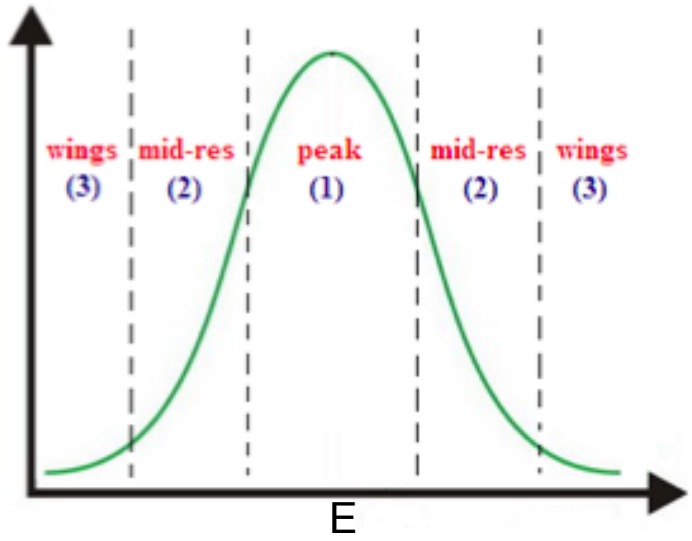
Mid resonance:

$$\sigma_{T,C,F}(T) \sim \sum_{k=0}^{\infty} e_k T^{k/2}$$



Wings of resonance:

$$\sigma_{T,C,F}(T) \sim \sum_{k=0}^{\infty} f_k T^k$$



Combined functional form :

$$\sigma_{T,C,F}(T) \sim \sum_{k=1}^{n} \frac{a_k}{T^{k/2}} + \sum_{k=1}^{n} b_k T^{k/2} + c$$

- for specific E, MT
- n varies for E, MT
- a_k, b_k, c tabulated for E, MT

Functional forms for temperature fitting based on multilevel **Adler-Adler** model, with expansions for peak, mid-res, wings

OTF Methodology – Fitting vs T (2)

- **For 1 nuclide, determine:**
  - **MT numbers** for reactions to be broadened
  - **Energy range** for broadening, E_{min} - E_{max}
    - Up to start of unresolved data, or high-threshold reactions (whichever smaller)
  - **Temperature range** T_{min} – T_{max} & interval ΔT for tolerance testing (input)
  - **Base set of $\sigma_x(e)$'s** from NJOY at T_{base}
    - "x" = any MT reaction that needs broadening
    - ACE data file from NJOY: Yesilyurt: T_{base}=0 K, Brown: T_{base}=293.6 K
  - **Union energy grid** for this nuclide & T range
  - **Maximum order for temperature fitting**
    - Adler-Adler based functional form, using powers of $T^{1/2}$ and $1/T^{1/2}$

- **For 1 nuclide, at each point in the union E grid:**
  - **Exact Doppler broadening from T_{base} to all T's in range**, using sigma1 method
  - **Least-squares fitting over T**
    - Singular value decomposition, least squares for temperature dependence
    - **Fitting order chosen adaptively for each energy & reaction so that fits accurate within 0.1% for all T's and all E's in range, for all MT's**
  - **Coefficients saved in files for MCNP use**

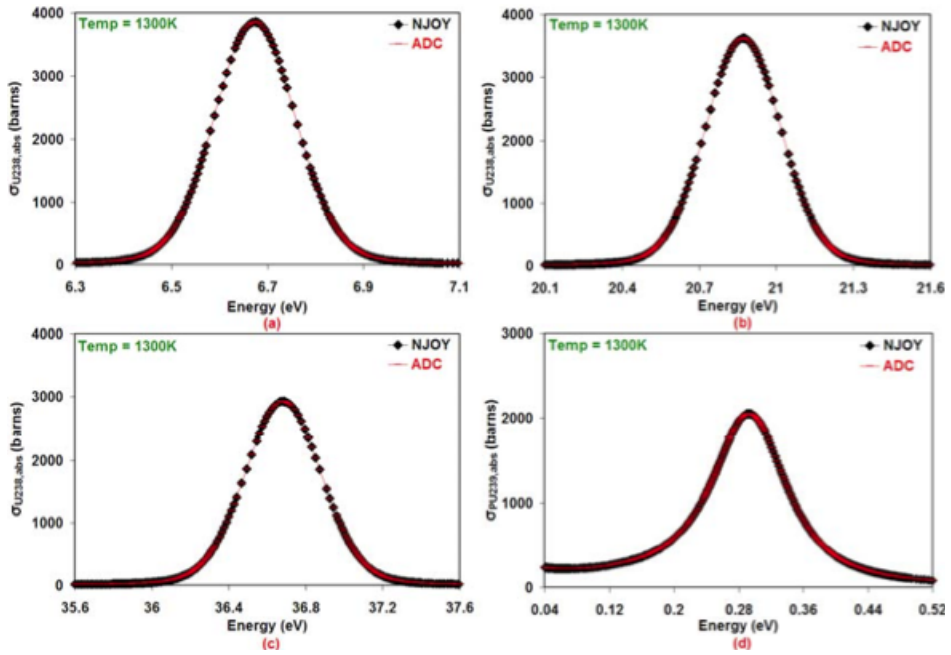
OTF Methodology – MCNP OTF

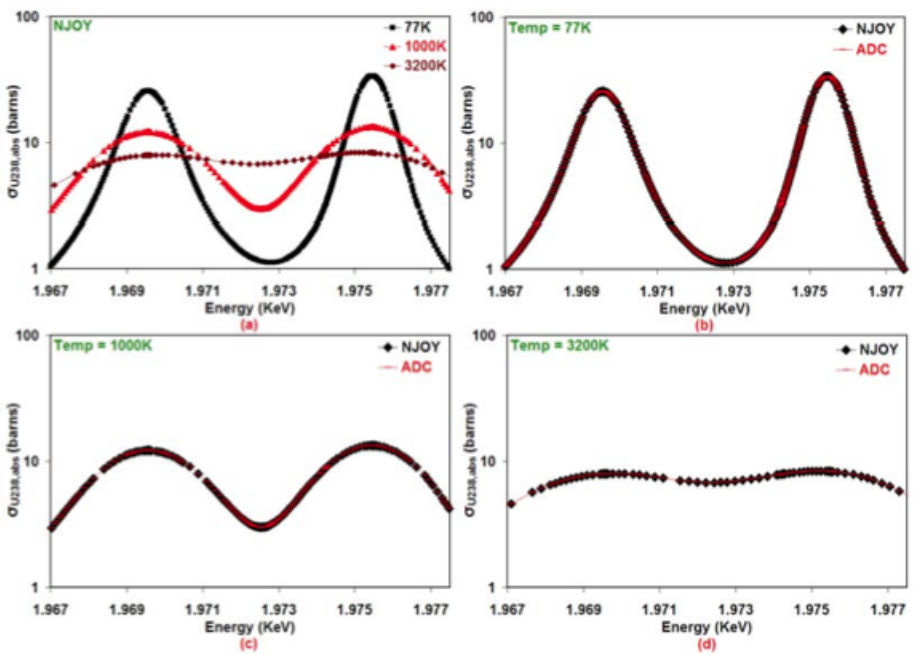
Monte Carlo Codes
XCP-3, LANL

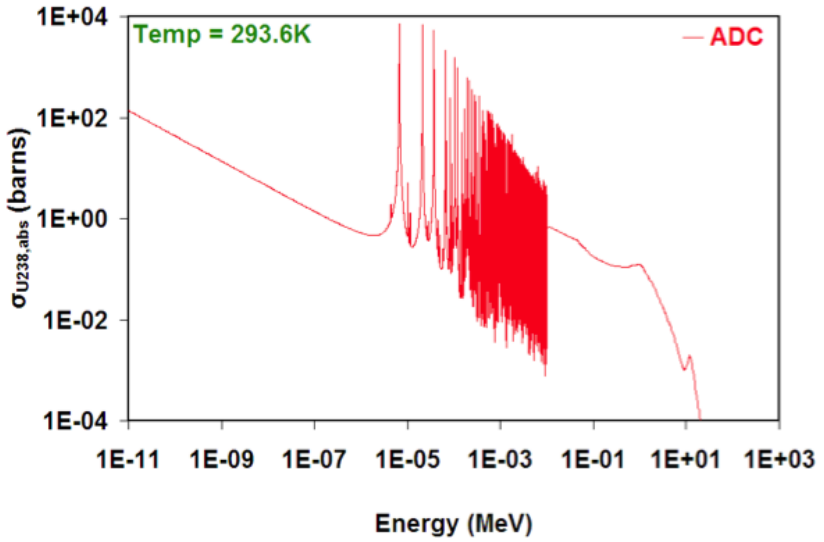
- **At problem setup, read in OTF data for various nuclides**
  - Each OTF nuclide set can have different fit orders & union E-grid & reactions
- **During simulation, if neutron in E-T range of fits**
  - Use OTF data for each nuclide to create on-the-fly Doppler broadened cross-sections at current cell temperature
  - If outside E-T range of OTF data, use standard ACE data
  - Collision physics (exit E & angles) uses standard ACE data
- **Only need to generate OTF datasets once, & then use for any problems**
- **Cost**
  - Extra storage for OTF data
  - Extra computing for evaluating OTF functions (typical <10% runtime)
- **Benefit**
  - Less storage for ACE data (no need for multiple temperatures)
  - Can solve problems with 1000s of T's or more, no limit
  - Greatly simplifies problem setup

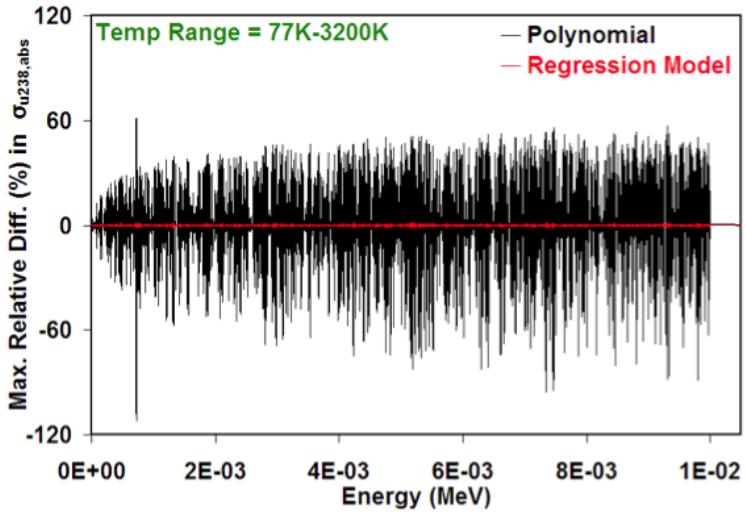
OTF Testing - Yesilyurt

Monte Carlo Codes
XCP-3, LANL

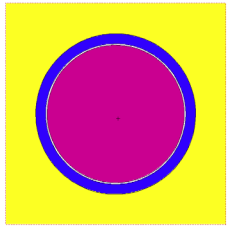








- **Doppler Reactivity Benchmark**
  - Compare k-effective for **HZP** (hot, zero power) and **HFP** (hot, full power) conditions for a unit fuel cell typical of a PWR
  - **Basic model:**



    - **PWR fuel pin cell** with reflecting BCs, various enrichments
    - **HZP** cases**:** **fuel at 600K**, clad/moderator at 600K
    - **HFP** cases: **fuel at 900K**, clad/moderator at 600K
    - Uniform temperature within each fuel, clad, moderator region.
    - Number densities and dimensions adjusted for the HFP thermal expansion
    - 5M active neutron histories per each of 28 MCNP runs

  - **NJOY+MCNP**: NJOY-broadened data at exact temperatures
  - **OTF+MCNP**: OTF data for ^{16}O, ^{234}U, ^{235}U, ^{238}U in fuel

  - **OTF details**
    - For union E-grid: T_{base}=293.6K, T range 300-1000K, ΔT=100K
    - For OTF fitting: 8^{th} order, T range 300-1000K, ΔT=10K
    - For general production use, would use larger T range & smaller ΔT's

Doppler Defect Benchmark Results

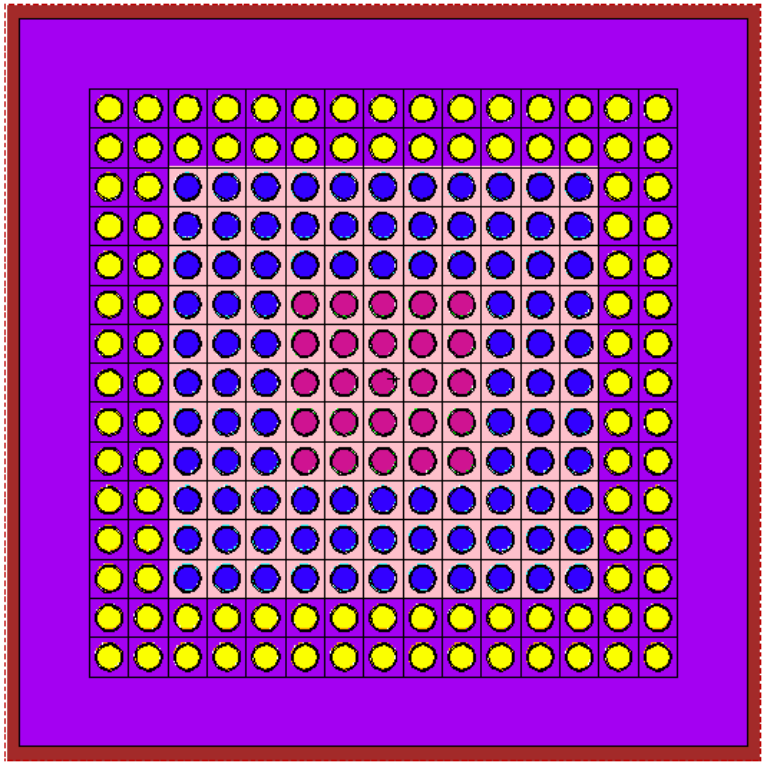
Monte Carlo Codes
XCP-3, LANL

		HZP	HFP	Doppler Coef. pcm/K
UO2 fuel pin	NJOY+MCNP	0.66556 (18)	0.65979 (19)	-4.38 (.20)
0.711% enrichment	OTF+MCNP	0.66567 (18)	0.66022 (19)	-4.13 (.20)
UO2 fuel pin	NJOY+MCNP	0.96094 (26)	0.95293 (25)	-2.92 (.13)
1.60% enrichment	OTF+MCNP	0.96026 (24)	0.95283 (23)	-2.71 (.13)
UO2 fuel pin	NJOY+MCNP	1.09912 (27)	1.08997 (26)	-2.55 (.10)
2.40% enrichment	OTF+MCNP	1.09923 (27)	1.08975 (28)	-2.64 (.10)
UO2 fuel pin	NJOY+MCNP	1.17718 (27)	1.16744 (27)	-2.36 (.09)
3.10% enrichment	OTF+MCNP	1.17703 (30)	1.16767 (30)	-2.27 (.10)
UO2 fuel pin	NJOY+MCNP	1.23967 (27)	1.22920 (30)	-2.29 (.09)
3.90% enrichment	OTF+MCNP	1.23953 (29)	1.22979 (29)	-2.13 (.09)
UO2 fuel pin	NJOY+MCNP	1.27501 (30)	1.26526 (27)	-2.01 (.09)
4.50% enrichment	OTF+MCNP	1.27534 (29)	1.26552 (29)	-2.03 (.09)
UO2 fuel pin	NJOY+MCNP	1.29901 (31)	1.28920 (29)	-1.95 (.08)
5.00% enrichment	OTF+MCNP	1.29907 (28)	1.28938 (29)	-1.93 (.08)

$$\rho = (1 / K_{HZP} - 1 / K_{HFP}) \times 10^5 / 300 \quad \text{pcm/K}$$

Results – Fuel Assembly

- **Simplified PWR 15 x 15 fuel assembly, with varying temperatures**
  - **From OECD/NEA fuel storage vault benchmark**
    - Fuel = 900 K, 600 K, 300 K
    - Clad = 900 K, 600 K, 300 K
    - Water = 600 K, 300 K
    - Outer iron rack = 293.6K
  - **Standard NJOY+MCNP5:**
    - ACE data at explicit temperatures
  - **OTF+MCNP5**
    - use 293.6K ACE data for all nuclides
    - OTF data for all nuclides (except iron)
  - **MCNP5**
    - 20,000 neutrons/cycle,
    - 10 inactive cycles, 1000 active cycle
    - Reflecting BCs



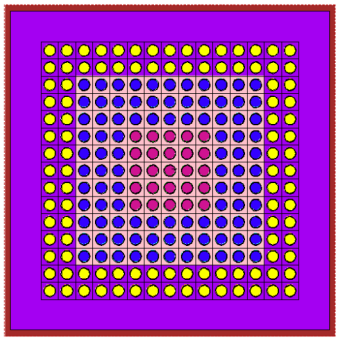
Fuel=900K, clad=900K, mod=600K
Fuel=600K, clad=600K, mod=600K
Fuel=300K, clad=300K, mod=300K

Results – Fuel Assembly

Monte Carlo Codes
XCP-3, LANL

k-effective:

STD	1.11599 (15)
OTF	1.11592 (15)



Fuel=900K, clad=900K, mod=600K
Fuel=600K, clad=600K, mod=600K
Fuel=300K, clad=300K, mod=300K

	900K	600K	300K
Total fission			
STD	.045140 (.08%)	.161186 (.04%)	.248782 (.03%)
OTF	.045081 (.08%)	.161329 (.04%)	.248731 (.03%)
Total capture in fuel			
STD	.027672 (.09%)	.096276 (.05%)	.116745 (.04%)
OTF	.027667 (.09%)	.096268 (.05%)	.116829 (.04%)
U235 capture in fuel			
STD	.008993 (.08%)	.031910 (.04%)	.045998 (.03%)
OTF	.008983 (.08%)	.031932 (.04%)	.045987 (.03%)
U238 capture in fuel			
STD	.018547 (.11%)	.063887 (.06%)	.070236 (.05%)
OTF	.018551 (.11%)	.063858 (.06%)	.070332 (.05%)
O16 capture in fuel			
STD	1.15E-04 (.23%)	4.18E-04 (.14%)	4.37E-04 (.13%)
OTF	1.15E-04 (.23%)	4.16E-04 (.14%)	4.37E-04 (.13%)

OTF Work in Progress

- **Better integration into MCNP (optimization)**
- **FIT_OTF fitting program**
  - Investigate scaling & Chebychev, for better numerical stability
  - Investigate regression, to vary fit order by energy & reaction **[done]**
- **U. Michigan work**
  - Create OTF libraries for all nuclides in ENDF/B-VII.0
  - Test various applications: fuel assemblies, 3D whole core, LWR, HTGR, ...
- **Methodology for Unresolved Resonances & S(α,β) data**
  - Probable 1st cut – tables with temperature interpolation
  - Possible thesis topic for PhD student
- **Implement corrected free-gas scatter model**
  - Demonstrated, needs robust implementation
- **Easy to extend to any temperature range**
  - Need to investigate broadening for high-threshold reactions

References

- **F.B. Brown, W.R. Martin, G. Yesilyurt, S. Wilderman**, “Progress with On-The-Fly Neutron Doppler Broadening in MCNP”, *Trans. Am. Nuc. Soc.* 106 [also LA-UR-12-00423] (2012).

- **G. Yesilyurt**, "Advanced Monte Carlo Methods for Analysis of Very High Temperature Reactors: On-the-Fly Doppler Broadening and Deterministic / Monte Carlo Methods," *PhD thesis*, Department of Nuclear Engineering and Radiological Sciences, University of Michigan, Ann Arbor, MI (2009).

- **G. Yesilyurt, W.R. Martin, F.B. Brown**, “On-The-Fly Doppler Broadening for Monte Carlo Codes”, accepted for publication, *Nuclear Science & Engineering.*

- **F.B. Brown, B.C. Kiedrowski, W.R. Martin, G. Yesilyurt**, “Advances in Monte Carlo Criticality Methods”, Invited Workshop for M&C-2009, Saratoga Springs, NY, May 3-7 [also, LA-UR-09-02442] (2009)

- **R.D. Mosteller**, "Computational Benchmarks for the Doppler Reactivity Defect", ANS Joint Benchmark Committee [LA-UR-06-2968] (2006).

- **R.E. Macfarlane and D.W. Muir**, ““NJOY99.0 - Code System for Producing Pointwise and Multigroup Neutron and Photon Cross Sections from ENDF/B Data,”” *PSR- 480/NJOY99.00*, Los Alamos National Laboratory, Los Alamos (2000).

- **T. Viitanen, J. Leppanen**, “Explicit Temperature Treatment in Monte Carlo Neutron Tracking Routines – First Results”, PHYSOR-2012, Knoxville, TN (2012).

Population Size and Fission Source Coverage

Effect of Population Size

- Classical analysis of issues has the assumption

  The population is sufficiently large such that all relevant regions of the problem are adequately sampled each iteration

- Interplay between batch size and number of batches
- Different issue than renormalization bias
- Typically problematic in loosely-coupled systems

Population Size Interplay

- Tally scoring density function changes each cycle
  - Result of stochastic noise in the fission source

    Amount of variation in source depends on batch size
  - Tally scoring density function mean within an individual cycle is biased by noise

    Infinite samples from a fission source calculated by a finite sample will yield wrong result!
  - Need to sample numerous fission sources to get correct tally mean

- How large is enough?
  - Depends on the desired result

    Highly-localized quantities magnify issues

Renormalization Bias Versus Coverage

- **Bias results from renormalization of the fission source based on a random variable**
  - **Random variation is such that calculated *k* with be lower than the true *k***
  - **The bias is inversely proportional to the batch size**
  - **Issue typically disappears for batch sizes > 10K**

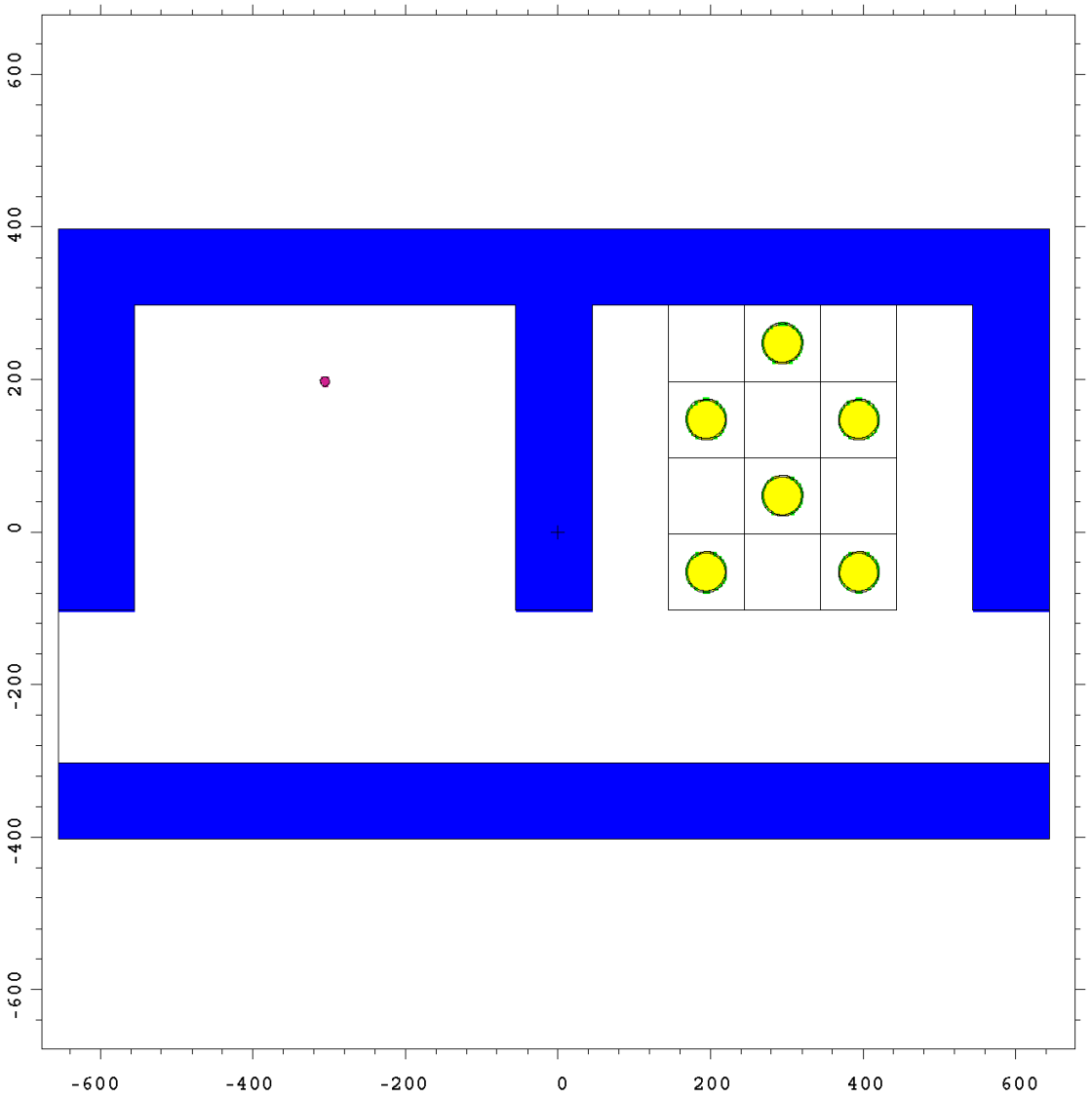
- **Undersampling and coverage deal with failure to sufficiently sample the phase space in a way that biases the results**

Example Problem

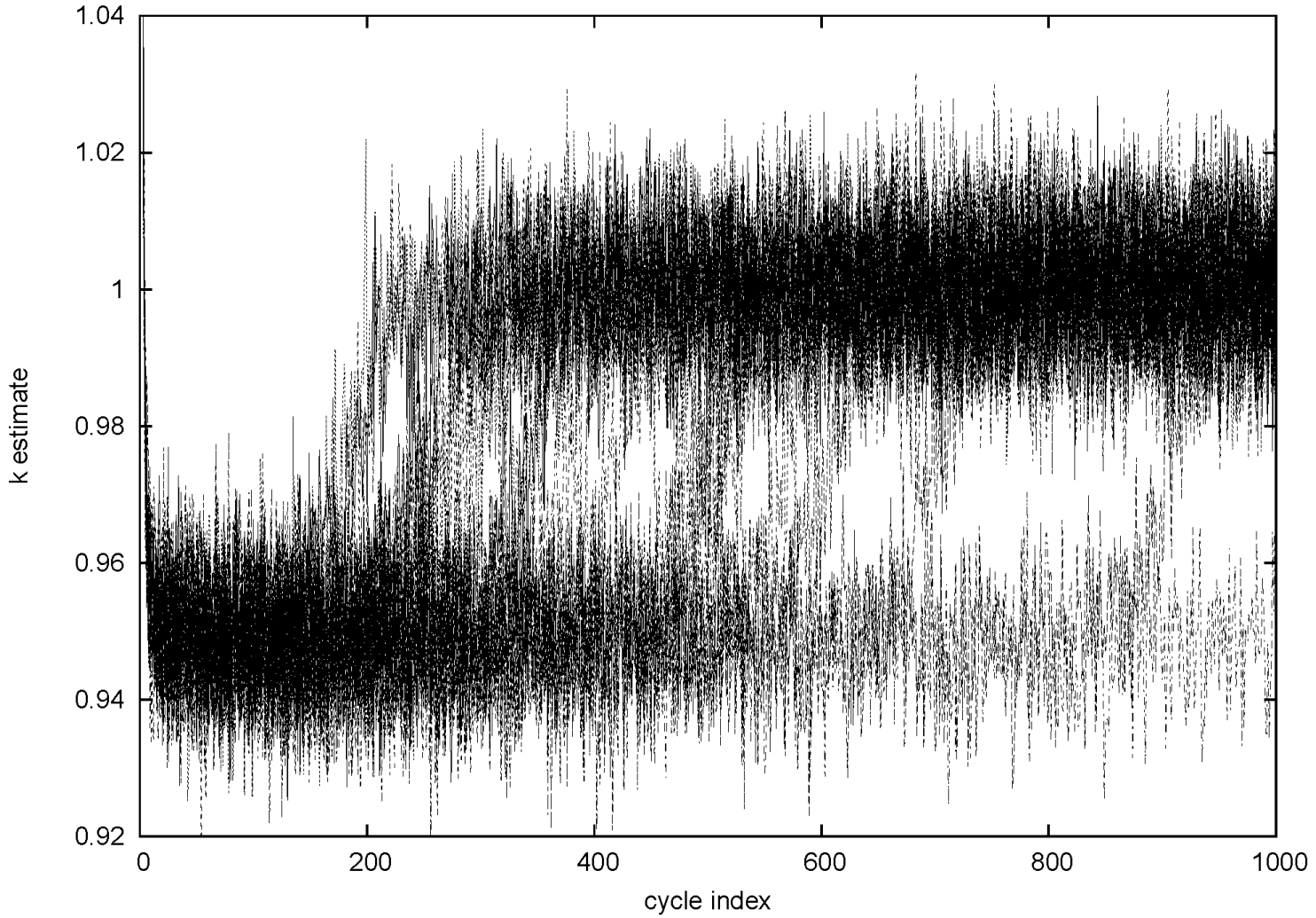
- Two rooms one containing Jezebel (critical) and a subcritical array of cans of plutonium nitrate solution
- Rooms separated by 1 meter of concrete or a hallway
- Bad source guess: all neutrons in the plutonium nitrate cans (500 inactive cycles, 1000 total)
- Run 25 independent random trials with various batch sizes and observe convergence in *k*

Problem Specifications

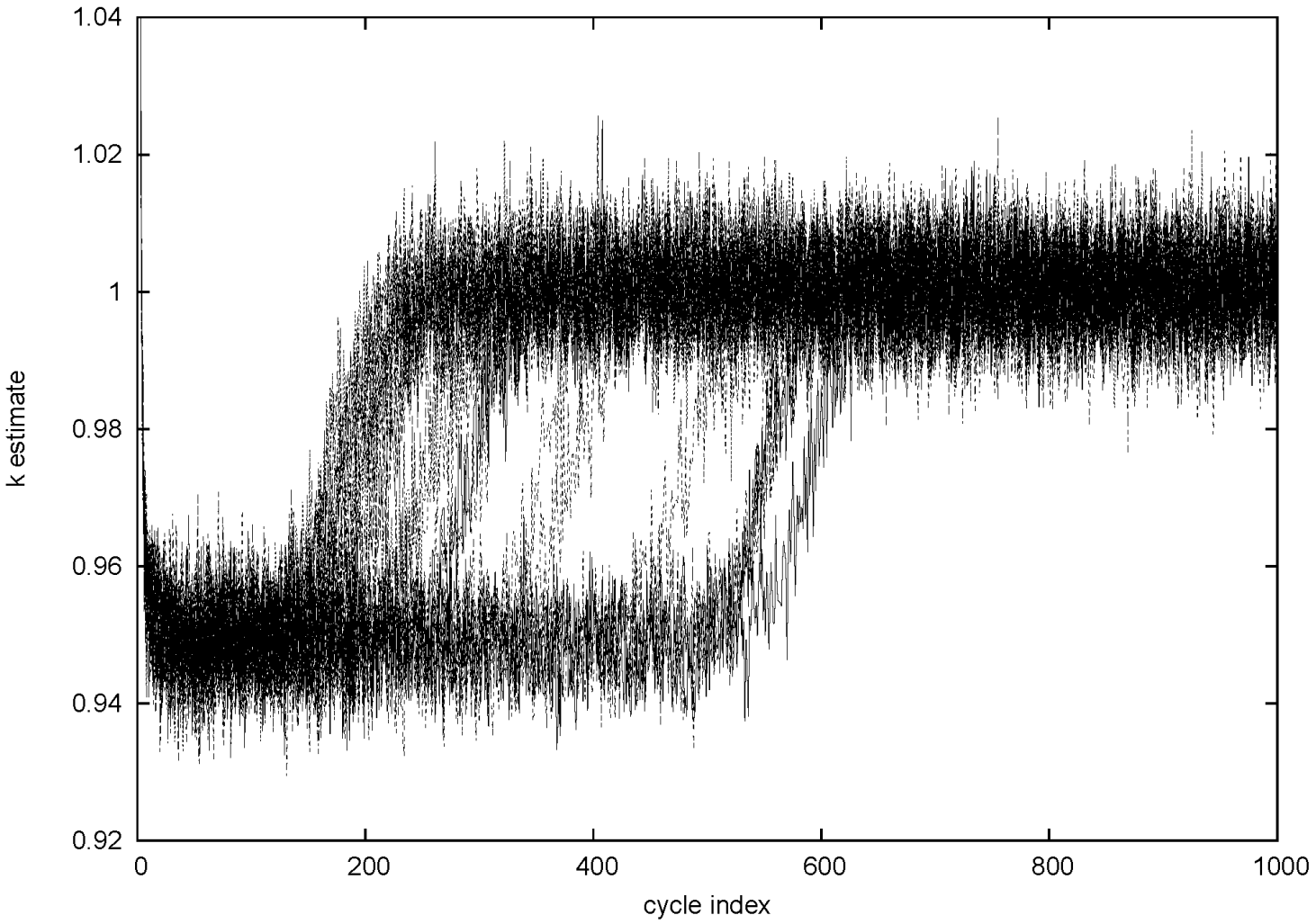
Monte Carlo Codes
XCP-3, LANL



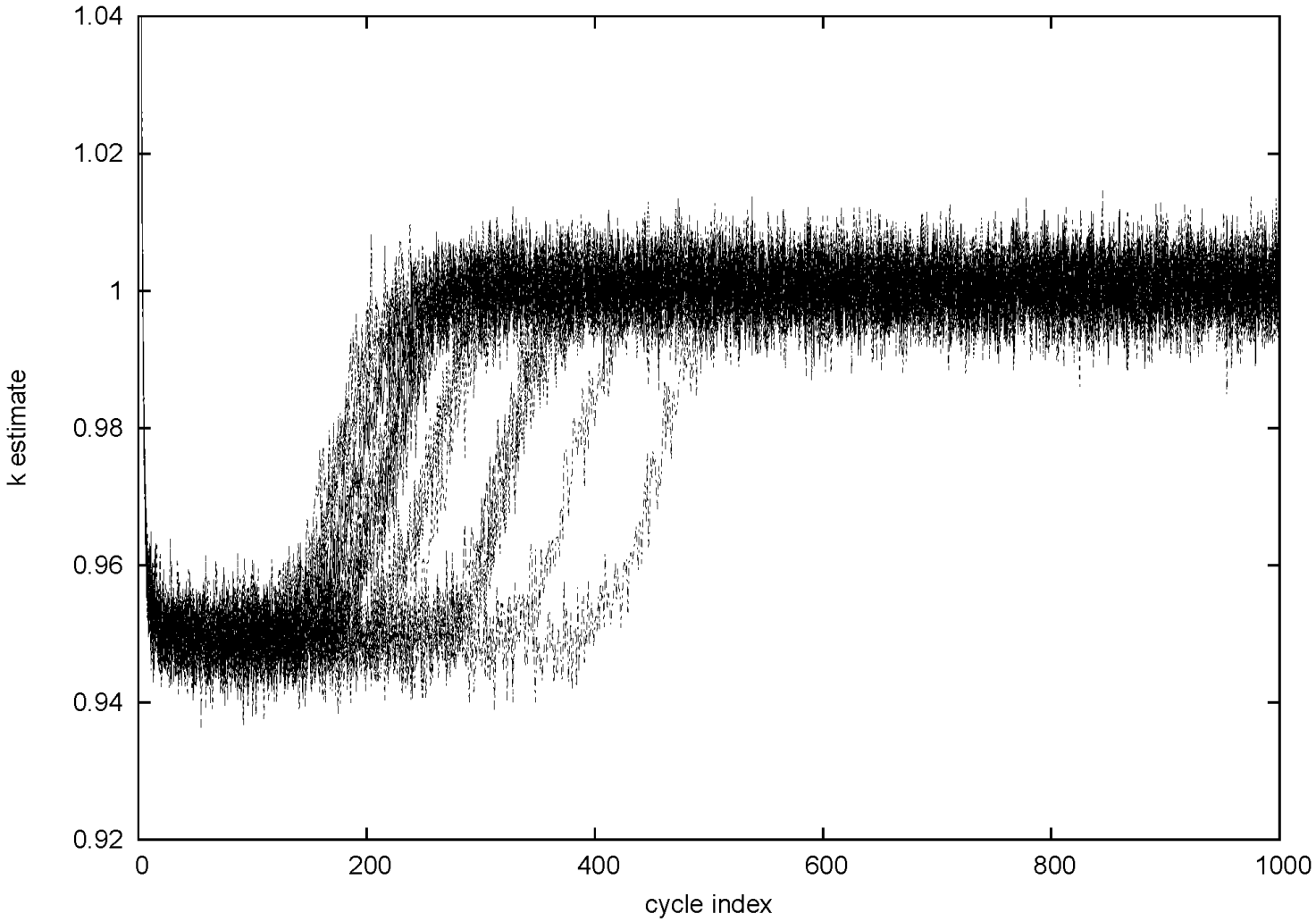
Batch Size: 10K



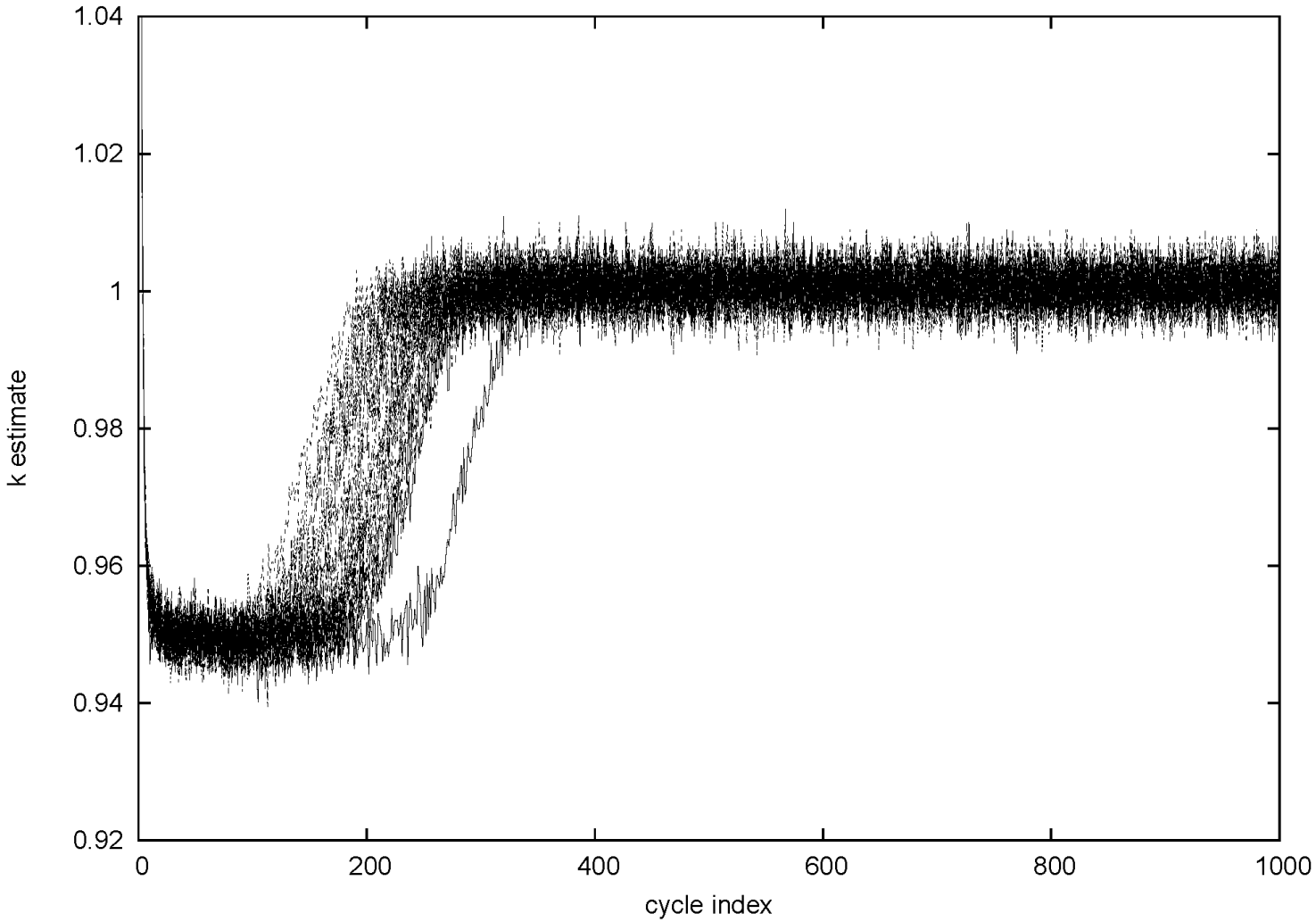
Batch Size: 20K



Batch Size: 50K



Batch Size: 100K



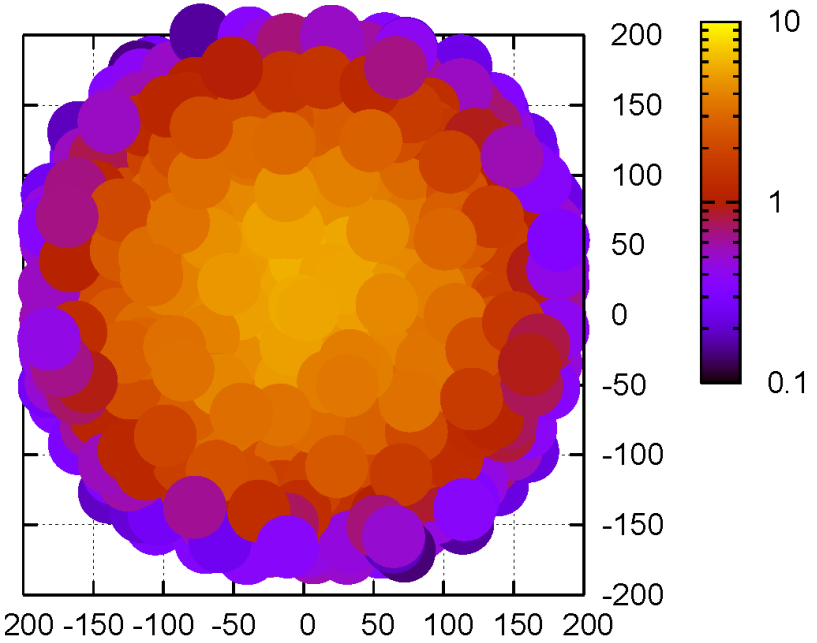
Discussion of Results

- Bad source guess may yield bad results, even if many cycles are skipped
  - Good guess produces correct results consistently
- Source converges on average at a constant rate, but has randomness
  - Bad guesses in tricky problems show this
- Problem is difficult because the communication to Jezebel is weak

Kernel Density Estimators for Fission Source

Monte Carlo Codes
XCP-3, LANL

- Automated placement routine based on distance between fission points
- Provides a more robust estimate of sampling fissionable material
- KDEs can be used to compute Shannon entropy as well



Fission Source Sampling Test Results

Monte Carlo Codes
XCP-3, LANL

Problem	Sample 99.9%	99% w/ Rel. Unc. < 10%
Godiva	< 20k	~ 1 M
3-D PWR Full Core	440 k	8.8 M
K-eff of the World	< 20k	6.6 M
OECD Fuel Pool	>> 100 M	>> 100 M

Alternate Eigenvalues for Criticality Searches

Motivation

- **Typically, reactors operate at criticality**

- **Temperature and depletion effects generally perturb the system from criticality**
  - Must use control mechanism to readjust
  - **Otherwise <u>spectrum is biased</u>**

- **Multiple iterations typically needed**
  - May be costly with Monte Carlo
  - Concern for statistical noise from random process

- **Steady-state solution of neutron transport equation desired**
  - Apply a multiplicative factor (eigenvalue) to one (or more) of the terms to achieve balance

- **k-eigenvalue equation (fission)**

$$(L + T - S) \cdot \Psi = \frac{1}{k} \cdot F \cdot \Psi$$

- **c-eigenvalue equation (collisions)**

$$(L + T) \cdot \Psi = \frac{1}{c} \cdot (S + F) \cdot \Psi$$

- **δ-eigenvalue equation (leakage)**

$$L \cdot \Psi = \frac{1}{\delta} \cdot (S + F - T) \cdot \Psi$$

The *c*-Eigenvalue

- **A generation is redefined as a collision producing any neutrons (including scattering)**
  - Power iteration method in MCNP otherwise unchanged

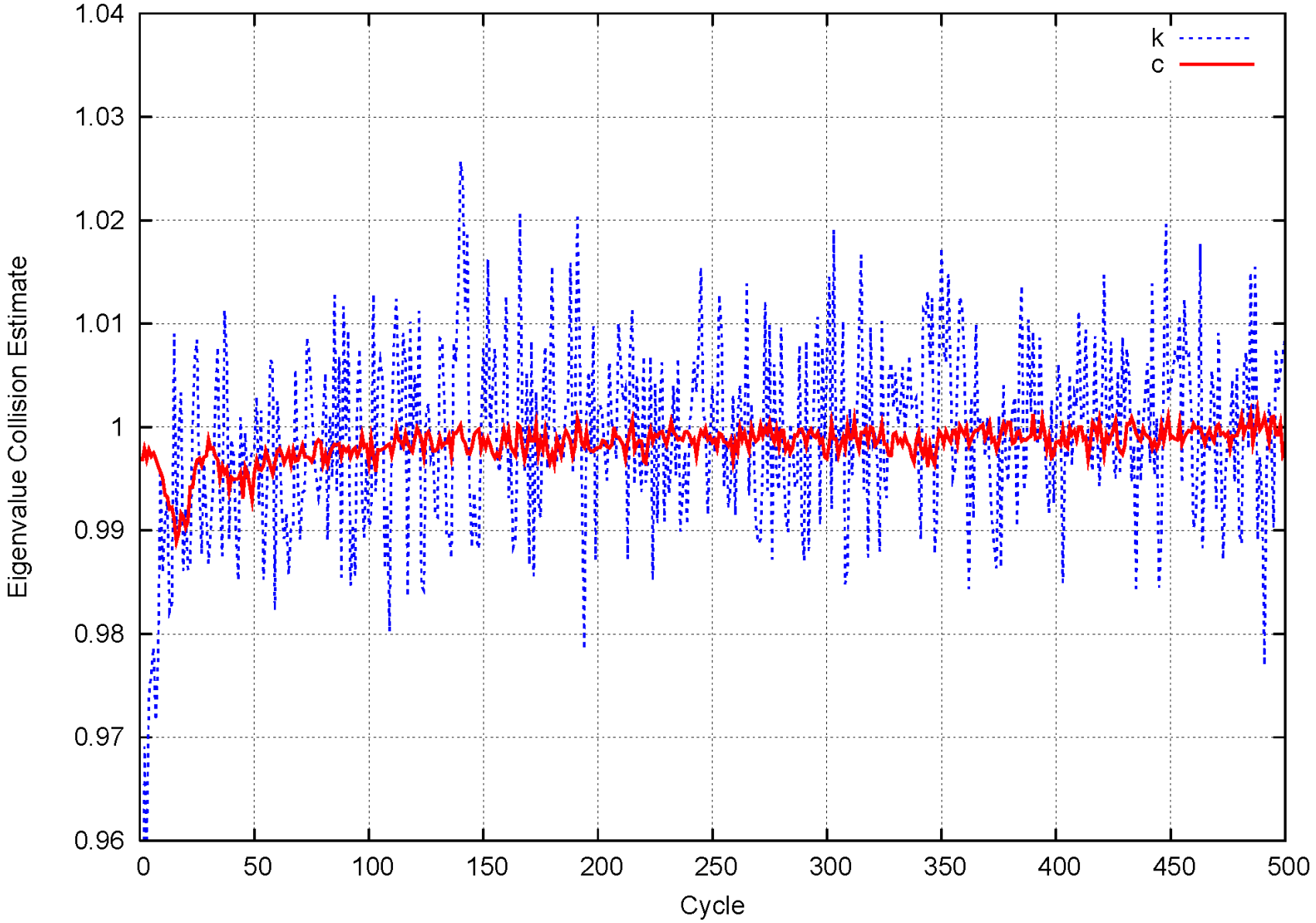
- **Effects on a calculation for reactors**
  - **Bad:** More cycles required for source convergence (spectrum now more important) and greater inter-cycle correlation
  - **Good:** Cycles very short and, if numbers of collisions is large, such as in an LWR, less statistical noise

k Versus *c*

	k	c	Gain
Reflected Sphere	**0.9955**	**0.9954**	**31**
Pu Soln. Can Array	**0.9866**	**0.9989**	**60**
Full-Core PWR	**0.9992**	**0.9986**	**200**

Hoogenboom-Martin Problem

Monte Carlo Codes
XCP-3, LANL



Time-Absorption Eigenvalues

- **Assume separation of time from spatial and momentum variables in transport equation**

$$\Psi = \sum_J \Psi_{\alpha_J} \cdot e^{\alpha_J \cdot t}$$

$$\left(L + T + \frac{\alpha_J}{v} \right) \cdot \Psi_{\alpha_J} = \left(S + \tilde{F}(\alpha_J) \right) \cdot \Psi_{\alpha_J}$$

$$\tilde{F} = \iint dE' \, d\Omega' \left(\chi_p \nu_p + \sum_l \frac{\lambda_l}{\lambda_l + \alpha_J} \cdot \chi_l \nu_l \right) \cdot \Sigma_F$$

α Eigenvalue Solution Schemes

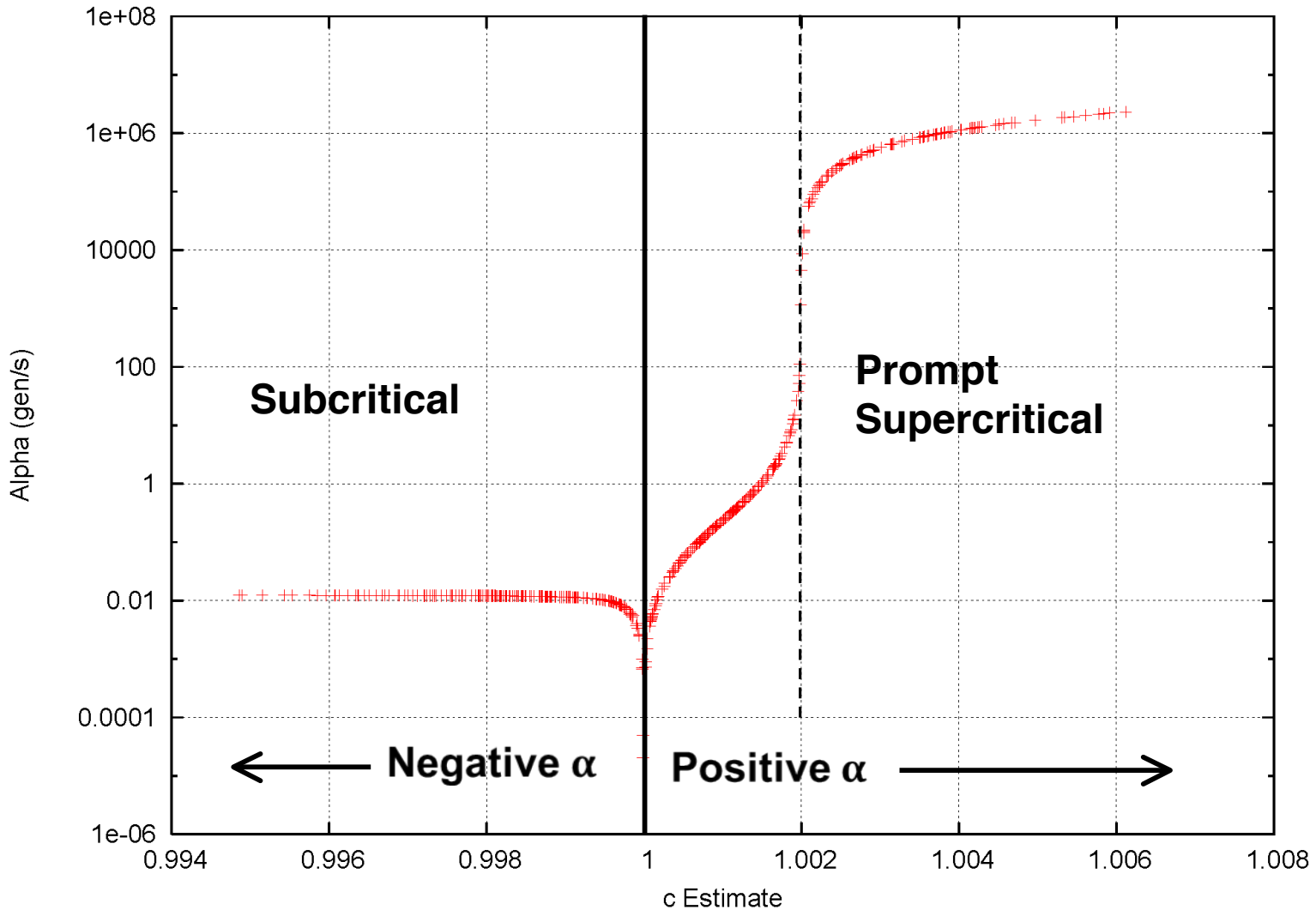
- In practice, it is difficult to solve for α directly
- Typical method: Solve for a different eigenvalue (k), and find α that makes system critical

$$\left(L+T-S+\frac{\alpha}{v}\right)\cdot\Psi = \frac{1}{k}\cdot\tilde{F}(\alpha)\cdot\Psi$$

$$\left(L+T+\frac{\alpha}{v}\right)\cdot\Psi = \frac{1}{c}\cdot\left(S+\tilde{F}(\alpha)\right)\cdot\Psi$$

- Preliminary results:
  - Using c to estimate α appears to have a FOM
  - 2-5 times higher than with k for certain systems

c vs α for Godiva Problem



Continuous-Energy Nuclear Data Sensitivities

C.E. Sensitivity Coefficients

- **MCNP6 can compute continuous-energy sensitivity coefficients to k**

$$S_{k,\sigma_x} = \frac{\sigma_x}{k} \cdot \frac{\partial k}{\partial \sigma_x}$$

- **Progress made on continuous-energy adjoint-based perturbation theory methods for continuous-energy sensitivity coefficients**
  - 2010: Fission, capture agree with TSUNAMI-3D, scattering disagree
  - 2012: Improved agreement for scattering for individual isotopes

C.E. Sensitivity Coefficients

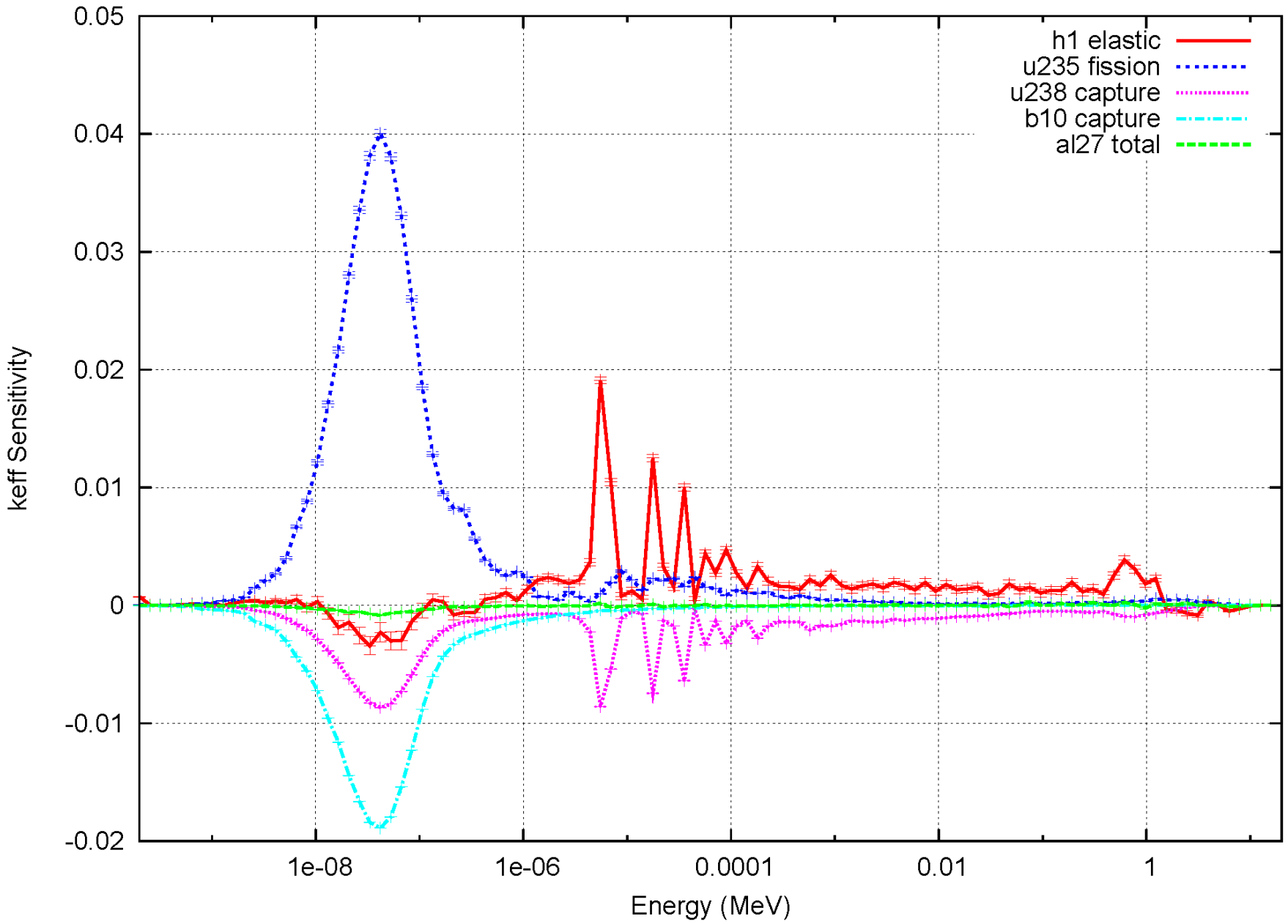
- **Results for B.T. Rearden Paraffin sphere problem:**

	TSUNAMI-3D	MCNP6	Calc/Ref	2010 Calc/Ref
Total	$+3.314 \times 10^{-1}$	$+3.336 \times 10^{-1}$	1.007	0.957
Capture	-5.081×10^{-1}	-4.995×10^{-1}	0.983	0.988
Fission	$+3.964 \times 10^{-1}$	$+3.960 \times 10^{-1}$	0.999	1.004
Elastic	$+4.115 \times 10^{-1}$	$+4.053 \times 10^{-1}$	0.985	1.025
Inelastic	$+2.950 \times 10^{-2}$	$+2.882 \times 10^{-2}$	0.977	0.745
n,2n	$+1.032 \times 10^{-3}$	$+1.089 \times 10^{-3}$	1.035	--

Note: TSUNAMI-3D is 238-group ENDF/B-VI, whereas MCNP6 uses continuous-energy ENDF/B-VII.0

Sensitivity Profile (B&W 11 Lattice Benchmark)

Monte Carlo Codes
XCP-3, LANL



Boundary Sensitivities

Boundary Sensitivities

- **Dimensions and positions of various components in benchmarks, experiments, systems, etc. are uncertain**

- **Can apply sensitivity theory to perform analysis**
  - Early theoretical work by Lewins (early 1960s)
  - Later work by Rahnema on boundary perturbations (1980s)
  - Sensitivity work with Sn by Favorite (Late 2000-2010s)
  - Continuous-Energy Monte Carlo (Today)

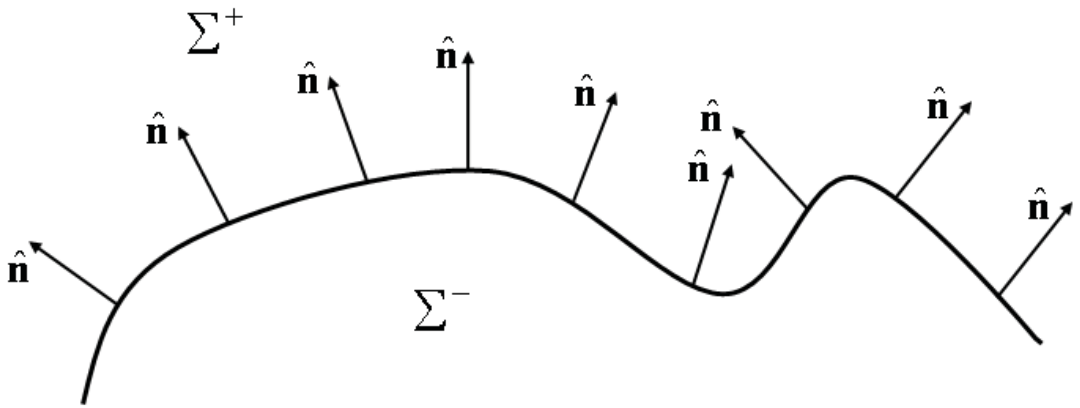
Boundary Sensitivity Theory

- **Classic expression from sensitivity theory:**

$$dk = -\frac{1}{M}\left\langle \psi^{\dagger}, \left(d\Sigma_t - dS - \lambda dF\right)\psi \right\rangle, \qquad M = \left\langle \psi^{\dagger}, \lambda^2 F\psi \right\rangle .$$

- **Treat perturbation as a material substitution, defining**

$$\Sigma(\mathbf{r}) = \Sigma^{-} + \Theta(r-b)(\Sigma^{+} - \Sigma^{-}),$$



System Dimension Sensitivity Theory

- Take derivatives and rearrange to obtain convenient grouping of terms:

$$\frac{dk}{db} = \frac{1}{M}\Big[\left\langle \psi^{\dagger}, \left(\Sigma_t^{+} - \Sigma_t^{-}\right)\psi\right\rangle_B + \left\langle \psi^{\dagger}, S^{-}\psi\right\rangle_B - \left\langle \psi^{\dagger}, S^{+}\psi\right\rangle_B + \left\langle \psi^{\dagger}, \lambda F^{-}\psi\right\rangle_B - \left\langle \psi^{\dagger}, \lambda F^{+}\psi\right\rangle_B\Big]$$

- Here b is the variable for the interface location, B subscript denotes the integral is over the contour being perturbed

Description of terms

Impact of change on collision rate

$$\frac{dk}{db} = \frac{1}{M}\left[\left\langle \psi^{\dagger}, \left(\Sigma_t^{+} - \Sigma_t^{-}\right)\psi \right\rangle_B + \left\langle \psi^{\dagger}, S^{-}\psi \right\rangle_B - \left\langle \psi^{\dagger}, S^{+}\psi \right\rangle_B + \left\langle \psi^{\dagger}, \lambda F^{-}\psi \right\rangle_B - \left\langle \psi^{\dagger}, \lambda F^{+}\psi \right\rangle_B\right]$$

Description of terms

Impact of gain in scattered neutrons from increasing material on "-" side

$$\frac{dk}{db} = \frac{1}{M}\left[\left\langle \psi^{\dagger}, \left(\Sigma_t^{+} - \Sigma_t^{-}\right)\psi\right\rangle_B + \left\langle \psi^{\dagger}, S^{-}\psi\right\rangle_B - \left\langle \psi^{\dagger}, S^{+}\psi\right\rangle_B + \left\langle \psi^{\dagger}, \lambda F^{-}\psi\right\rangle_B - \left\langle \psi^{\dagger}, \lambda F^{+}\psi\right\rangle_B\right]$$

Impact of loss in scattered neutrons from decreasing material on "+" side

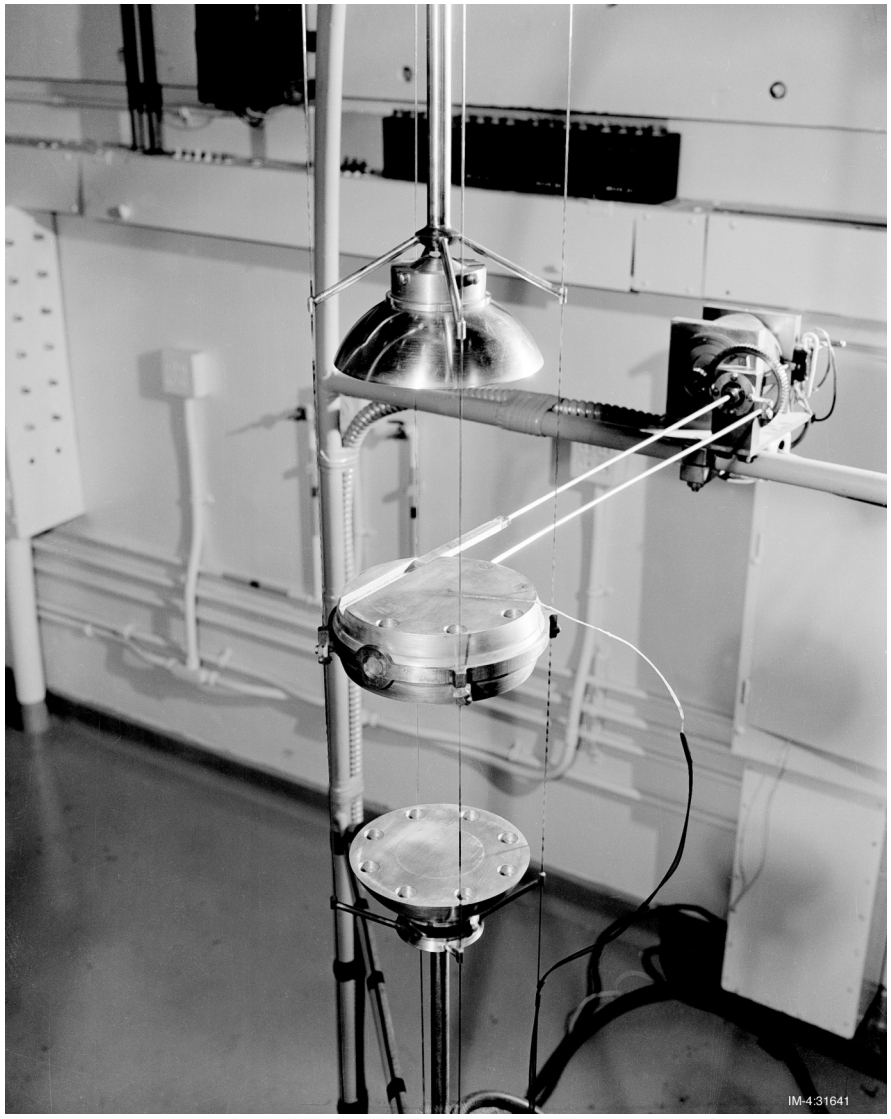
Description of terms

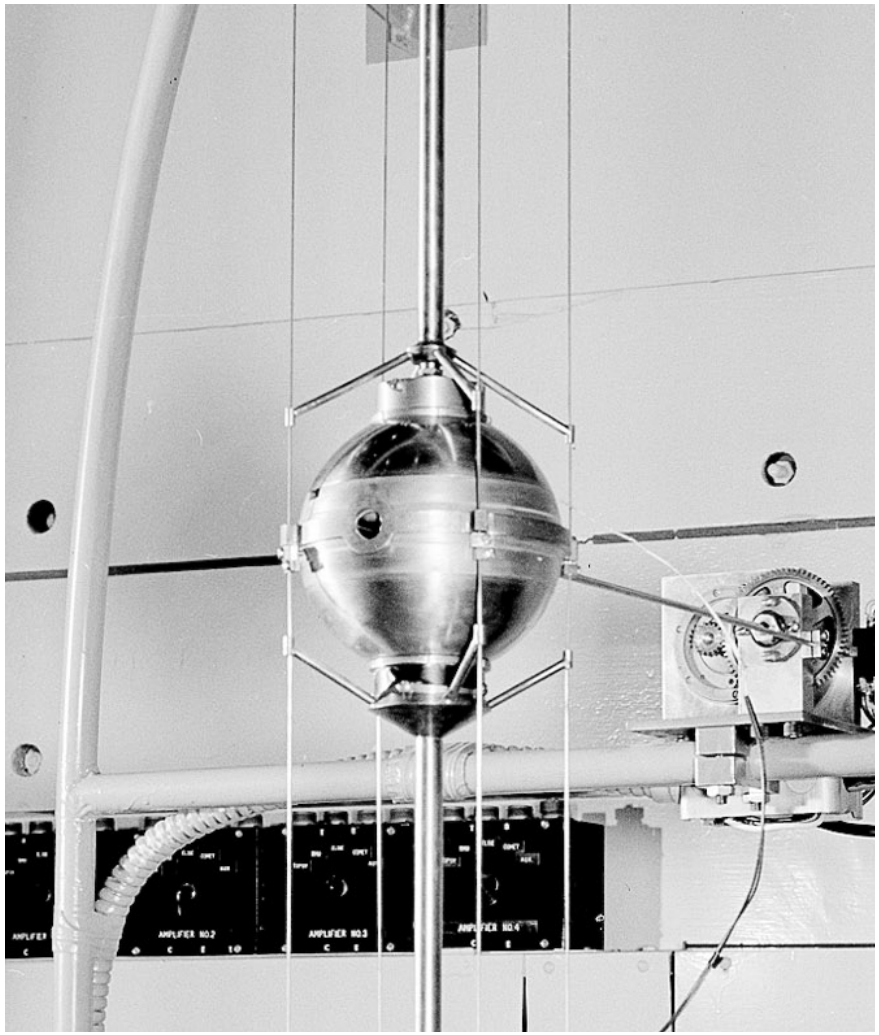
Impact of gain in fission neutrons from increasing material on "-" side

$$\frac{dk}{db} = \frac{1}{M}\Big[\left\langle \psi^\dagger, \left(\Sigma_t^+ - \Sigma_t^-\right)\psi\right\rangle_B + \left\langle \psi^\dagger, S^-\psi\right\rangle_B - \left\langle \psi^\dagger, S^+\psi\right\rangle_B + \left\langle \psi^\dagger, \lambda F^-\psi\right\rangle_B - \left\langle \psi^\dagger, \lambda F^+\psi\right\rangle_B\Big]$$

Impact of loss in fission neutrons from decreasing material on "+" side

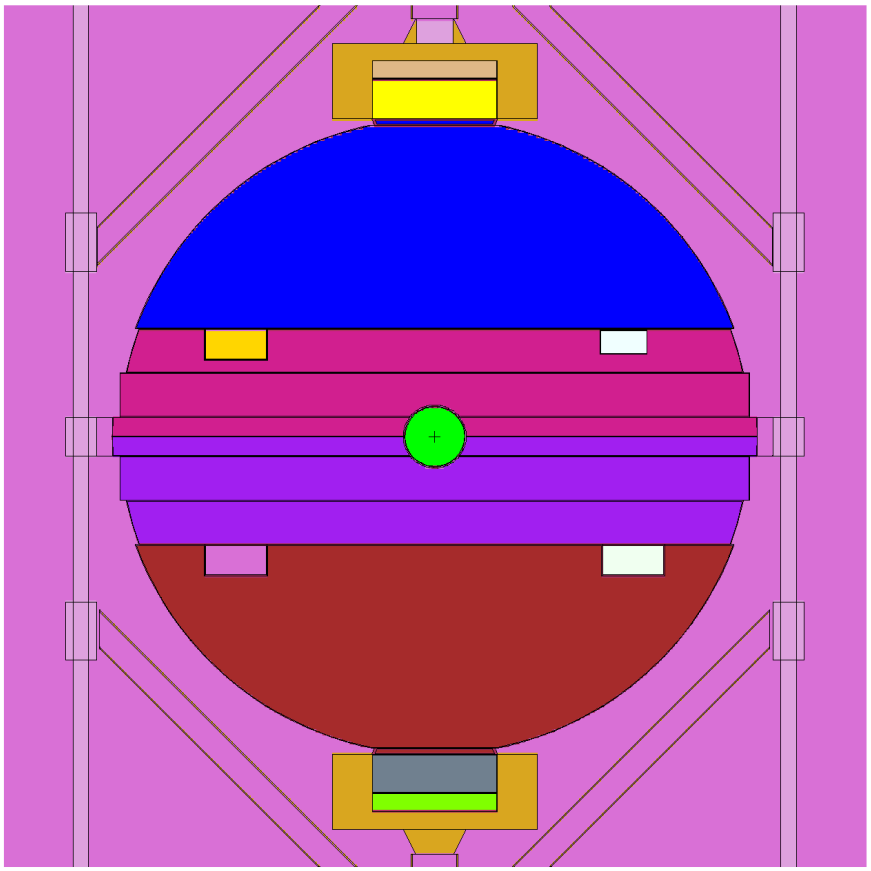
Analysis of Detailed Jezebel Model

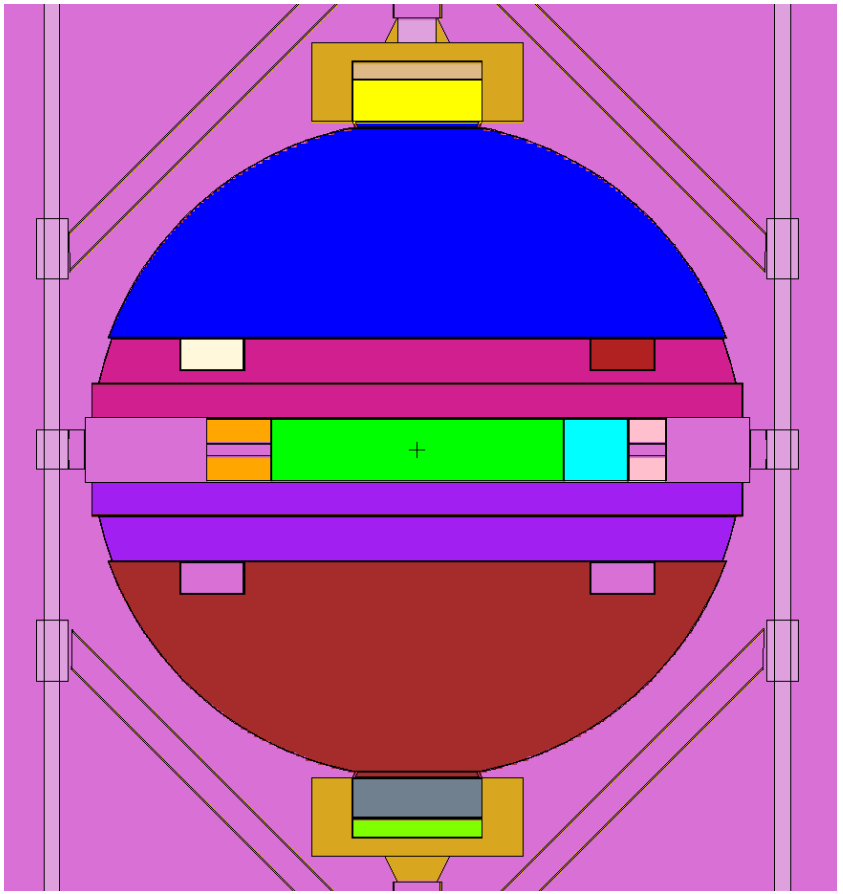




Analysis of Detailed Jezebel Model

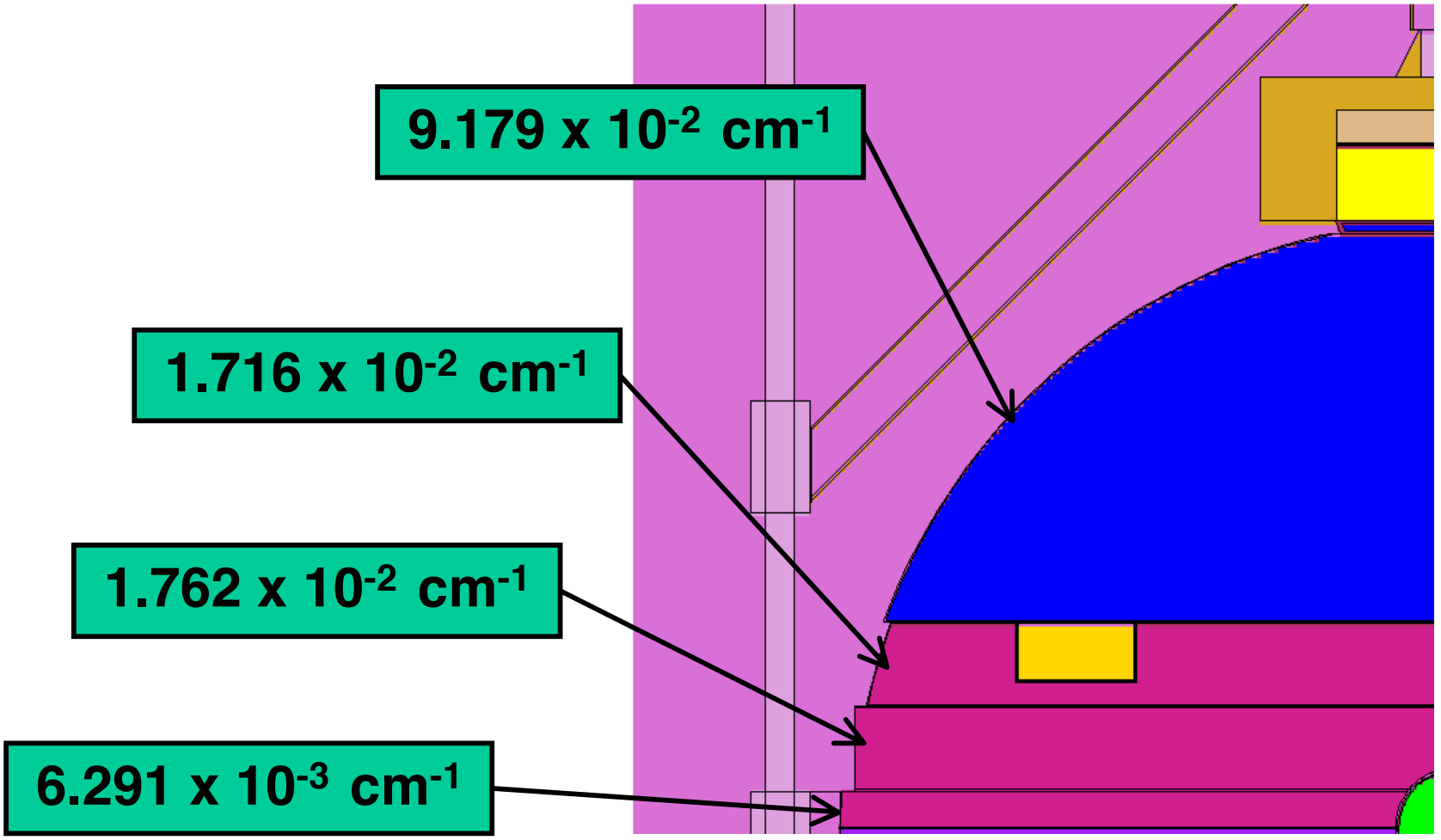
Monte Carlo Codes
XCP-3, LANL





Analysis of Detailed Jezebel Model

Monte Carlo Codes
XCP-3, LANL



Total outer radius sensitivity: 1.329×10^{-1} cm^{-1}

Simple sphere radius sensitivity: 1.341×10^{-1} cm^{-1}

Release of the ENDF/B-VII.1 Evaluated Nuclear Data File

David Brown

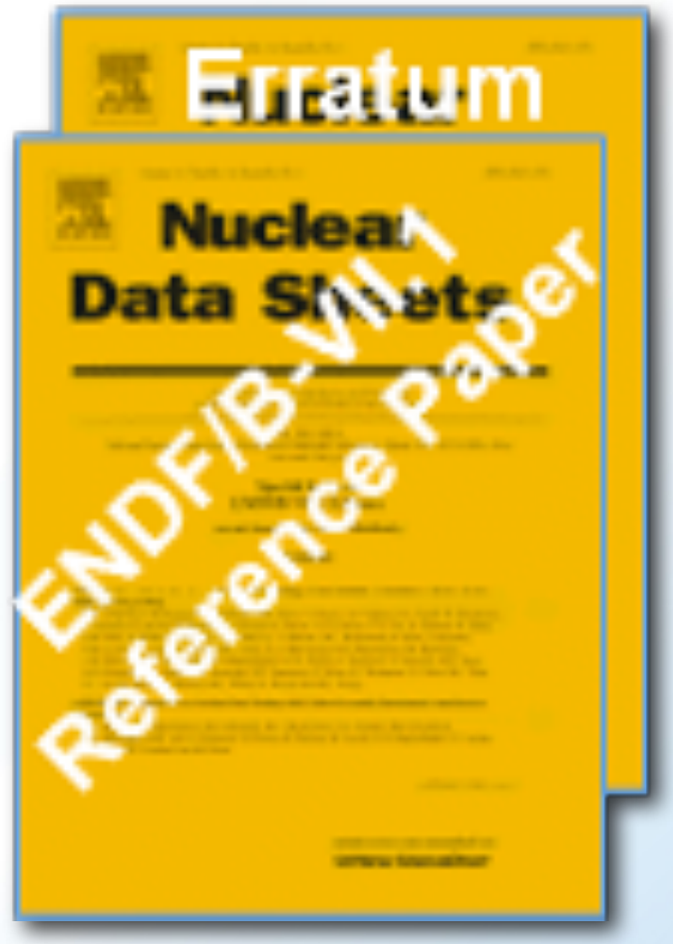
BROOKHAVEN NATIONAL LABORATORY

a passion for discovery

U.S. DEPARTMENT OF ENERGY | Office of Science

ENDF/B-VII.1 was released on Dec. 22, 2011

- ENDF/B is arguably most important nuclear data library for all nuclear applications
- Many more full evaluations in neutron sublibrary than in any other release
  - ENDF/B-VII.0 contains 393 evaluations
  - ENDF/B-VII.1 contains 423 evaluations
- Extensive collection of covariance data (190 evaluations)
- **Library summarized in Dec. 2011 issue of Nuclear Data Sheets**
- **See also http://www.nndc.bnl.gov/exfor/endfb7.1.jsp**



Only four sublibraries updated; Summarized in the "Big Paper"

ENDF B-VII.1

Available online at www.sciencedirect.com
SciVerse ScienceDirect
Nuclear Data Sheets
Nuclear Data Sheets 112 (2011) 2887–2996
www.elsevier.com/locate/nds

ENDF/B-VII.1 Nuclear Data for Science and Technology: Cross Sections, Covariances, Fission Product Yields and Decay Data

M.B. Chadwick,[1,*] M. Herman,[2] P. Obložinský,[2] M.E. Dunn,[3] Y. Danon,[4] A.C. Kahler,[1] D.L. Smith,[5] B. Pritychenko,[2] G. Arbanas,[3] R. Arcilla,[2] R. Brewer,[1] D.A. Brown,[2,6] R. Capote,[7] A.D. Carlson,[8] Y.S. Cho,[13] H. Derrien,[3] K. Guber,[3] G.M. Hale,[1] S. Hoblit,[2] S. Holloway,[1] T.D. Johnson,[2] T. Kawano,[1] B.C. Kiedrowski,[1] H. Kim,[13] S. Kunieda,[1,15] N.M. Larson,[3] L. Leal,[3] J.P. Lestone,[1] R.C. Little,[1] E.A. McCutchan,[2] R.E. MacFarlane,[1] M. MacInnes,[1] C.M. Mattoon,[6] R.D. McKnight,[5] S.F. Mughabghab,[2] G.P.A. Nobre,[2] G. Palmiotti,[14] A. Palumbo,[2] M.T. Pigni,[3] V.G. Pronyaev,[9] R.O. Sayer,[3] A.A. Sonzogni,[2] N.C. Summers,[6] P. Talou,[1] I.J. Thompson,[6] A. Trkov,[10] R.L. Vogt,[6] S.C. van der Marck,[11] A. Wallner, [12] M.C. White,[1] D. Wiarda,[3] P.G. Young[1]
[1] *Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[2] *Brookhaven National Laboratory, Upton, NY 11973-5000, USA*
[3] *Oak Ridge National Laboratory, Oak Ridge, TN 37831-6171, USA*
[4] *Rensselaer Polytechnic Institute, Troy, NY 12180, USA*
[5] *Argonne National Laboratory, Argonne, IL 60439-4842 USA*
[6] *Lawrence Livermore National Laboratory, Livermore, CA 94551-0808, USA*
[7] *International Atomic Energy Agency, Vienna-A-1400, PO Box 100, Austria*
[8] *National Institute of Standards and Technology, Gaithersburg, MD 20899-8463, USA*
[9] *Institute of Physics and Power Engineering, Obninsk, Russian Federation*
[10] *Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*
[11] *Nuclear Research and Consultancy Group, P.O. Box 25, NL-1755, ZG Petten, The Netherlands*
[12] *Faculty of Physics, University of Vienna, Waehringer Strasse 17, A-1090 Vienna, Austria*
[13] *Korea Atomic Energy Research Institute, Daejeon, Korea*
[14] *Idaho National Laboratory, Idaho Falls, ID 83415, USA and*
[15] *Japan Atomic Energy Agency, Tokai-mura Naka-gun, Ibaraki 319-1195, Japan*
(Received 12 July 2011; revised received 22 September 2011; accepted 17 October 2011)

The ENDF/B-VII.1 library is our latest recommended evaluated nuclear data file for use in nuclear science and technology applications, and incorporates advances made in the five years since the release of ENDF/B-VII.0. These advances focus on neutron cross sections, covariances, fission product yields and decay data, and represent work by the US Cross Section Evaluation Working Group (CSEWG) in nuclear data evaluation that utilizes developments in nuclear theory, modeling, simulation, and experiment.
The principal advances in the new library are: (1) An increase in the breadth of neutron reaction cross section coverage, extending from 393 nuclides to 423 nuclides; (2) Covariance uncertainty data for 190 of the most important nuclides, as documented in companion papers in this edition; (3) R-matrix analyses of neutron reactions on light nuclei, including isotopes of He, Li, and Be; (4) Resonance parameter analyses at lower energies and statistical high energy reactions for isotopes of Cl, K, Ti, V, Mn, Cr, Ni, Zr and W; (5) Modifications to thermal neutron reactions on fission products (isotopes of Mo, Tc, Rh, Ag, Cs, Nd, Sm, Eu) and neutron absorber materials (Cd, Gd); (6) Improved minor actinide evaluations for isotopes of U, Np, Pu, and Am (we are not making changes to the major actinides ^{235,238}U and ^{239}Pu at this point, except for delayed neutron data and covariances, and instead we intend to update them after a further period of research in experiment and theory), and our adoption of JENDL-4.0 evaluations for isotopes of Cm, Bk, Cf, Es, Fm, and some other minor actinides; (7) Fission energy release evaluations; (8) Fission product yield advances for fission-spectrum neutrons and 14 MeV neutrons incident on ^{239}Pu; and (9) A new decay data sublibrary.
Integral validation testing of the ENDF/B-VII.1 library is provided for a variety of quantities: For nuclear criticality, the VII.1 library maintains the generally-good performance seen for VII.0 for a wide range of MCNP simulations of criticality benchmarks, with improved performance coming from new structural material evaluations, especially for Ti, Mn, Cr, Zr and W. For Be we see some improvements although the fast assembly data appear to be mutually inconsistent. Actinide cross section updates are also assessed through comparisons of fission and capture reaction rate measurements in critical assemblies and fast reactors, and improvements are evident. Maxwellian-averaged capture cross sections at 30 keV are also provided for astrophysics applications.
We describe the cross section evaluations that have been updated for ENDF/B-VII.1 and the measured data and calculations that motivated the changes, and therefore this paper augments the ENDF/B-VII.0 publication [1].

*) Electronic address: mbchadwick@lanl.gov

doi:10.1016/j.nds.2011.11.002

No.	NSUB	Sublibrary name	Short name	VII.1	VII.0	VI.8
1	0	Photonuclear	g	163	163	-
2	3	Photo-atomic	photo	100	100	100
3	4	Radioactive decay	decay	3817	3838	979
4	5	Spont. fis. yields	s/fpy	9	9	9
5	6	Atomic relaxation	ard	100	100	100
6	10	Neutron	n	423	393	328
7	11	Neutron fis.yields	n/fpy	31	31	31
8	12	Thermal scattering	tsl	21	20	15
9	19	Standards	std	8	8	8
10	113	Electro-atomic	e	100	100	100
11	10010	Proton	p	48	48	35
12	10020	Deuteron	d	5	5	2
13	10030	Triton	t	3	3	1
14	20030	^{3}He	he3	2	2	1

M. B. Chadwick, M. Herman, P. Oblozinsky, et al., "ENDF/B-VII.1 nuclear data for science and technology: Cross sections, covariances, fission product yields and decay data", Nuclear Data Sheets, 112(12):2887-2996 (2011).

Library underwent comprehensive testing; Summarized in "Benchmark Paper"

Available online at www.sciencedirect.com

SciVerse ScienceDirect

Nuclear Data Sheets

Nuclear Data Sheets 112 (2011) 2997–3036

www.elsevier.com/locate/nds

ENDF/B-VII.1 Neutron Cross Section Data Testing with Critical Assembly Benchmarks and Reactor Experiments

A. C. Kahler,[1,*] R. E. MacFarlane,[1] R. D. Mosteller,[1] B. C. Kiedrowski,[1] S. C. Frankle,[1] M. B. Chadwick,[1] R. D. McKnight,[2] R. M. Lell,[2] G. Palmiotti,[3] H. Hiruta,[3] M. Herman,[4] R. Arcilla,[4] S. F. Mughabghab,[4] J. C. Sublet,[5] A. Trkov,[6] T. H. Trumbull,[7] and M. Dunn[8]

[1]*Los Alamos National Laboratory, Los Alamos, NM 87545, USA*
[2]*Argonne National Laboratory, Argonne, IL 60349, USA*
[3]*Idaho National Laboratory, Idaho Falls, ID 83415, USA*
[4]*Brookhaven National Laboratory, Upton, NY 11973, USA*
[5]*Culham Center for Fusion Energy, Abingdon, OX14 3DB, UK*
[6]*Jozef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*
[7]*Knolls Atomic Power Laboratory, Schenectady, NY 12309, USA*
[8]*Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*

(Received 9 August 2011; revised received 21 September 2011; accepted 17 October 2011)

The ENDF/B-VII.1 library is the latest revision to the United States' Evaluated Nuclear Data File (ENDF). The ENDF library is currently in its seventh generation, with ENDF/B-VII.0 being released in 2006. This revision expands upon that library, including the addition of new evaluated files (was 393 neutron files previously, now 423 including replacement of elemental vanadium and zinc evaluations with isotopic evaluations) and extension or updating of many existing neutron data files. Complete details are provided in the companion paper [1]. This paper focuses on how accurately application libraries may be expected to perform in criticality calculations with these data. Continuous energy cross section libraries, suitable for use with the MCNP Monte Carlo transport code, have been generated and applied to a suite of nearly one thousand critical benchmark assemblies defined in the International Criticality Safety Benchmark Evaluation Project's International Handbook of Evaluated Criticality Safety Benchmark Experiments. This suite covers uranium and plutonium fuel systems in a variety of forms such as metallic, oxide or solution, and under a variety of spectral conditions, including unmoderated (i.e., bare), metal reflected and water or other light element reflected. Assembly eigenvalues that were accurately predicted with ENDF/B-VII.0 cross sections such as unmoderated and uranium reflected ^{235}U and ^{239}Pu assemblies, HEU solution systems and LEU oxide lattice systems that mimic commercial PWR configurations continue to be accurately calculated with ENDF/B-VII.1 cross sections, and deficiencies in predicted eigenvalues for assemblies containing selected materials, including titanium, manganese, cadmium and tungsten are greatly reduced. Improvements are also confirmed for selected actinide reaction rates such as ^{236}U, ^{238,242}Pu and ^{241,243}Am capture in fast systems. Other deficiencies, such as the overprediction of Pu solution system critical eigenvalues and a decreasing trend in calculated eigenvalue for ^{233}U fueled systems as a function of Above-Thermal Fission Fraction remain. The comprehensive nature of this critical benchmark suite and the generally accurate calculated eigenvalues obtained with ENDF/B-VII.1 neutron cross sections support the conclusion that this is the most accurate general purpose ENDF/B cross section library yet released to the technical community.

Contents

I. INTRODUCTION 2998

II. DATA TESTING 2998
A. NJOY Processing 2998
B. ICSBEP Benchmark Overview 2999
C. Fast Systems 2999
D. Thermal Systems 3005
1. Solution Systems 3005
2. Low Enriched Lattice Systems 3008
E. ^{233}U/^{232}Th and Systems with Zr 3011
F. Argonne ZPR Systems 3012
1. Criticality Measurements 3013
2. Beta-effective (β_{eff}) Measurements 3014
3. Measurements of Sodium Void Worth (ρ_{Na}) 3015
4. Worth Measurements of Control Rods and Control Positions 3016

*Electronic address: akahler@lanl.gov

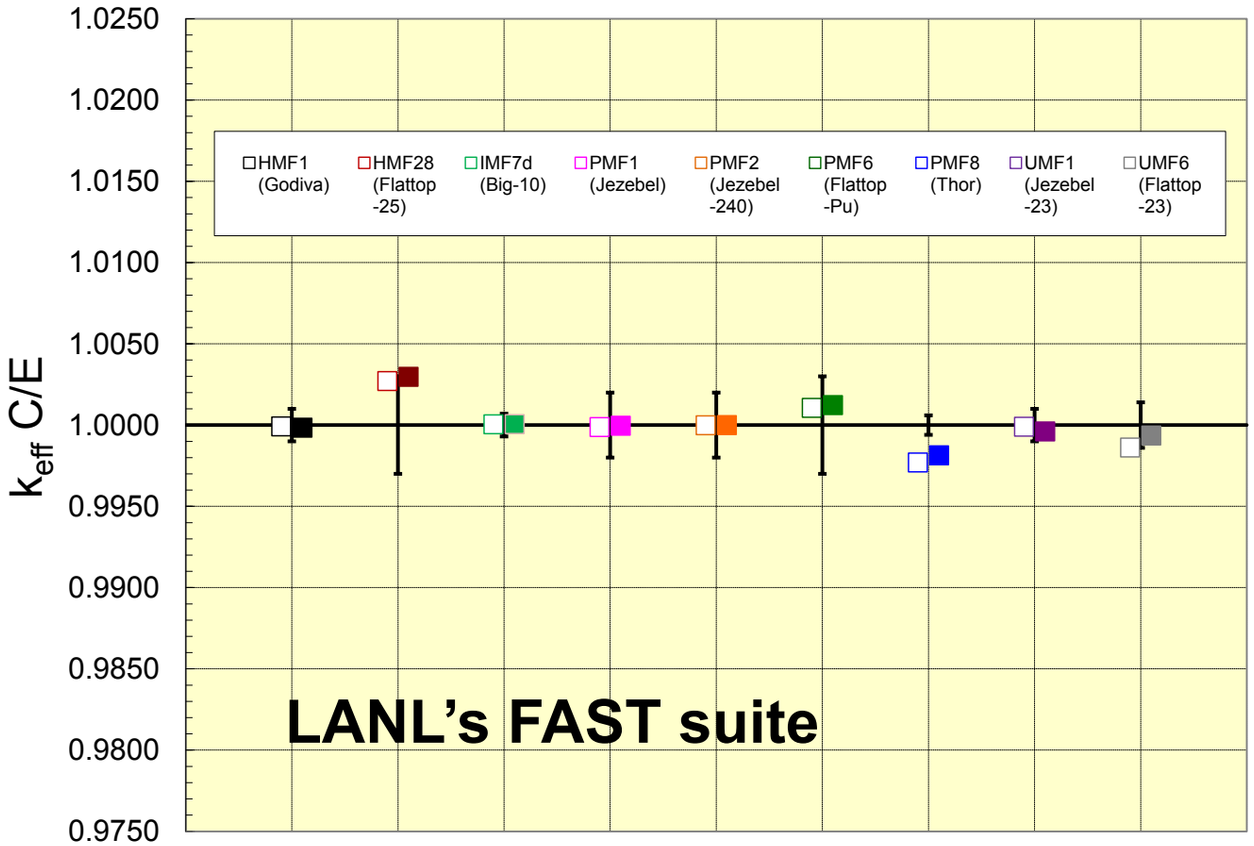
doi:10.1016/j.nds.2011.11.003

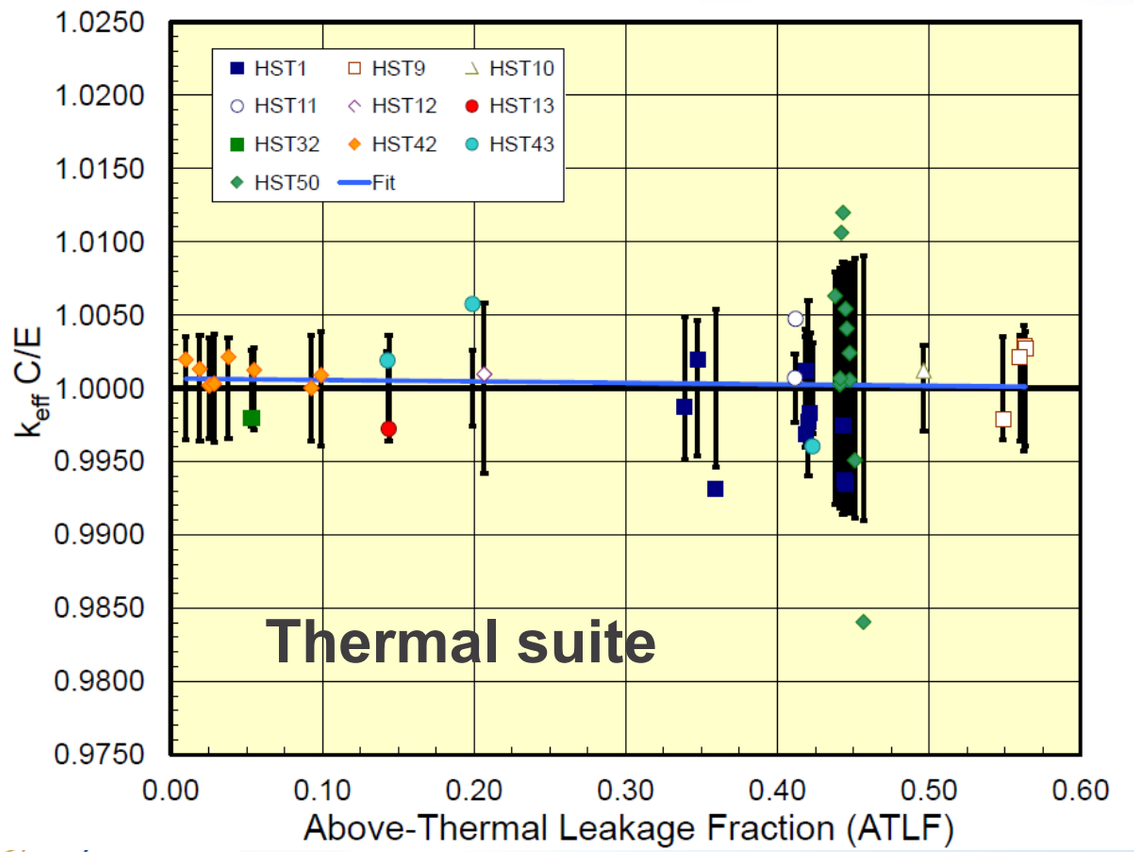
- ***"Do no harm"*** -- If we had accurate results before, we must ensure we do not make them worse
- Did we improve poorly performing systems? Can we attribute it to data improvements?
- Did something unexpected change?

A. Kahler, R. MacFarlane, R. Mosteller, et al., "ENDF/B-VII.1 Neutron Cross Section Data Testing with Critical Assembly Benchmarks and Reactor Experiments", Nuclear Data Sheets, 112(12): 2997-3036 (2011).

Key fast and thermal benchmarks are unchanged

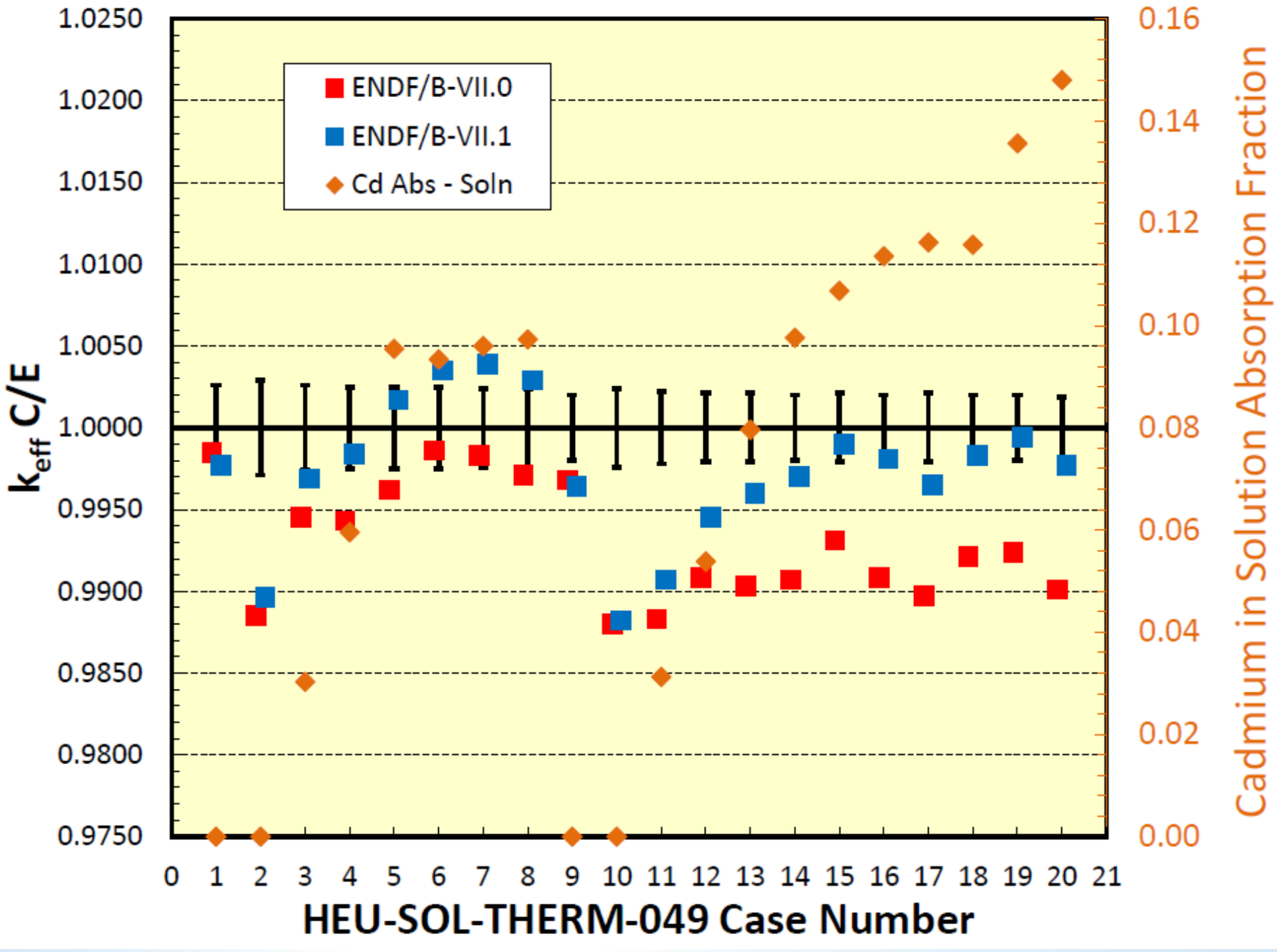
ENDF B-VII.1





- These tests and all others in this talk are taken from the ICSBEP benchmark book
- Data processed with NJOY into ACE format
- Tests run with MCNP by A. Kahler, et al.

Generally, results are better for ENDF/B-VII.1



Large variation in calculated eigenvalues, but in general E71 based results are superior to E70.

Slide from S. Kahler

One of the main thrusts was the addition of covariance data; They are detailed in 3 papers

ENDF B-VII.1

Available online at www.sciencedirect.com
SciVerse ScienceDirect
Nuclear Data Sheets 112 (2011) 3037–3053
Nuclear Data Sheets
www.elsevier.com/locate/nds

Evaluated Nuclear Data Covariances: The Journey From ENDF/B-VII.0 to ENDF/B-VII.1

Donald L. Smith*[1]
[1]Argonne National Laboratory, 1710 Avenida Del Mundo #1506, Coronado, CA 92118, USA
(Received 24 June 2011; revised received 23 September 2011; accepted 9 October 2011)

Recent interest from data users on applications that utilize the uncertainties of evaluated nuclear reaction data has stimulated the data evaluation community to focus on producing covariance data to a far greater extent than ever before. Although some uncertainty information has been available in the ENDF/B libraries since the 1970's, this content has been fairly limited in scope, the quality quite variable, and the use of covariance data confined to only a few application areas. Today, covariance data are more widely and extensively utilized than ever before in neutron dosimetry, in advanced fission reactor design studies, in nuclear criticality safety assessments, in national security applications, and even in certain fusion energy applications. The main problem that now faces the ENDF/B evaluator community is that of providing covariances that are adequate both in quantity and quality to meet the requirements of contemporary nuclear data users in a timely manner. In broad terms, the approach pursued during the past several years has been to purge any legacy covariance information contained in ENDF/B-VI.8 that was judged to be subpar, to include in ENDF/B-VII.0 (released in 2006) only those covariance data deemed then to be of reasonable quality for contemporary applications, and to subsequently devote as much effort as the available time and resources allowed to producing additional covariance data of suitable scope and quality for inclusion in ENDF/B-VII.1. Considerable attention has also been devoted during the five years since the release of ENDF/B-VII.0 to examining and improving the methods used to produce covariance data from thermal energies up to the highest energies addressed in the ENDF/B library, to processing these data in a robust fashion so that they can be utilized readily in contemporary nuclear applications, and to developing convenient covariance data visualization capabilities. Other papers included in this issue discuss in considerable detail various aspects of the data producer community's efforts to improve the evaluation methods and to add covariance content to the ENDF/B library. The present paper offers just a brief glimpse of these activities by drawing material from covariance papers presented at meetings, workshops and international conferences during the past five years. Highlighted are: advances in methods for producing and processing covariance data, recently developed covariance visualization capabilities, and the development and implementation of quality assurance (QA) requirements that should be satisfied for covariance data to be included in ENDF/B-VII.1.

Contents

I. INTRODUCTION 3038
A. Overview 3038
B. Covariances in ENDF/B-VI.8, -VII.0, and -VII.1 3038
C. The Role of ENDF/A 3038
II. MEETINGS, WORKSHOPS AND CONFERENCES 3039
A. AccApp'07 3039
B. ND-2007 Conference 3039
C. Port Jefferson 2008 Workshop 3040
D. Port Jefferson 2009 Workshop 3040
E. ND-2010 Conference 3040
F. IAEA 2010 Workshop 3041
G. CSEWG Annual Meetings 3041
III. COVARIANCE EVALUATION METHODS 3041
A. Low-Energy Region 3041
B. High-Energy Region 3042
C. Light Nuclei 3045
D. Neutron Emission Spectra 3045
E. Standards 3046
F. Low Fidelity Covariances 3047
G. Neutron Multiplicity (nu-bar) 3047
IV. COVARIANCE FORMATS AND DATA PROCESSING 3048

*Electronic address: Donald.L.Smith@anl.gov

doi:10.1016/j.nds.2011.11.004

D. Smith, "Evaluated Nuclear Data Covariances: The Journey From ENDF/B-VII.0 to ENDF/B-VII.1", Nuclear Data Sheets, 112(12):3037-3053(2011).

Available online at www.sciencedirect.com
SciVerse ScienceDirect
Nuclear Data Sheets 112 (2011) 3054–3074
Nuclear Data Sheets
www.elsevier.com/locate/nds

Quantification of Uncertainties for Evaluated Neutron-Induced Reactions on Actinides in the Fast Energy Range

P. Talou*, P.G. Young, and T. Kawano
T-2, Nuclear Physics Group, Theoretical Division,
Los Alamos National Laboratory, Los Alamos, NM 87545, USA

M. Rising
Department of Nuclear Engineering, University of New Mexico, Albuquerque, NM

M.B. Chadwick
X-CP, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
(Received 12 July 2011; revised received 4 October 2011; accepted 7 October 2011)

Covariance matrix evaluations in the fast energy range were performed for a large number of actinides, either using low-fidelity techniques or more sophisticated methods that rely on both experimental data as well as model calculations. The latter covariance evaluations included in the ENDF/B-VII.1 library are discussed for each actinide separately.

Contents

I. INTRODUCTION
II. METHODOLOGY
A. General Statements
B. Combining Model Calculations and Experimental Data
C. Types of Data Considered
D. Experimental Data Uncertainties
E. Codes Used
F. Present Limitations
III. RESULTS
A. ^{235}U
B. ^{238}U
C. ^{238}Pu
D. ^{239}Pu
E. ^{240}Pu
F. ^{241}Pu
G. Other Actinide Evaluations
IV. SUMMARY AND OUTLOOK
Acknowledgments
References

*Electronic address: talou@lanl.gov

doi:10.1016/j.nds.2011.11.005

I. INTRODUCTION

The process of evaluating nuclear data remains incomplete as long as no associated uncertainties are specified. Because of the often intrinsically cumbersome nature of the evaluation procedure, reasonable estimates of uncertainty have eluded the data evaluators for quite some time, except in specific situations for which the evaluation relied on a least-square fit of experimental data only.

This situation has changed dramatically in the past few years due to the availability of large computing capabilities as well as to a renewed interest in uncertainty quantification (UQ). Modern computers have allowed nuclear model calculations used in evaluations in the fast energy range to run very quickly, and therefore to be run numerous times in order to study the sensitivity of the results to small changes in input model parameters around their evaluated central values. The strong renewed interest in UQ is driven by applications- nuclear reactors, stockpile stewardship, *etc*, which now require a more scientifically-based approach to their quantification of safety, performance, and economic margins. For instance, the recent COMMARA-2.0 33-group covariance matrix library for advanced reactor applications [1] is the result of a multi-year, multi-lab effort mostly funded through the Advanced Fuel Cycle Initiative (AFCI) and now the Fuel Cycle R&D (FCRD) Department of Energy programs in the US.

At LANL, we started working on UQ for evaluated nuclear data about 6 years ago, just before the release of the ENDF/B-VII.0 library [2]. This VII.0 library constitutes a milestone in reliability, completeness and accuracy for many nuclear data. However, it contains close to zero

P. Talou, P. Young, T. Kawano, et al., "Quantification of Uncertainties for Evaluated Neutron-Induced Reactions on Actinides in the Fast Region", Nuclear Data Sheets, 112(12): 3054-3074(2011).

Available online at www.sciencedirect.com
SciVerse ScienceDirect
Nuclear Data Sheets 112 (2011) 3075–3097
Nuclear Data Sheets
www.elsevier.com/locate/nds

Neutron Cross Section Covariances for Structural Materials and Fission Products

S. Hoblit,* Y.-S. Cho,† M. Herman, C.M. Mattoon,† S.F. Mughabghab, P. Obložinský,§ M.T. Pigni,¶ A.A. Sonzogni[1]
[1]National Nuclear Data Center, Brookhaven National Laboratory, Upton, NY 11973-5000
(Received 19 September 2011; revised received 3 October 2011; accepted 19 October 2011)

We describe neutron cross section covariances for 78 structural materials and fission products produced for the new US evaluated nuclear reaction library ENDF/B-VII.1. Neutron incident energies cover full range from 10^{-5} eV to 20 MeV and covariances are primarily provided for capture, elastic and inelastic scattering as well as (n,2n). The list of materials follows priorities defined by the Advanced Fuel Cycle Initiative, the major application being data adjustment for advanced fast reactor systems. Thus, in addition to 28 structural materials and 49 fission products, the list includes also ^{23}Na which is important fast reactor coolant. Due to extensive amount of materials, we adopted a variety of methodologies depending on the priority of a specific material. In the resolved resonance region we primarily used resonance parameter uncertainties given in Atlas of Neutron Resonances and either applied the kernel approximation to propagate these uncertainties into cross section uncertainties or resorted to simplified estimates based on integral quantities. For several priority materials we adopted MF32 covariances produced by SAMMY at ORNL, modified by us by adding MF33 covariances to account for systematic uncertainties. In the fast neutron region we resorted to three methods. The most sophisticated was EMPIRE-KALMAN method which combines experimental data from EXFOR library with nuclear reaction modeling and least-squares fitting. The two other methods used simplified estimates, either based on the propagation of nuclear reaction model parameter uncertainties or on a dispersion analysis of central cross section values in recent evaluated data files. All covariances were subject to quality assurance procedures adopted recently by CSEWG. In addition, tools were developed to allow inspection of processed covariances and computed integral quantities, and for comparing these values to data from the Atlas and the astrophysics database KADoNiS.

Contents

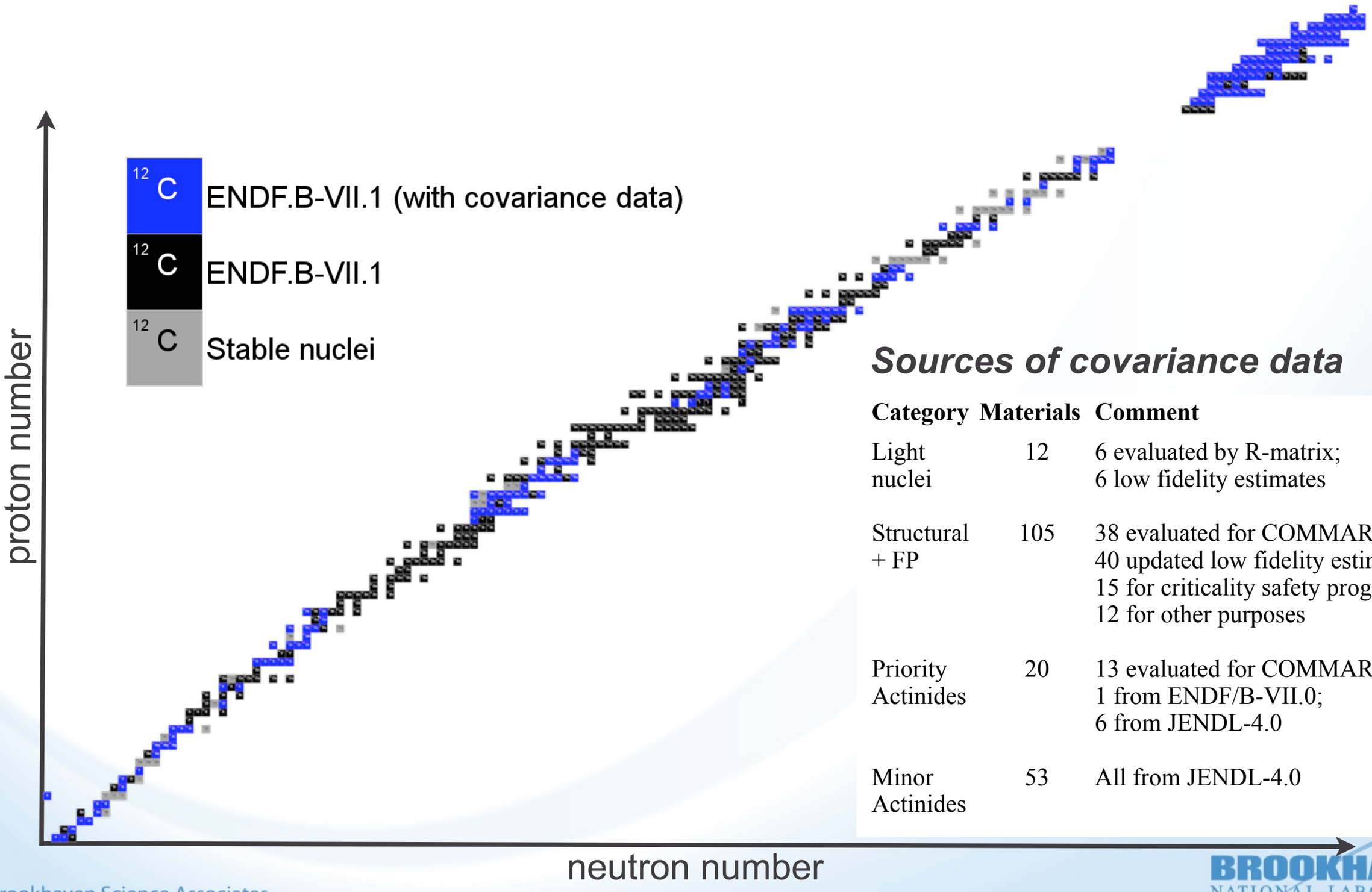
I. INTRODUCTION 3076
II. COVARIANCE METHODOLOGY IN THE RESONANCE REGION 3076
A. Integral Method 3077
B. Kernel Method 3077
1. Radiative capture 3077
2. Elastic scattering 3079
C. SAMMY + BNL Method 3081
III. COVARIANCE METHODOLOGY IN THE FAST NEUTRON REGION 3082
A. EMPIRE-KALMAN Method 3082
B. Model-Based Method 3083
C. Dispersion Analysis 3084
IV. STRUCTURAL MATERIALS 3084
A. ^{23}Na and Major Structural Materials 3084
1. ^{23}Na 3084
2. ^{54,56,57}Fe 3085
3. ^{50,52,53}Cr 3086
4. ^{58,60}Ni 3088
5. $^{90-96}$Zr 3088
6. ^{204,206,207,208}Pb 3089
7. ^{209}Bi 3089
B. Minor Structural Materials 3089
1. ^{24,25,26}Mg 3089
2. ^{27}Al 3090
3. ^{28,29,30}Si 3090
4. ^{55}Mn 3090
V. FISSION PRODUCTS 3090
A. Major Fission Products 3090
1. ^{92,94,95,96,97,98,100}Mo 3090
2. ^{99}Tc 3091
3. ^{109}Ag 3091
4. ^{133,135}Cs 3091
5. ^{141}Pr 3091
6. ^{143,145,146,148}Nd 3092
7. ^{155,156,157,158,160}Gd 3092

*Electronic address: hoblit@bnl.gov
†On sabbatical leave from Nuclear Data Lab, KAERI, Korea
‡Current address: LLNL L-059, Livermore, CA 94550
§Current address: Na Riviére 30, 84104 Bratislava, Slovakia
¶Current address: ORNL, P.O. Box 2008, Oak Ridge, TN 37831

doi:10.1016/j.nds.2011.11.006

S. Hoblit, Y.-S. Cho, M. Herman, et al., "Neutron Cross Section Covariances for Structural Materials and Fission Products", Nuclear Data Sheets, 112(12): 3075-3097(2011).

An overview of the library



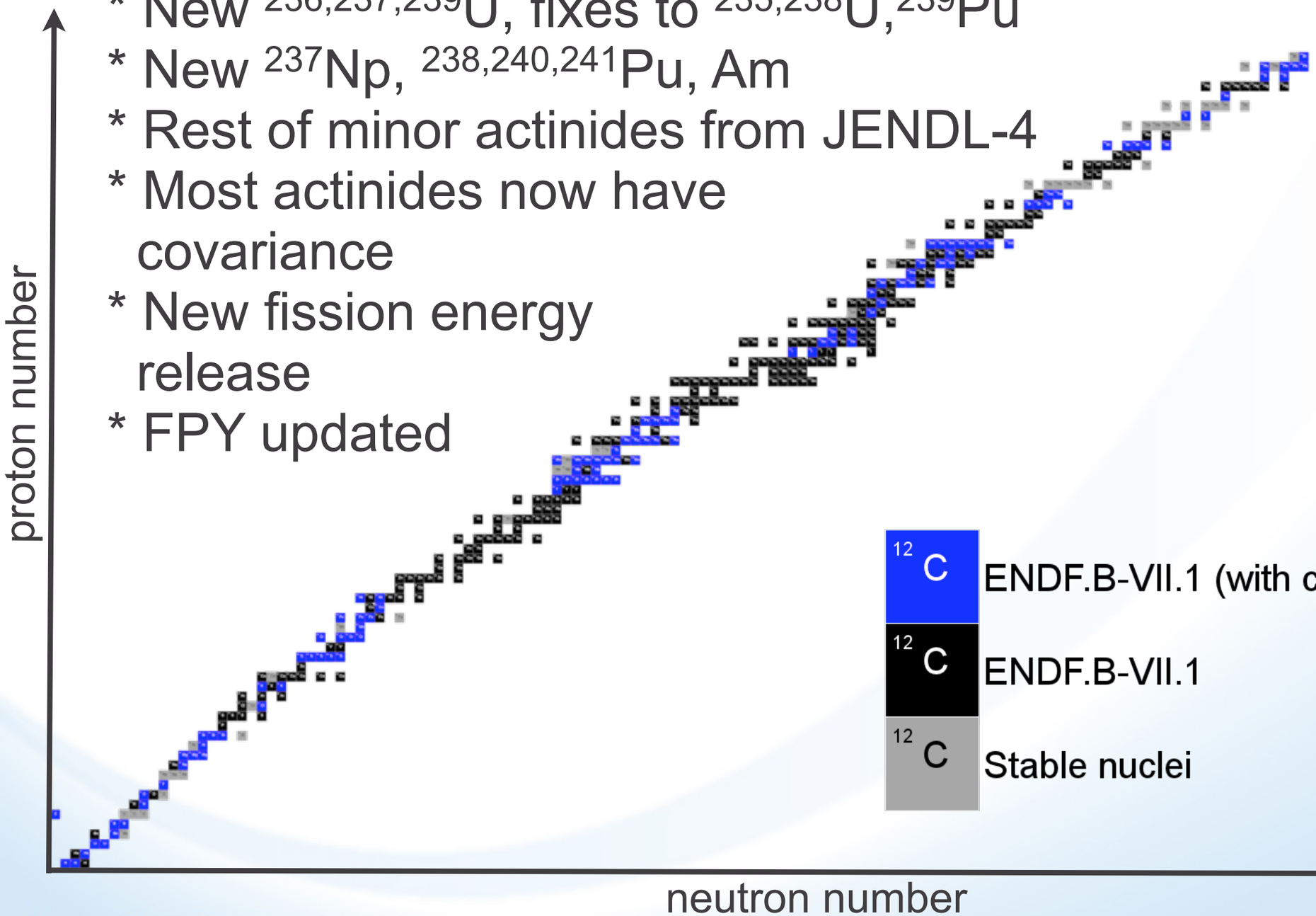
Sources of covariance data

Category	Materials	Comment
Light nuclei	12	6 evaluated by R-matrix; 6 low fidelity estimates
Structural + FP	105	38 evaluated for COMMARA-2.0; 40 updated low fidelity estimates; 15 for criticality safety programs; 12 for other purposes
Priority Actinides	20	13 evaluated for COMMARA-2.0; 1 from ENDF/B-VII.0; 6 from JENDL-4.0
Minor Actinides	53	All from JENDL-4.0

An overview of the library

ENDF B-VII.1

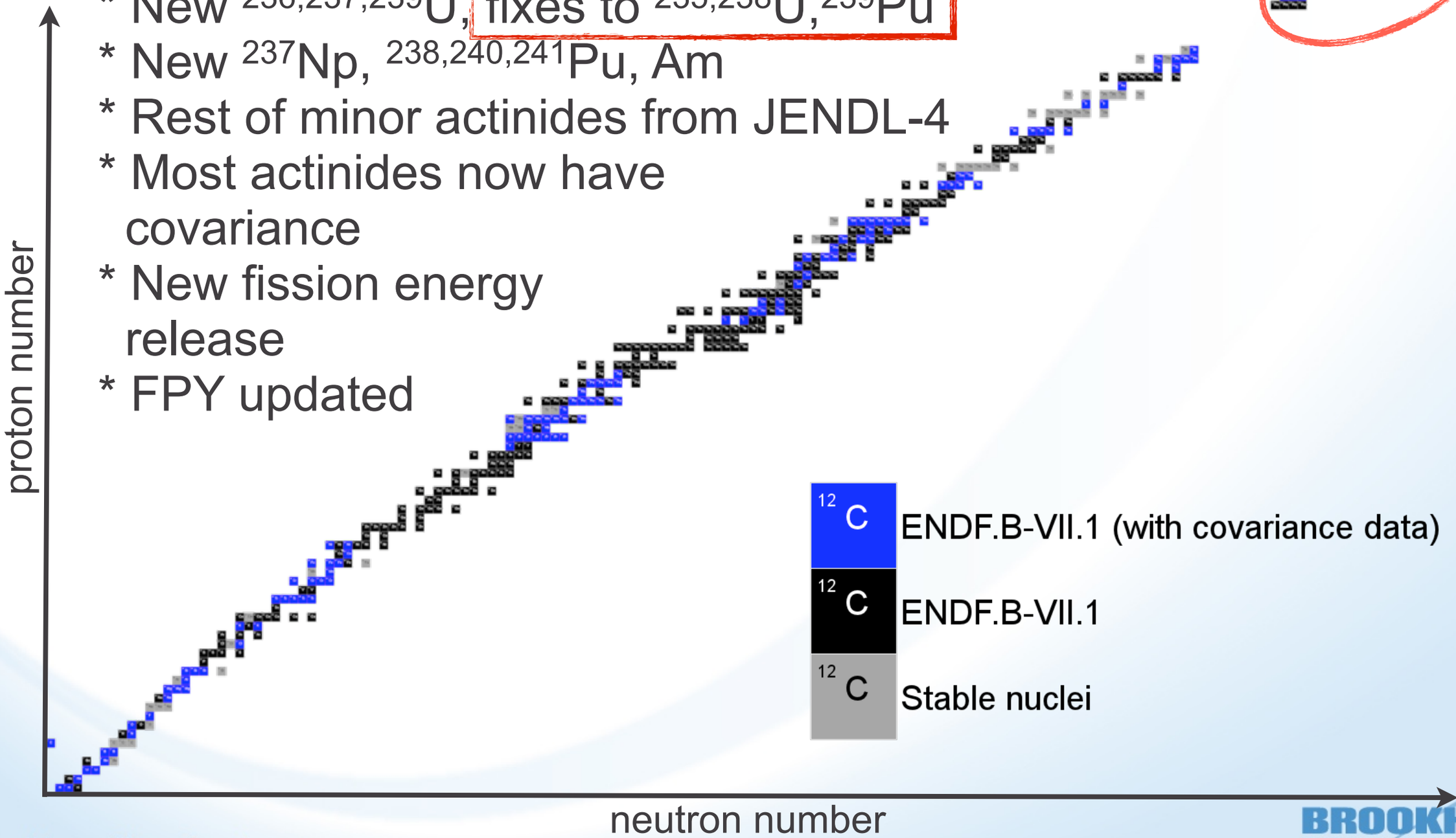
* Major actinides essentially unchanged,
* New ^{236,237,239}U, fixes to ^{235,238}U,^{239}Pu
* New ^{237}Np, ^{238,240,241}Pu, Am
* Rest of minor actinides from JENDL-4
* Most actinides now have covariance
* New fission energy release
* FPY updated



An overview of the library

ENDF B-VII.1

* Major actinides essentially unchanged,
* New ^{236,237,239}U, fixes to ^{235,238}U,^{239}Pu
* New ^{237}Np, ^{238,240,241}Pu, Am
* Rest of minor actinides from JENDL-4
* Most actinides now have covariance
* New fission energy release
* FPY updated

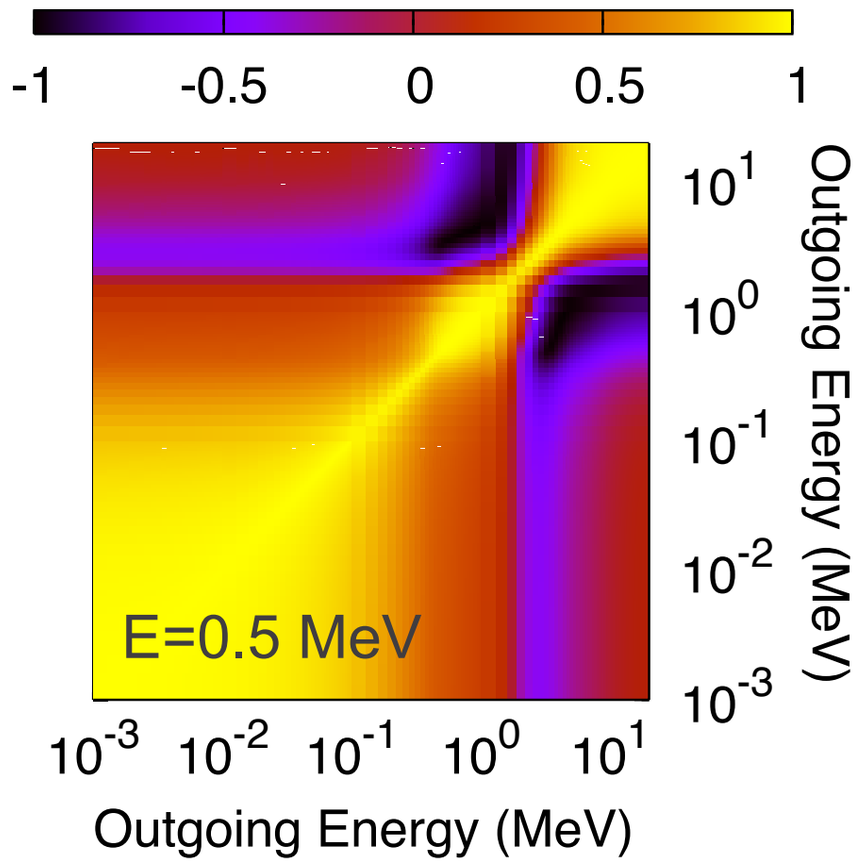


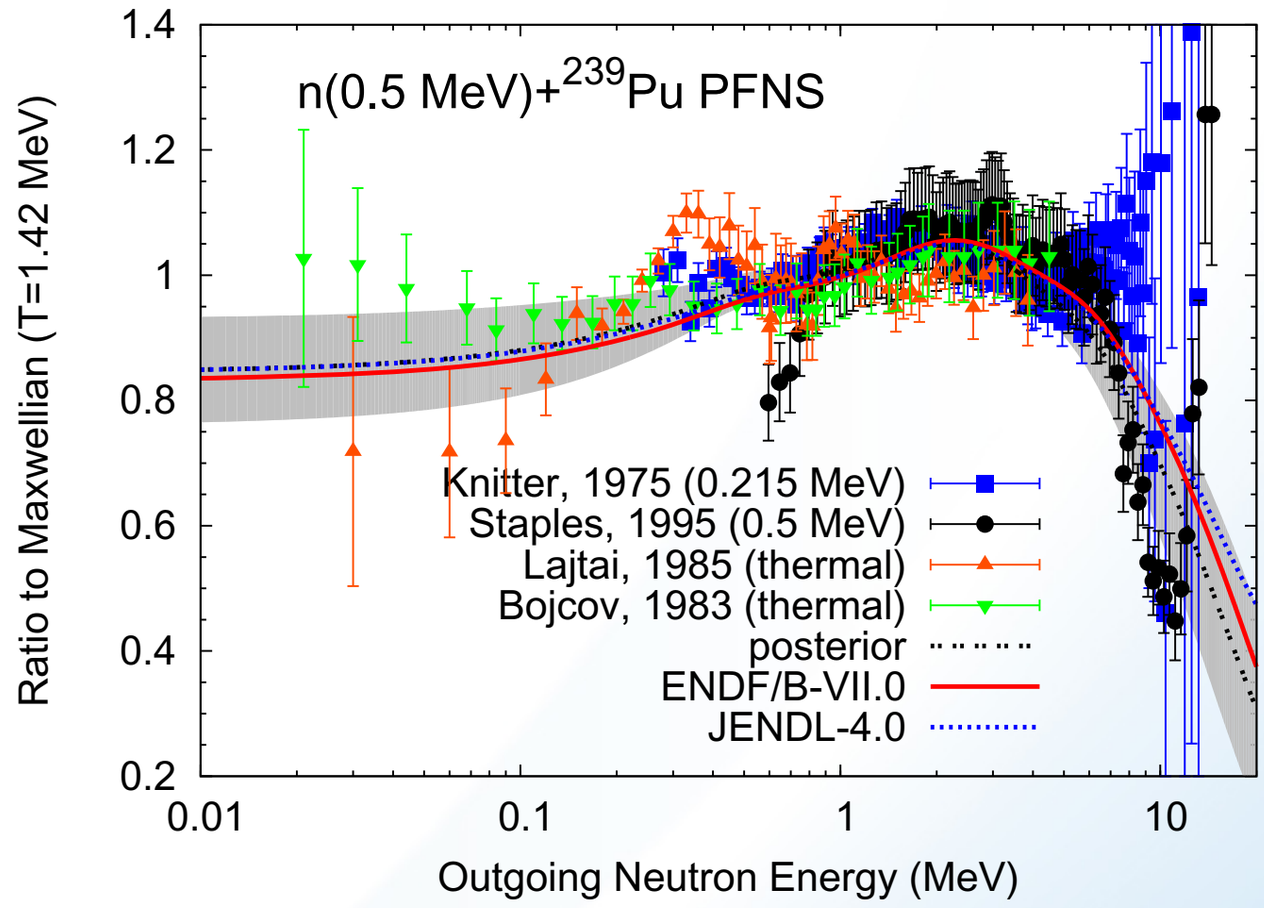
Delayed neutron data in ^{235,238}U, ^{239}Pu reverted to ENDF/B-VI.8

“Based upon unfavorable feedback there is evidence to suggest that the ENDF/B-VII.0 delayed neutron data are not as reflective of physical reality as the earlier ENDF/B-VI.8 delayed data”.

Only substantial change to ^{239}Pu: addition of prompt fission neutron spectrum covariance

ENDF B-VII.1



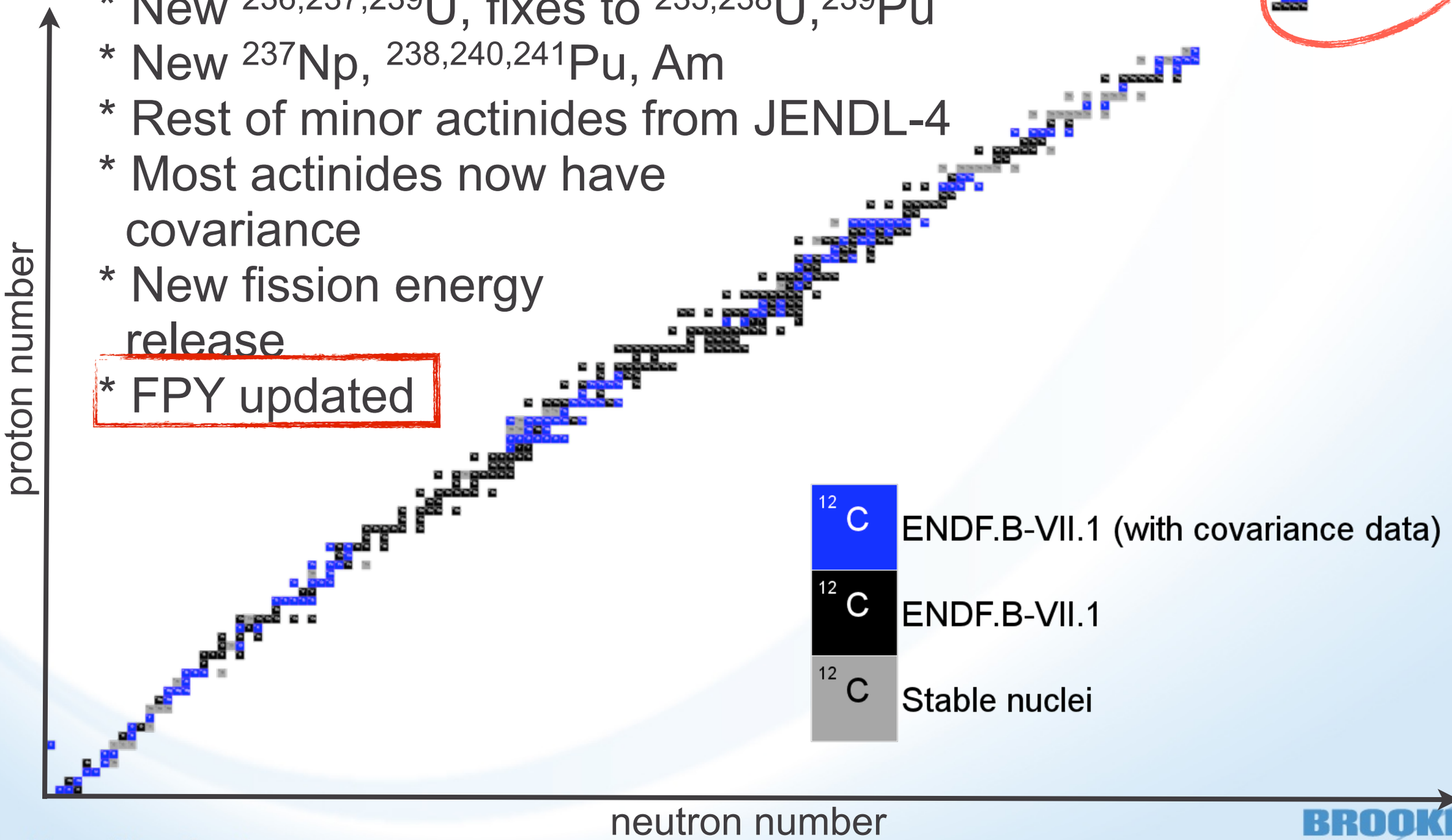


- Talou et al (LANL) retrofitted using Madland-Nix model
- Valuable contribution enabling full QMU studies in Pu systems (previously only nubar and cross section covariance available)

An overview of the library

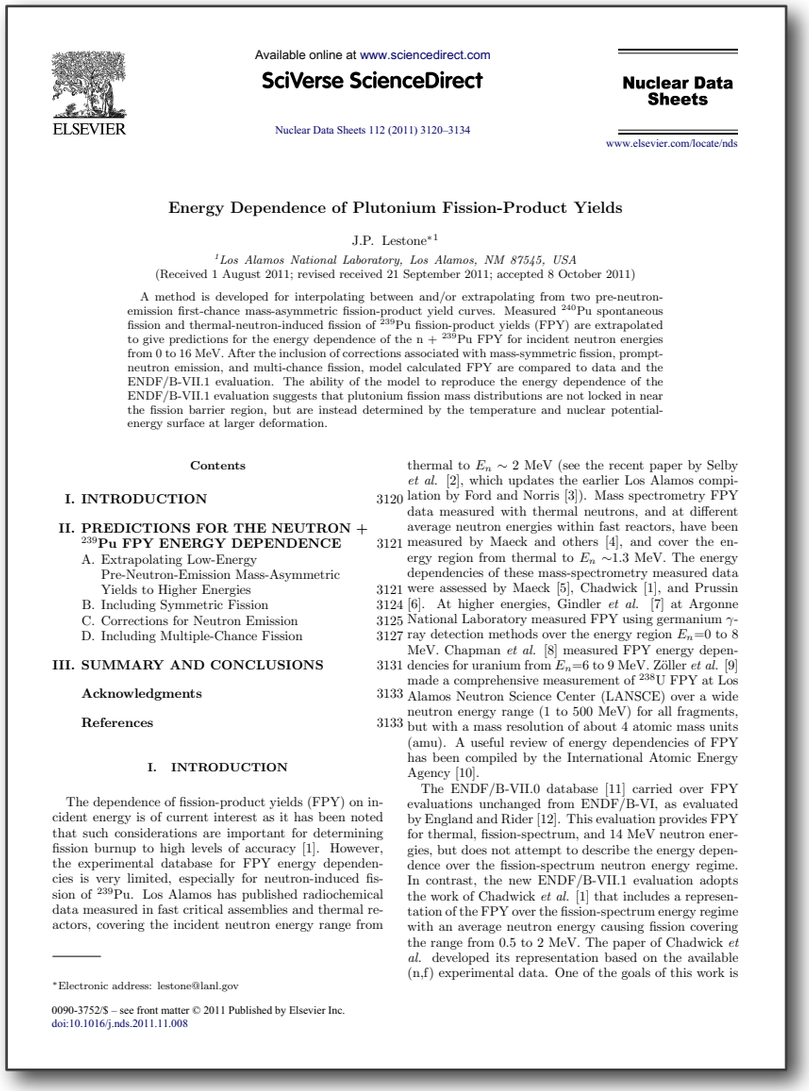
ENDF B-VII.1

* Major actinides essentially unchanged,
* New ^{236,237,239}U, fixes to ^{235,238}U,^{239}Pu
* New ^{237}Np, ^{238,240,241}Pu, Am
* Rest of minor actinides from JENDL-4
* Most actinides now have covariance
* New fission energy release
* FPY updated



Fission Product Yield work summarized in two reports, in addition to the "Big Paper"

ENDF B-VII.1



Available online at www.sciencedirect.com
SciVerse ScienceDirect
Nuclear Data Sheets 112 (2011) 3120–3134
Nuclear Data Sheets
www.elsevier.com/locate/nds

Energy Dependence of Plutonium Fission-Product Yields

J.P. Lestone*[1]
[1]Los Alamos National Laboratory, Los Alamos, NM 87545, USA
(Received 1 August 2011; revised received 21 September 2011; accepted 8 October 2011)

A method is developed for interpolating between and/or extrapolating from two pre-neutron-emission first-chance mass-asymmetric fission-product yield curves. Measured ^{240}Pu spontaneous fission and thermal-neutron-induced fission of ^{239}Pu fission-product yields (FPY) are extrapolated to give predictions for the energy dependence of the n + ^{239}Pu FPY for incident neutron energies from 0 to 16 MeV. After the inclusion of corrections associated with mass-symmetric fission, prompt-neutron emission, and multi-chance fission, model calculated FPY are compared to data and the ENDF/B-VII.1 evaluation. The ability of the model to reproduce the energy dependence of the ENDF/B-VII.1 evaluation suggests that plutonium fission mass distributions are not locked in near the fission barrier region, but are instead determined by the temperature and nuclear potential-energy surface at larger deformation.

Contents

I. INTRODUCTION 3120
II. PREDICTIONS FOR THE NEUTRON + ^{239}Pu FPY ENERGY DEPENDENCE
A. Extrapolating Low-Energy Pre-Neutron-Emission Mass-Asymmetric Yields to Higher Energies
B. Including Symmetric Fission
C. Corrections for Neutron Emission
D. Including Multiple-Chance Fission
III. SUMMARY AND CONCLUSIONS
Acknowledgments
References

I. INTRODUCTION

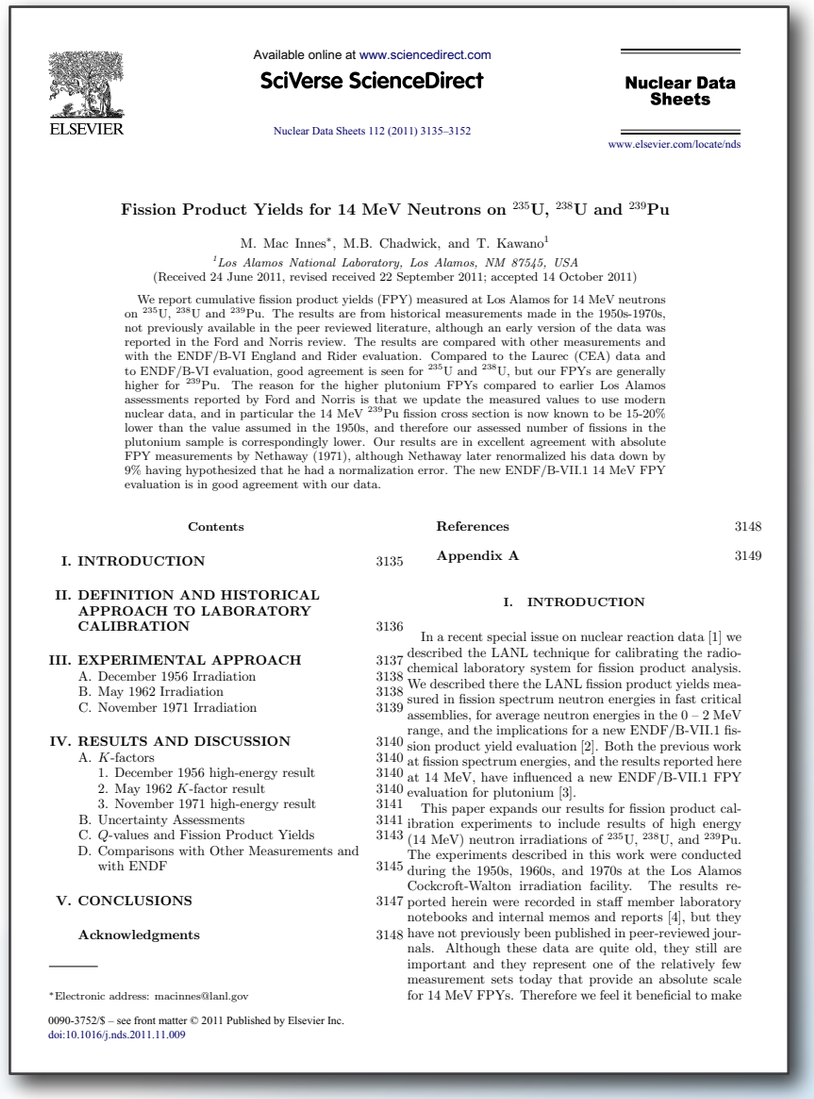
The dependence of fission-product yields (FPY) on incident energy is of current interest as it has been noted that such considerations are important for determining fission burnup to high levels of accuracy [1]. However, the experimental database for FPY energy dependencies is very limited, especially for neutron-induced fission of ^{239}Pu. Los Alamos has published radiochemical data measured in fast critical assemblies and thermal reactors, covering the incident neutron energy range from thermal to $E_n \sim 2$ MeV (see the recent paper by Selby *et al.* [2], which updates the earlier Los Alamos compilation by Ford and Norris [3]). Mass spectrometry FPY data measured with thermal neutrons, and at different average neutron energies within fast reactors, have been measured by Maeck and others [4], and cover the energy region from thermal to E_n ~1.3 MeV. The energy dependencies of these mass-spectrometry measured data were assessed by Maeck [5], Chadwick [1], and Prussin [6]. At higher energies, Gindler *et al.* [7] at Argonne National Laboratory measured FPY using germanium γ-ray detection methods over the energy region E_n=0 to 8 MeV. Chapman *et al.* [8] measured FPY energy dependencies for uranium from E_n=6 to 9 MeV. Zöller *et al.* [9] made a comprehensive measurement of ^{238}U FPY at Los Alamos Neutron Science Center (LANSCE) over a wide neutron energy range (1 to 500 MeV) for all fragments, but with a mass resolution of about 4 atomic mass units (amu). A useful review of energy dependencies of FPY has been compiled by the International Atomic Energy Agency [10].

The ENDF/B-VII.0 database [11] carried over FPY evaluations unchanged from ENDF/B-VI, as evaluated by England and Rider [12]. This evaluation provides FPY for thermal, fission-spectrum, and 14 MeV neutron energies, but does not attempt to describe the energy dependence over the fission-spectrum neutron energy regime. In contrast, the new ENDF/B-VII.1 evaluation adopts the work of Chadwick *et al.* [1] that includes a representation of the FPY over the fission-spectrum energy regime with an average neutron energy causing fission covering the range from 0.5 to 2 MeV. The paper of Chadwick *et al.* developed its representation based on the available (n,f) experimental data. One of the goals of this work is

*Electronic address: lestone@lanl.gov

0090-3752/$ – see front matter © 2011 Published by Elsevier Inc.
doi:10.1016/j.nds.2011.11.008

J. Lestone, "Energy Dependence of Plutonium Fission-Product Yields", Nuclear Data Sheets, 112(12):3120-3134 (2011).



Available online at www.sciencedirect.com
SciVerse ScienceDirect
Nuclear Data Sheets 112 (2011) 3135–3152
Nuclear Data Sheets
www.elsevier.com/locate/nds

Fission Product Yields for 14 MeV Neutrons on ^{235}U, ^{238}U and ^{239}Pu

M. Mac Innes*, M.B. Chadwick, and T. Kawano[1]
[1]Los Alamos National Laboratory, Los Alamos, NM 87545, USA
(Received 24 June 2011, revised received 22 September 2011; accepted 14 October 2011)

We report cumulative fission product yields (FPY) measured at Los Alamos for 14 MeV neutrons on ^{235}U, ^{238}U and ^{239}Pu. The results are from historical measurements made in the 1950s-1970s, not previously available in the peer reviewed literature, although an early version of the data was reported in the Ford and Norris review. The results are compared with other measurements and with the ENDF/B-VI England and Rider evaluation. Compared to the Laurec (CEA) data and to ENDF/B-VI evaluation, good agreement is seen for ^{235}U and ^{238}U, but our FPYs are generally higher for ^{239}Pu. The reason for the higher plutonium FPYs compared to earlier Los Alamos assessments reported by Ford and Norris is that we update the measured values to use modern nuclear data, and in particular the 14 MeV ^{239}Pu fission cross section is now known to be 15-20% lower than the value assumed in the 1950s, and therefore our assessed number of fissions in the plutonium sample is correspondingly lower. Our results are in excellent agreement with absolute FPY measurements by Nethaway (1971), although Nethaway later renormalized his data down by 9% having hypothesized that he had a normalization error. The new ENDF/B-VII.1 14 MeV FPY evaluation is in good agreement with our data.

Contents

I. INTRODUCTION 3135
II. DEFINITION AND HISTORICAL APPROACH TO LABORATORY CALIBRATION
III. EXPERIMENTAL APPROACH
A. December 1956 Irradiation
B. May 1962 Irradiation
C. November 1971 Irradiation
IV. RESULTS AND DISCUSSION
A. K-factors
1. December 1956 high-energy result
2. May 1962 K-factor result
3. November 1971 high-energy result
B. Uncertainty Assessments
C. Q-values and Fission Product Yields
D. Comparisons with Other Measurements and with ENDF
V. CONCLUSIONS
Acknowledgments
References 3148
Appendix A 3149

I. INTRODUCTION

In a recent special issue on nuclear reaction data [1] we described the LANL technique for calibrating the radiochemical laboratory system for fission product analysis. We described there the LANL fission product yields measured in fission spectrum neutron energies in fast critical assemblies, for average neutron energies in the 0 – 2 MeV range, and the implications for a new ENDF/B-VII.1 fission product yield evaluation [2]. Both the previous work at fission spectrum energies, and the results reported here at 14 MeV, have influenced a new ENDF/B-VII.1 FPY evaluation for plutonium [3].

This paper expands our results for fission product calibration experiments to include results of high energy (14 MeV) neutron irradiations of ^{235}U, ^{238}U, and ^{239}Pu. The experiments described in this work were conducted during the 1950s, 1960s, and 1970s at the Los Alamos Cockcroft-Walton irradiation facility. The results reported herein were recorded in staff member laboratory notebooks and internal memos and reports [4], but they have not previously been published in peer-reviewed journals. Although these data are quite old, they still are important and they represent one of the relatively few measurement sets today that provide an absolute scale for 14 MeV FPYs. Therefore we feel it beneficial to make

*Electronic address: macinnes@lanl.gov

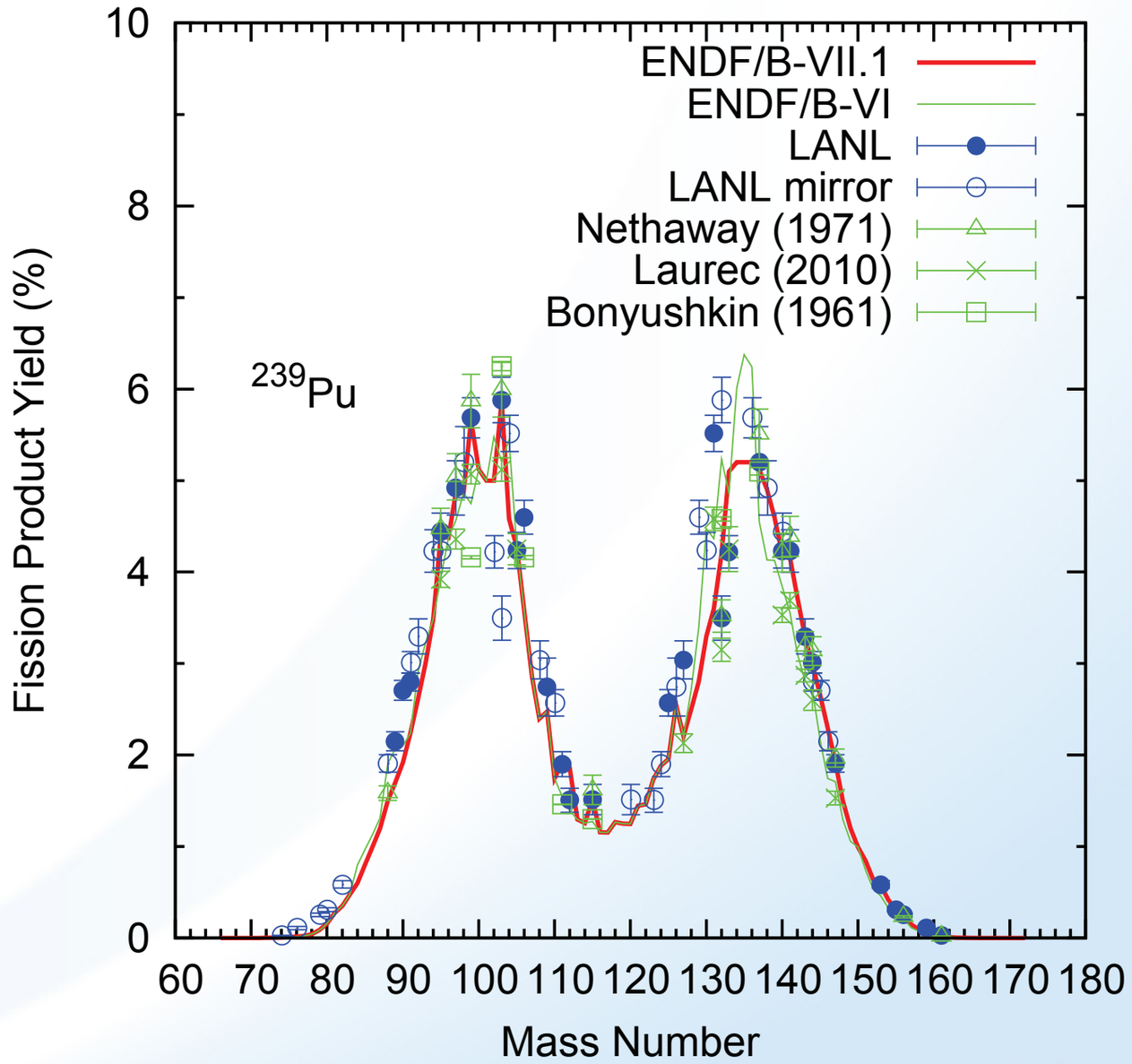
0090-3752/$ – see front matter © 2011 Published by Elsevier Inc.
doi:10.1016/j.nds.2011.11.009

M. MacInnes, M. Chadwick, T. Kawano, "Fission Product Yields for 14 MeV Neutrons on 235U, 238U and 239Pu", Nuclear Data Sheets, 112(12):3135-3152 (2011).

^{239}Pu Fission Product Yields reevaluated and 14 MeV point changed

ENDF B-VII.1

- **^{239}Pu**
  - Thermal FPY data are unchanged
  - Fission and 14 MeV energy FPY's are revised
    - Fission energy includes 0.5 MeV and 2.0 MeV incident neutron energy
      - Documented in Chadwick *et al*, *Nuclear Data Sheets*, **111**, 2923 (2010).
    - 14 MeV results documented in MacInnes *et al*, *Nuclear Data Sheets*, **112**, 3135 (2011).

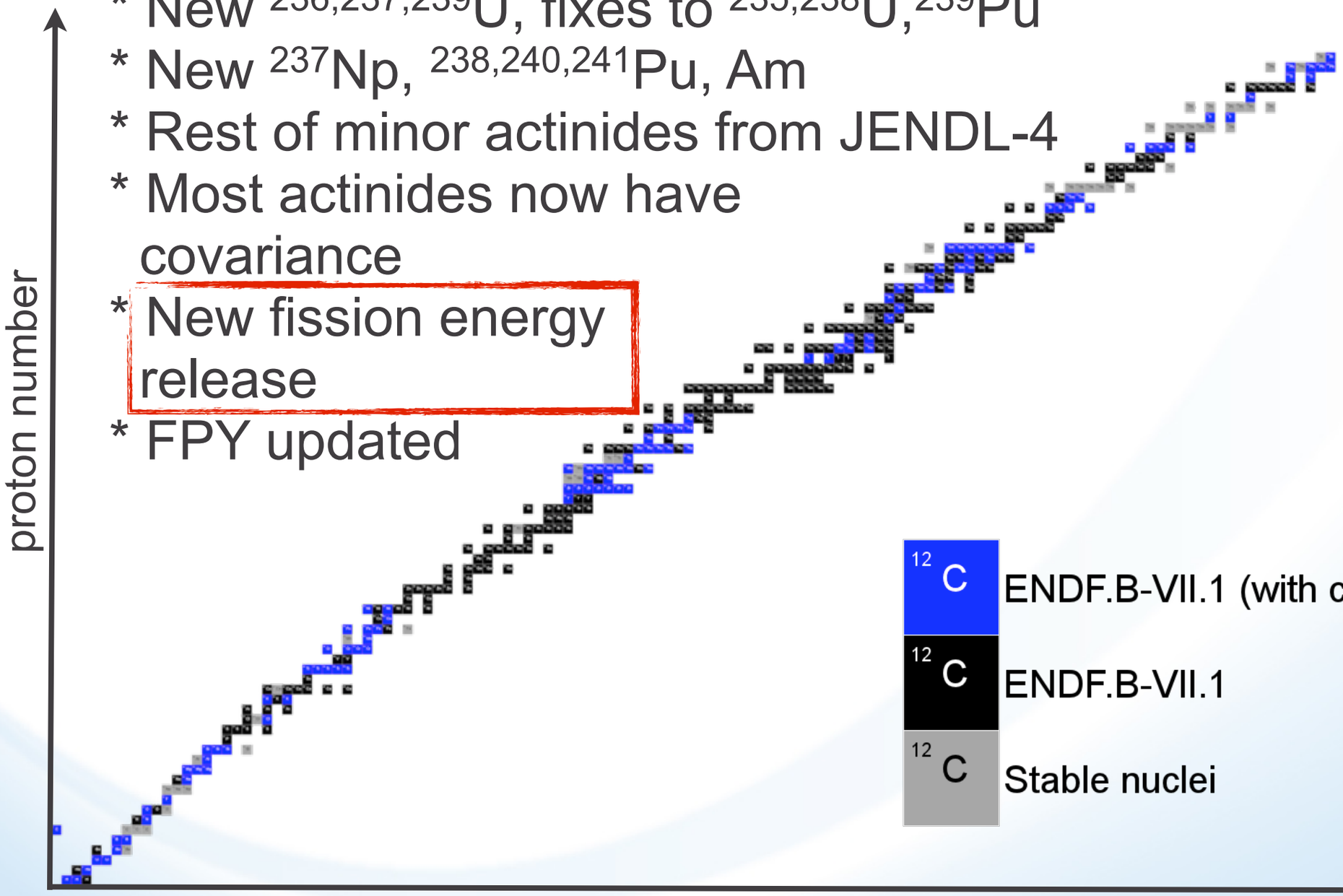


Slide from S. Kahler

An overview of the library

ENDF B-VII.1

* Major actinides essentially unchanged,
* New ^{236,237,239}U, fixes to ^{235,238}U,^{239}Pu
* New ^{237}Np, ^{238,240,241}Pu, Am
* Rest of minor actinides from JENDL-4
* Most actinides now have covariance
* New fission energy release
* FPY updated



Fission energy release added to all actinides without this type of data

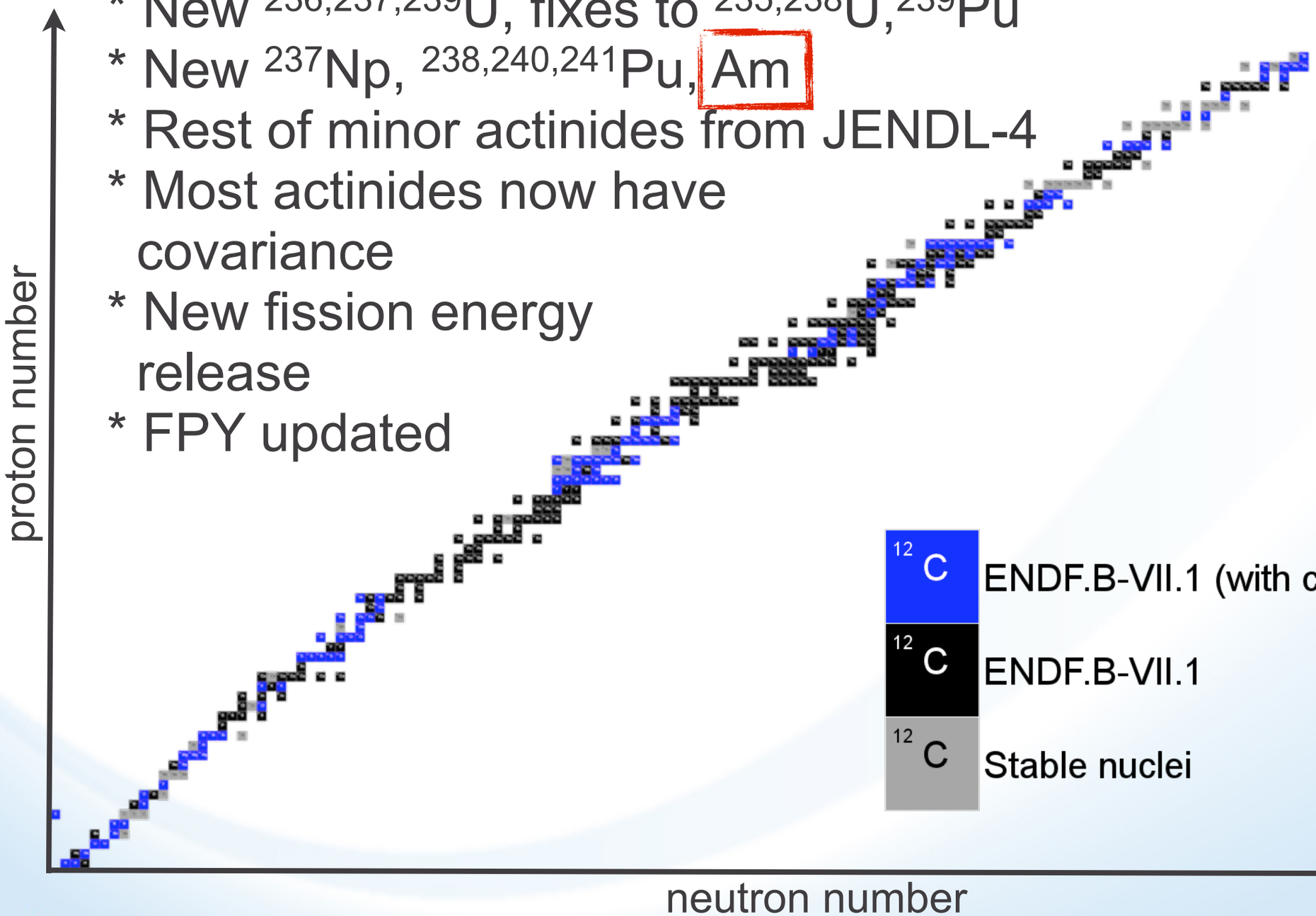
ENDF B-VII.1

ENDF/B-VII.0:
^{232}Th, ^{233,234,236,240}U, ^{237}Np, ^{240,241}Pu, ^{241,243}Am
Madland2006:
^{235,238}U, ^{239}Pu
Vogt2010:
^{225,226,227}Ac, ^{228,230,231,233,234}Th ^{229,230,231,232,233}Pa, ^{230,231,237,239,241}U ^{234,235,236,239}Np, ^{236,237,238,243,244,246}Pu ^{240,242,242m,244,244m}Am, ^{240,241,247,249,250}Cm ^{245,246,247,248,249,250}Bk, ^{246,248,250,252,253,254}Cf
JENDL-4.0:
^{227,229}Th, ^{232}U, ^{238}Np, ^{242}Pu ^{242,243,244,245,246,248}Cm, ^{249,251}Cf, ^{254}Es, ^{255}Bk
Missing:
^{251,252,253,254m,255}Es

An overview of the library

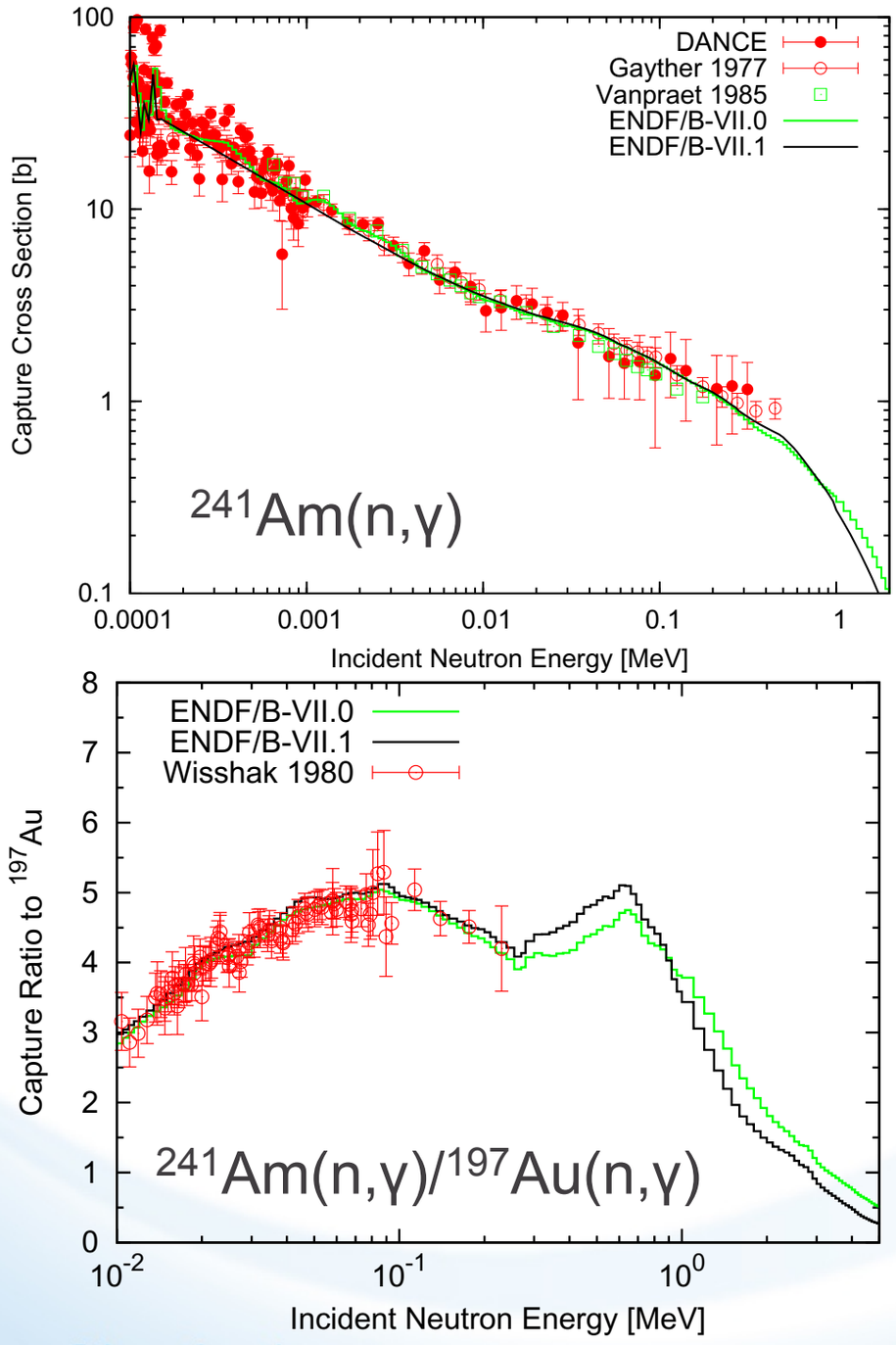
ENDF B-VII.1

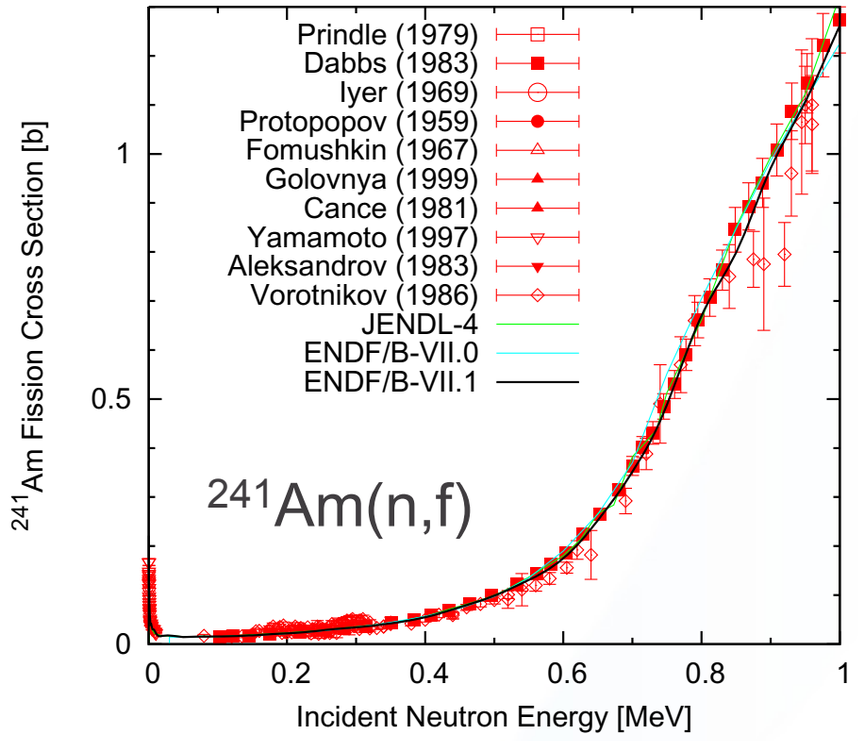
* Major actinides essentially unchanged,
* New ^{236,237,239}U, fixes to ^{235,238}U,^{239}Pu
* New ^{237}Np, ^{238,240,241}Pu, Am
* Rest of minor actinides from JENDL-4
* Most actinides now have covariance
* New fission energy release
* FPY updated

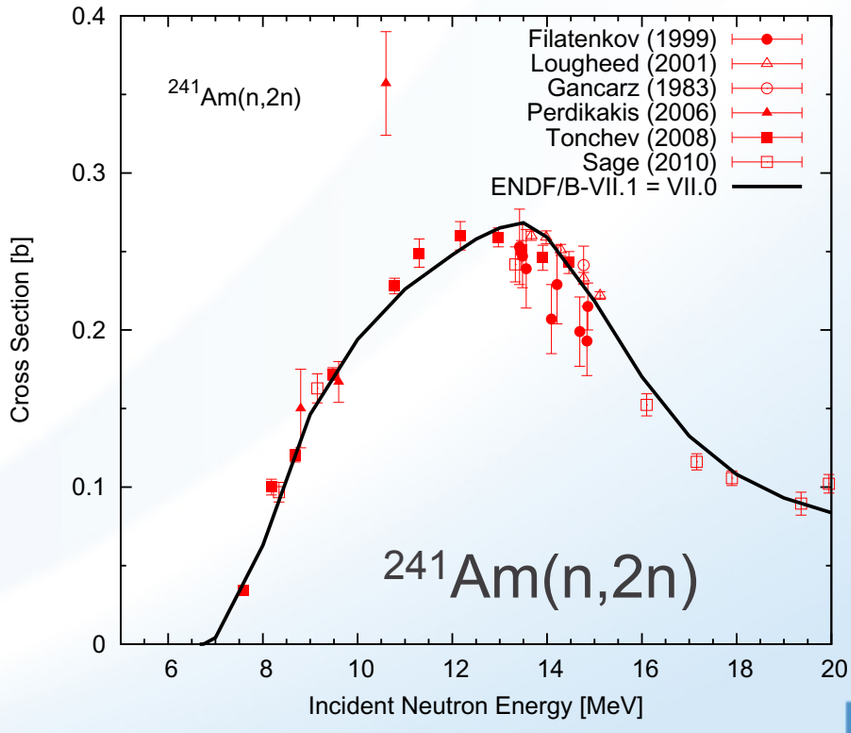


^{241,243}Am updated using GNASH, tuned with SOK to new LANCE data

ENDF B-VII.1

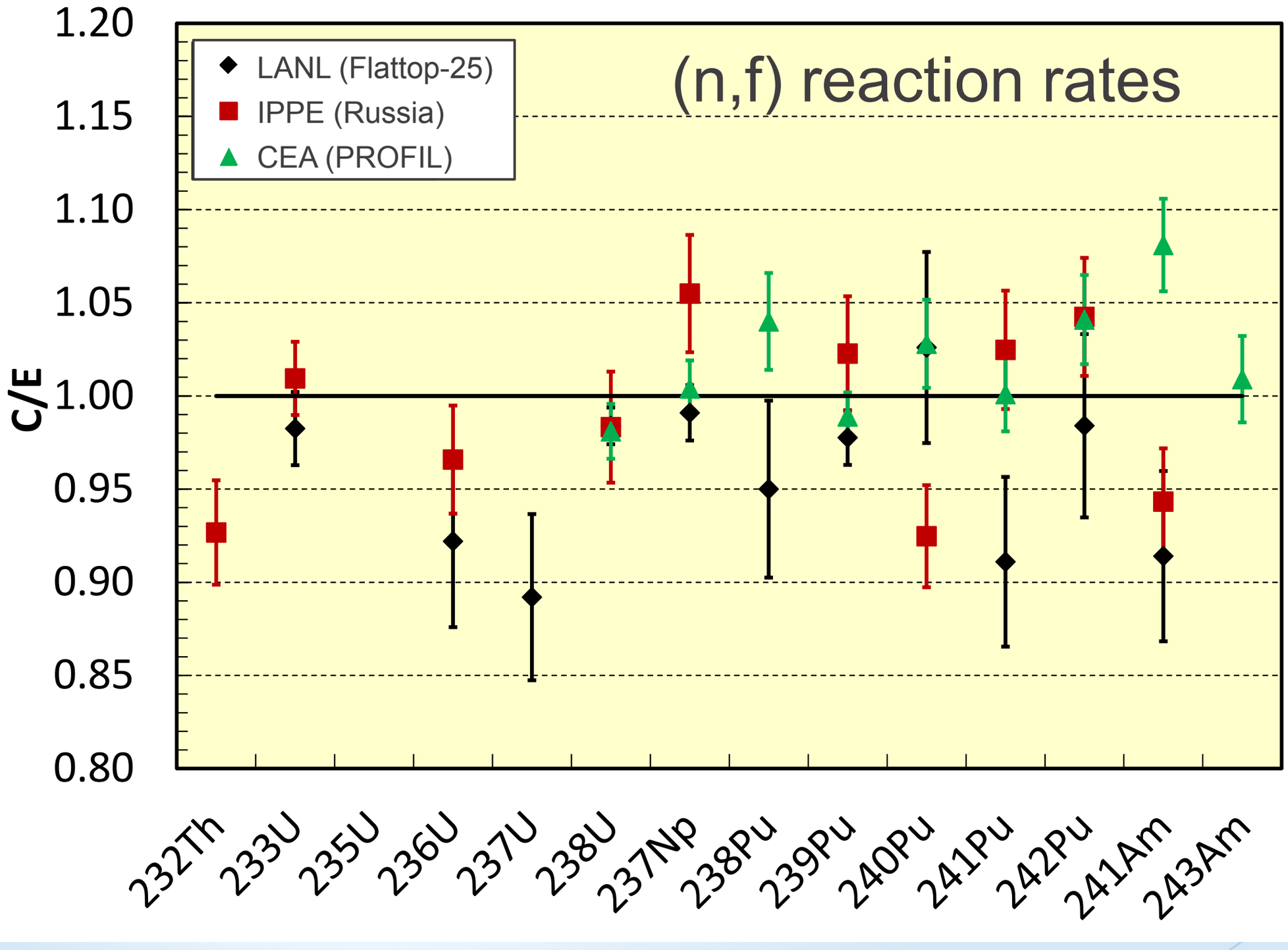






Sample activation benchmarks target individual reactions and show excellent (n,f) agreement

ENDF B-VII.1



as well as excellent (n,γ) agreement

ENDF B-VII.1

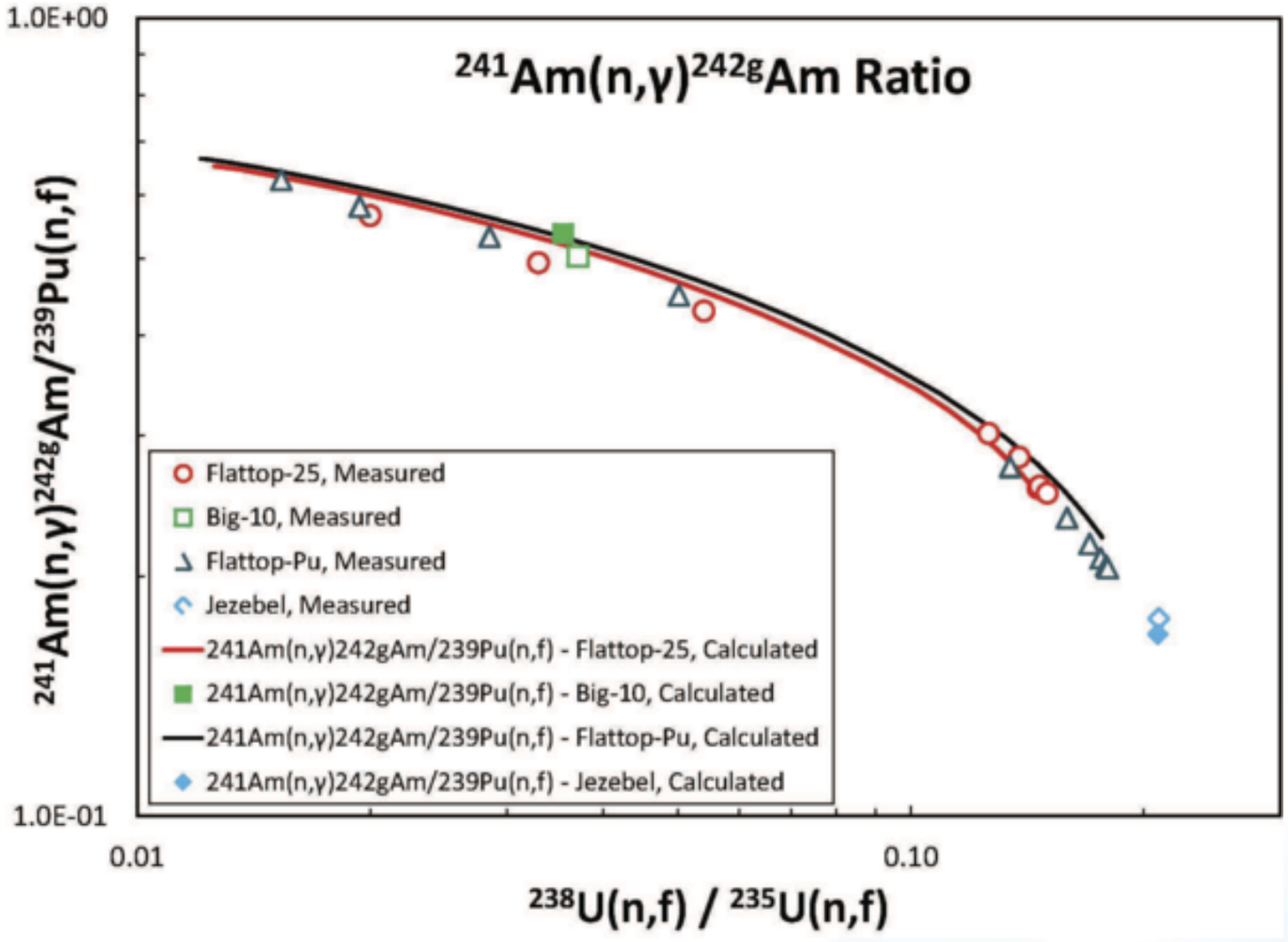
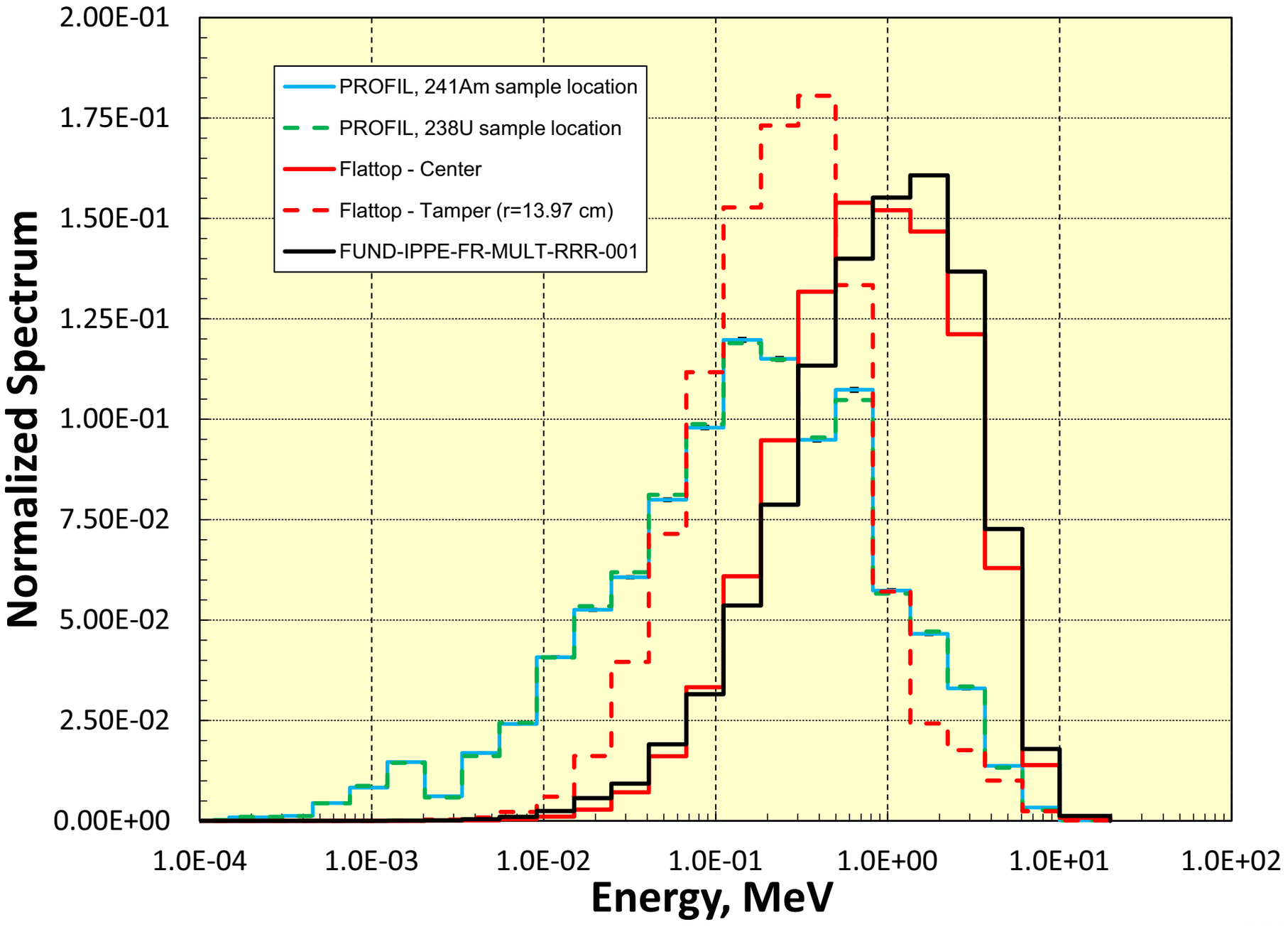


FIG. 93: The integral ^{241}Am neutron capture rate (divided by the ^{239}Pu fission rate) as a function of spectral index for different critical assembly locations. In this case the measurements, which detect the ^{242}Cm are divided by 0.827 to account for the fraction of ^{242g}Am that beta decays to ^{242}Cm.

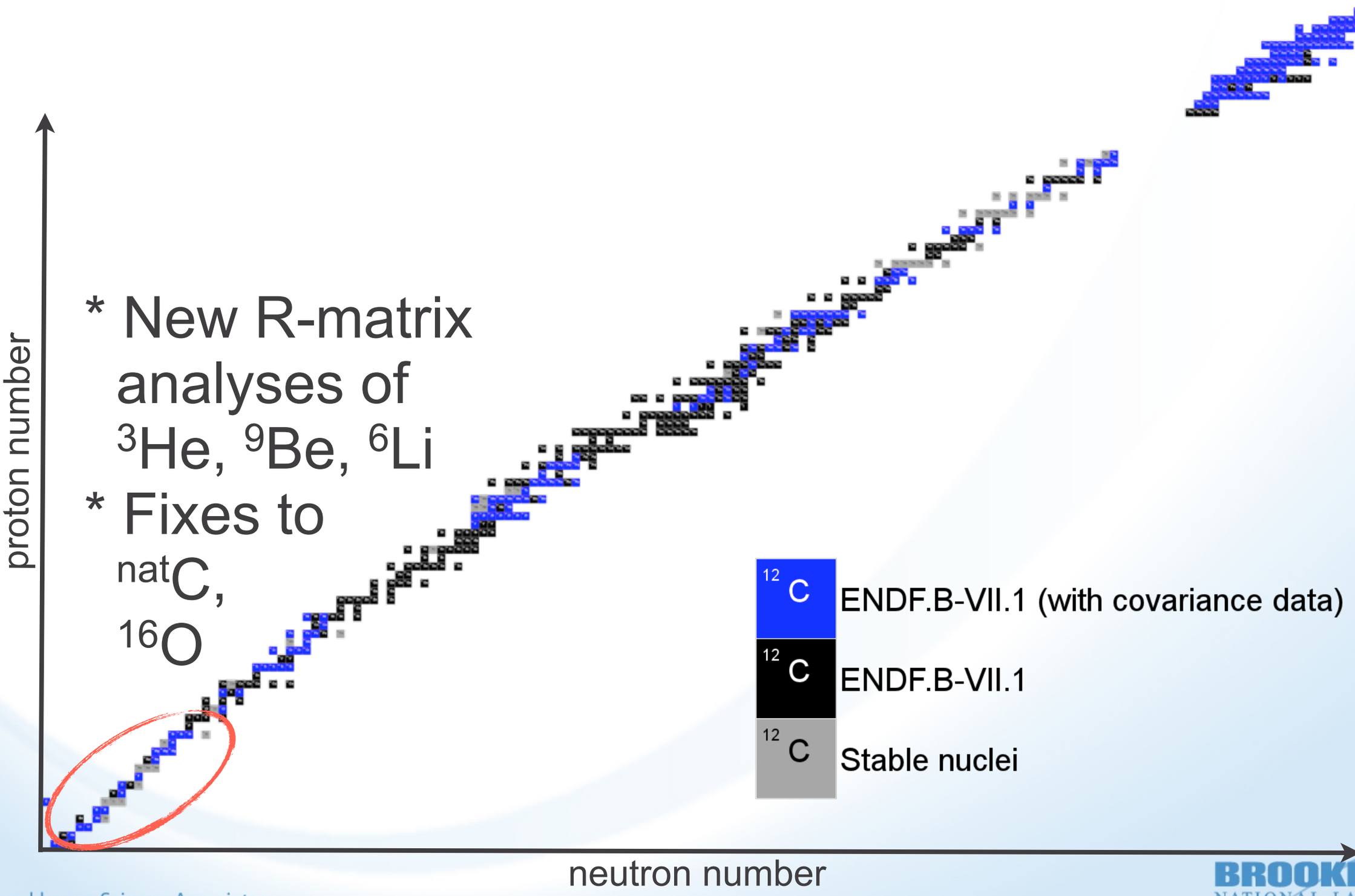
These are the spectra the samples were activated in



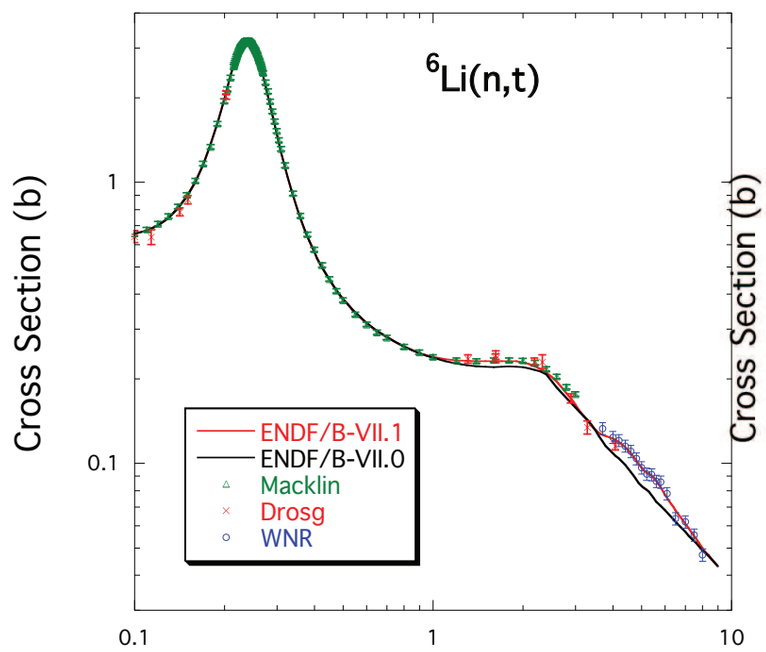
An overview of the library

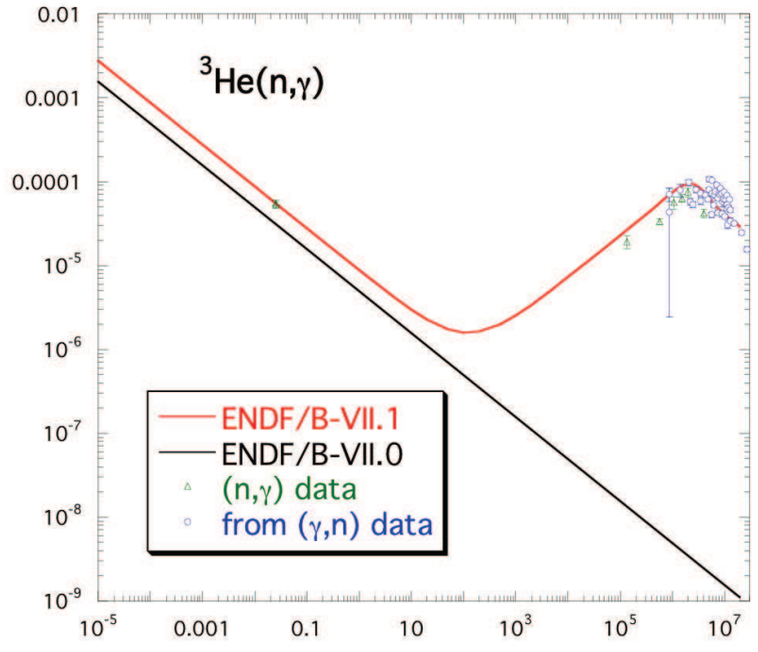
ENDF B-VII.1

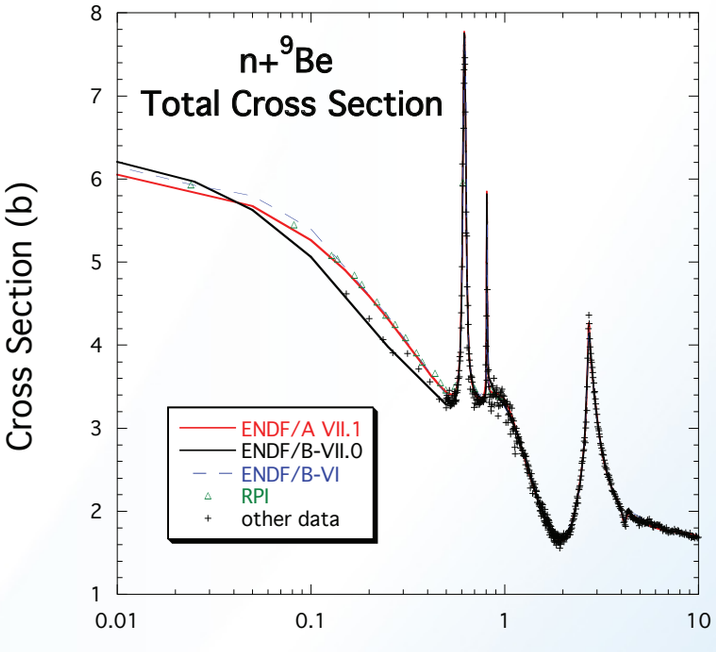
* New R-matrix analyses of ^{3}He, ^{9}Be, ^{6}Li
* Fixes to ^{nat}C, ^{16}O

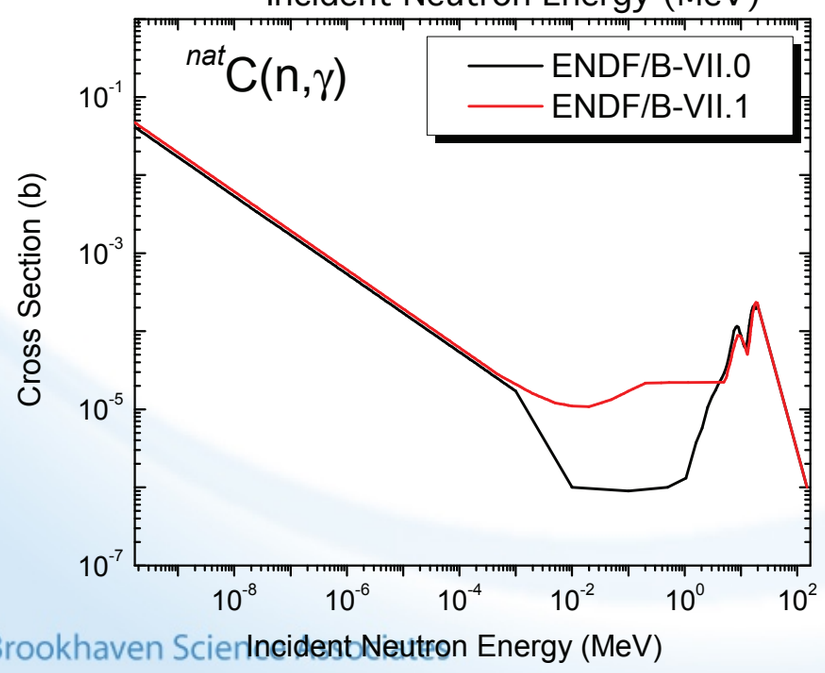


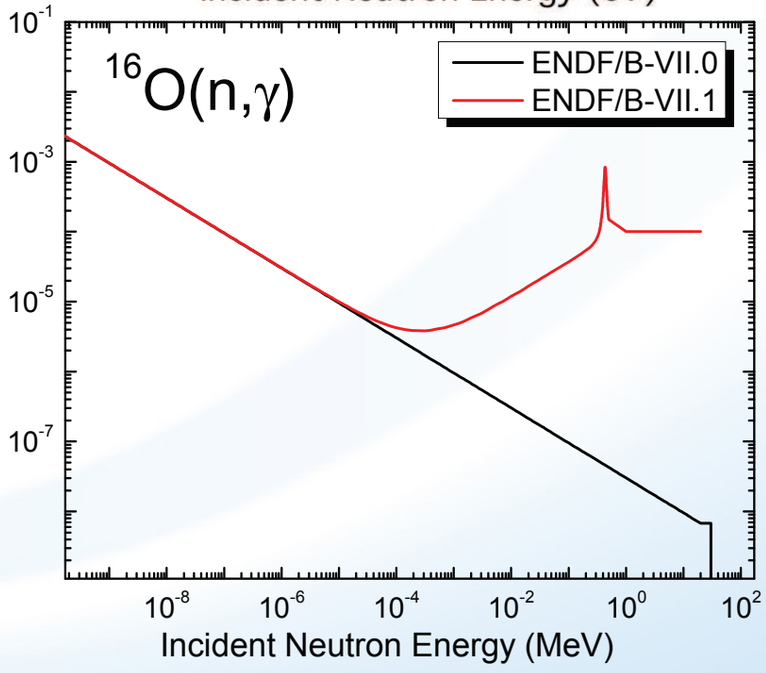
Many of the changes to the light nuclei were quite dramatic

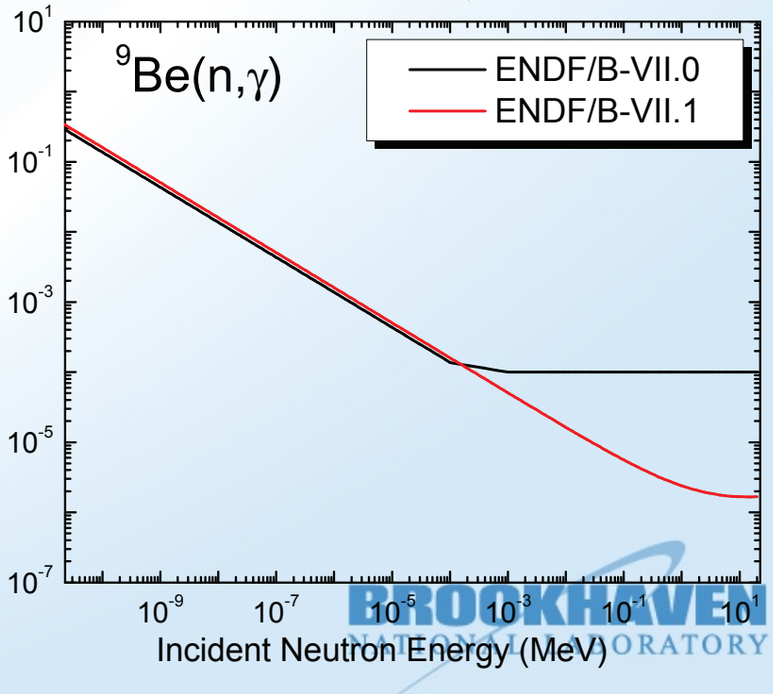












Be is looking good

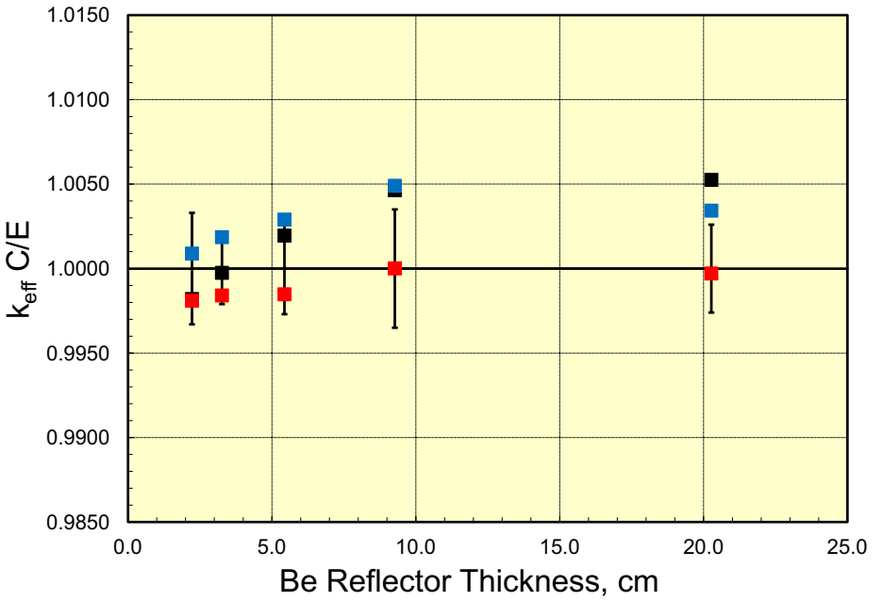


FIG. 6: Calculated eigenvalues with recent ENDF/B cross section libraries (black symbol is ENDF/B-VI.8; red symbol is ENDF/B-VII.0 and blue symbol is ENDF/B-VII.1) for the HMF58 benchmark.

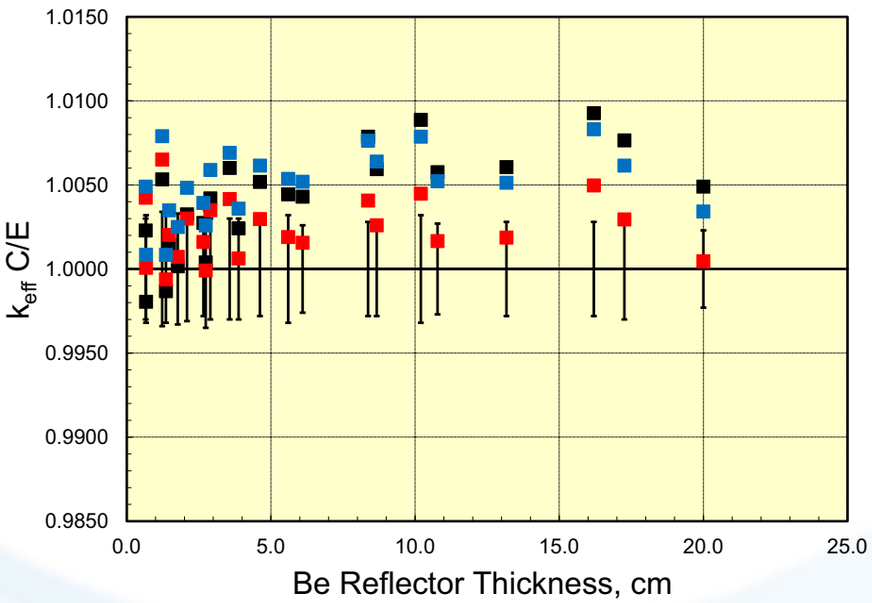


FIG. 7: Calculated eigenvalues with recent ENDF/B cross section libraries (black symbol is ENDF/B-VI.8; red symbol is ENDF/B-VII.0 and blue symbol is ENDF/B-VII.1) for the MMF7 benchmark.

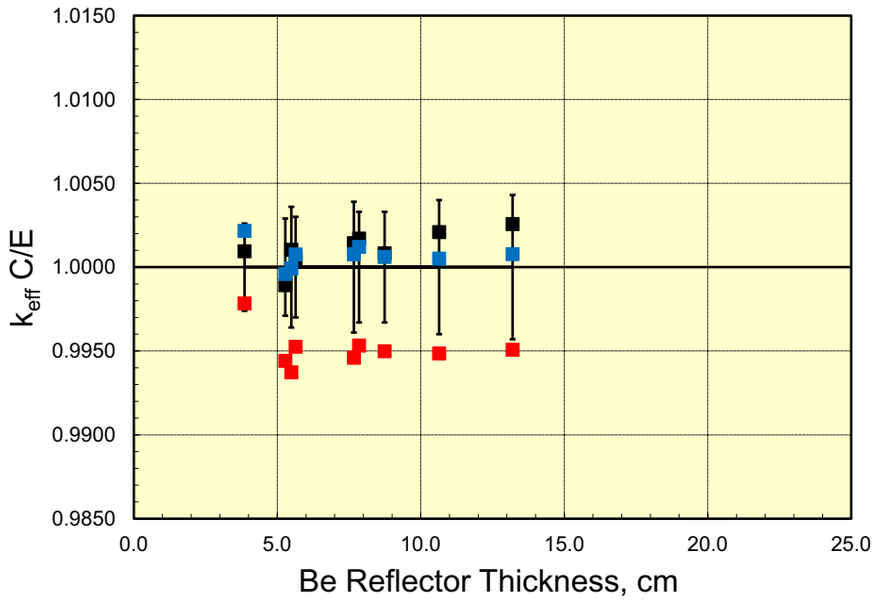


FIG. 8: Calculated eigenvalues with recent ENDF/B cross section libraries (black symbol is ENDF/B-VI.8; red symbol is ENDF/B-VII.0 and blue symbol is ENDF/B-VII.1) for the HMF66 benchmark.

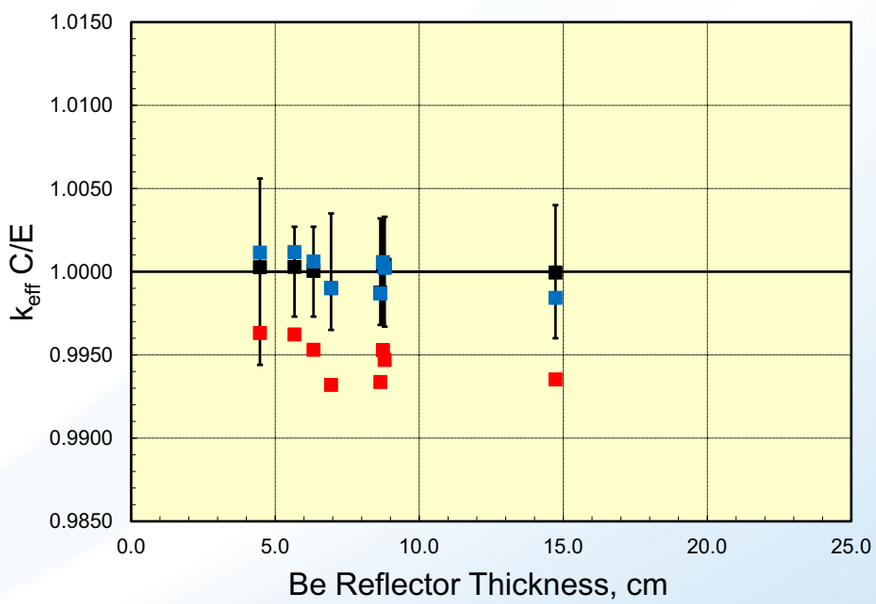
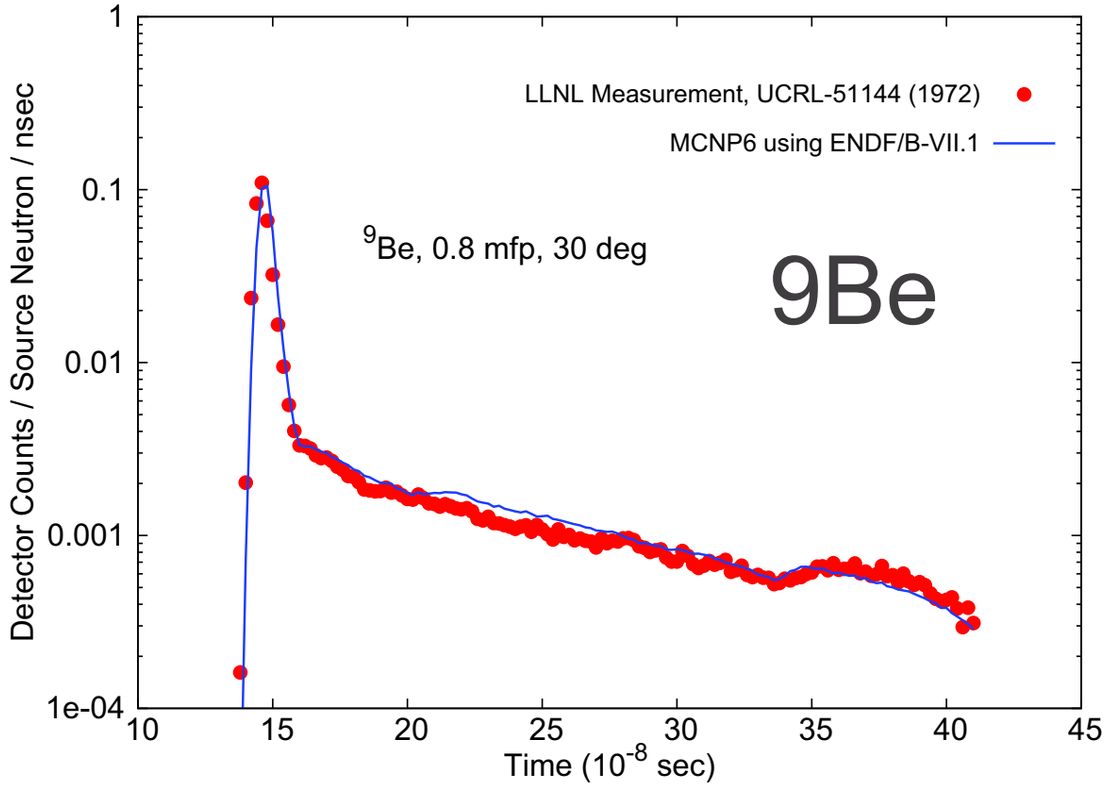
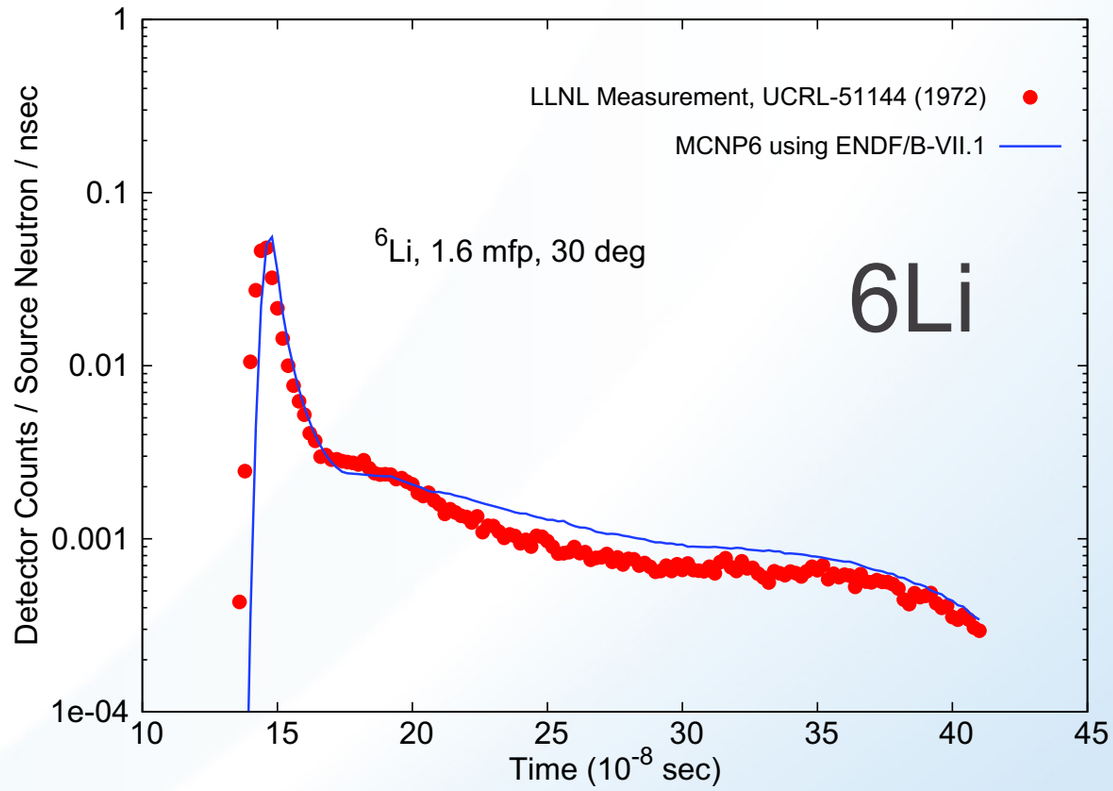


FIG. 9: Calculated eigenvalues with recent ENDF/B cross section libraries (black symbol is ENDF/B-VI.8; red symbol is ENDF/B-VII.0 and blue symbol is ENDF/B-VII.1) for the HMF77 benchmark.

Tests with LLNL Pulsed Spheres (14 MeV pulsed d-t source) indicate ^{9}Be and ^{6}Li performing well





An overview of the library

ENDF B-VII.1

Fission Products and Other Evaluations

1. ^{95}Mo
2. ^{92}Mo
3. ^{99}Tc
4. ^{103}Rh
5. ^{109}Ag
6. ^{133}Cs
7. ^{143}Nd
8. ^{145}Nd
9. ^{147}Nd
10. ^{147}Sm
11. ^{149}Sm
12. ^{152}Sm
13. ^{153}Eu
14. ^{58}Co
15. ^{62}Ni
16. Zr
17. ^{113}Cd
18. ^{157}Gd

Structural Material Evaluations

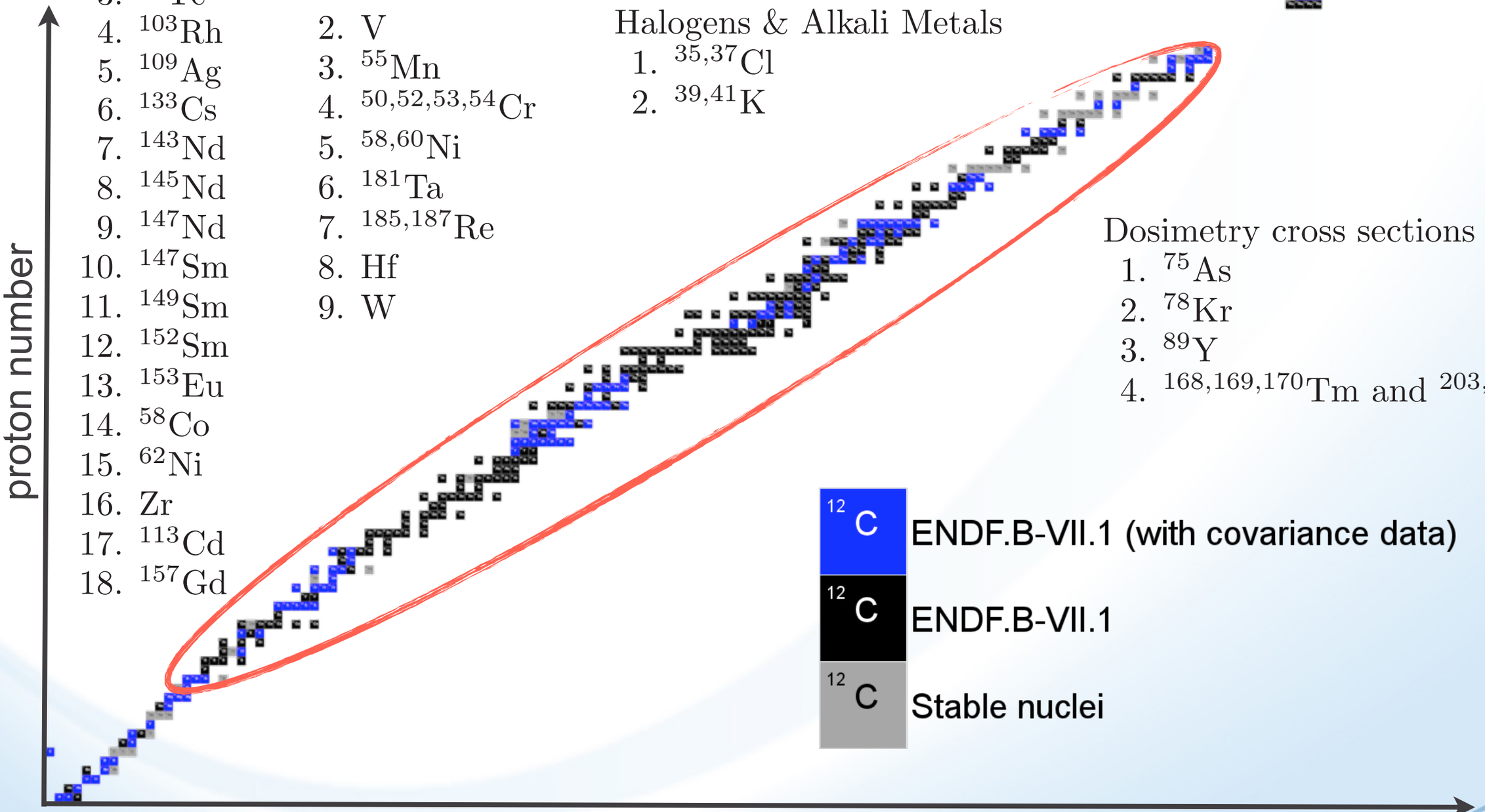
1. Ti
2. V
3. ^{55}Mn
4. ^{50,52,53,54}Cr
5. ^{58,60}Ni
6. ^{181}Ta
7. ^{185,187}Re
8. Hf
9. W

Halogens & Alkali Metals

1. ^{35,37}Cl
2. ^{39,41}K

Dosimetry cross sections

1. ^{75}As
2. ^{78}Kr
3. ^{89}Y
4. ^{168,169,170}Tm and ^{203,205}Tl



An overview of the library

ENDF B-VII.1

Fission Products and Other Evaluations

1. ^{95}Mo
2. ^{92}Mo
3. ^{99}Tc
4. ^{103}Rh
5. ^{109}Ag
6. ^{133}Cs
7. ^{143}Nd
8. ^{145}Nd
9. ^{147}Nd
10. ^{147}Sm
11. ^{149}Sm
12. ^{152}Sm
13. ^{153}Eu
14. ^{58}Co
15. ^{62}Ni
16. Zr
17. ^{113}Cd
18. ^{157}Gd

Structural Material Evaluations

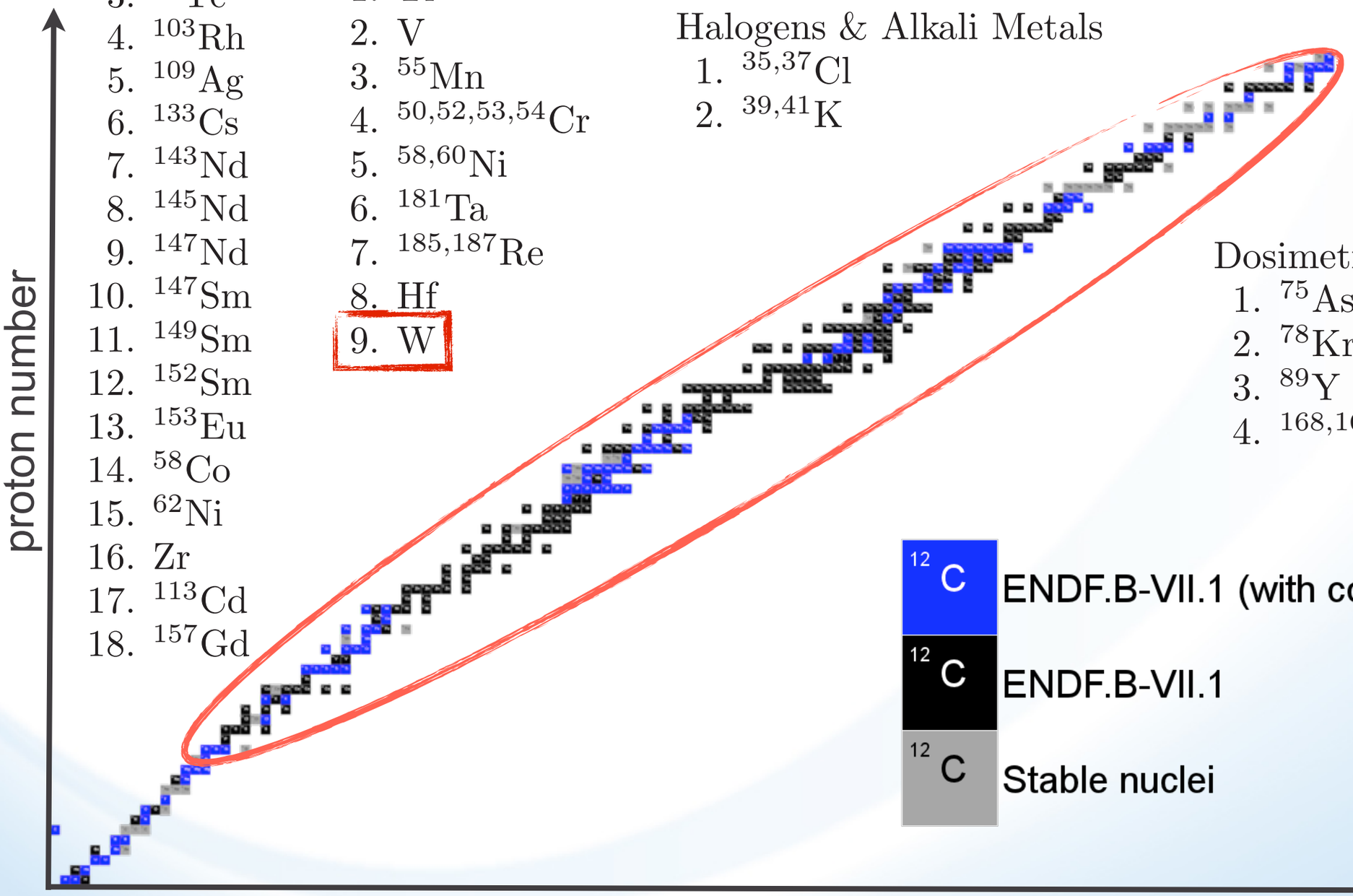
1. Ti
2. V
3. ^{55}Mn
4. ^{50,52,53,54}Cr
5. ^{58,60}Ni
6. ^{181}Ta
7. ^{185,187}Re
8. Hf
9. W

Halogens & Alkali Metals

1. ^{35,37}Cl
2. ^{39,41}K

Dosimetry cross sections

1. ^{75}As
2. ^{78}Kr
3. ^{89}Y
4. ^{168,169,170}Tm and ^{203,205}Tl



^{12}C ENDF.B-VII.1 (with covariance data)

^{12}C ENDF.B-VII.1

^{12}C Stable nuclei

EMPIRE-GANDR system used for ^{55}Mn, W and ^{232}Th

ENDF B-VII.1

Available online at www.sciencedirect.com

SciVerse ScienceDirect

Nuclear Data Sheets

Nuclear Data Sheets 112 (2011) 3098–3119

www.elsevier.com/locate/nds

Covariances of Evaluated Nuclear Cross Section Data for ^{232}Th, ^{180,182,183,184,186}W and ^{55}Mn

A. Trkov,[1] R. Capote*,[2] E.Sh. Soukhovitskii,[3] L.C. Leal,[4] M. Sin,[5] I. Kodeli,[1] and D.W. Muir[6]

[1] *Jožef Stefan Institute, Jamova 39, 1000 Ljubljana, Slovenia*
[2] *NAPC–Nuclear Data Section, International Atomic Energy Agency, P.O. Box 100, A–1400 Vienna, Austria*
[3] *Joint Institute for Power and Nuclear Research – Sosny, BY-220109 Minsk, Belarus*
[4] *Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6171, USA*
[5] *Nuclear Physics Department, Bucharest University, 077125 Bucharest-Magurele, Romania*
[6] *Special Term Appointee, Argonne National Laboratory, 9229 Rosewater Lane, Jacksonville, FL 32256, USA*

(Received 31 August 2011; revised received 27 September 2011; accepted 10 October 2011)

The EMPIRE code system is a versatile package for nuclear model calculations that is often used for nuclear data evaluation. Its capabilities include random sampling of model parameters, which can be utilised to generate a full covariance matrix of all scattering cross sections, including cross-reaction correlations. The EMPIRE system was used to prepare the prior covariance matrices of reaction cross sections of ^{232}Th, ^{180,182,183,184,186}W and ^{55}Mn nuclei for incident neutron energies up to 60 MeV. The obtained modelling prior was fed to the GANDR system, which is a package for a global assessment of nuclear data, based on the Generalised Least-Squares method. By introducing experimental data from the EXFOR database into GANDR, the constrained covariance matrices and cross section adjustment functions were obtained. Applying the correction functions on the cross sections and formatting the covariance matrices, the final evaluations in ENDF-6 format including covariances were derived. In the resonance energy range, separate analyses were performed to determine the resonance parameters with their respective covariances. The data files thus obtained were then subjected to detailed testing and validation. Described evaluations with covariances of ^{232}Th, ^{180,182,183,184,186}W and ^{55}Mn nuclei are included into the ENDF/B-VII.1 library release.

Contents

I. INTRODUCTION 3098
A. Overview of the Evaluations 3099

II. COVARIANCE EVALUATION METHODOLOGY 3100
A. Resonance Region 3100
B. Fast Neutron Region: Uncertainty of the Reaction Models and Model-Parameter Uncertainties 3100
C. Combining Modelling Uncertainty and Experimental Data: GANDR System 3102
D. Cross-Reaction and Cross-Material Covariances 3103
E. Covariance Formats and Data Processing 3103

III. EVALUATION OF THORIUM 3103
A. EMPIRE Model Calculations 3103
B. Selection of Experimental Data 3104
C. Analysis of Obtained Covariances 3106

IV. EVALUATION OF TUNGSTEN ISOTOPES 3106
A. EMPIRE Model Calculations 3106
B. Selection of Experimental Data 3107
1. ^{180}W 3107
2. ^{182}W 3108
3. ^{183}W 3109
4. ^{184}W 3111
5. ^{186}W 3112
C. Analysis of Obtained Covariances 3112

V. EVALUATION OF MANGANESE 3115
A. EMPIRE Model Calculations 3115
B. Selection of Experimental Data 3116
C. Analysis of Obtained Covariances 3116

VI. SUMMARY AND CONCLUSIONS 3117

Acknowledgments 3117

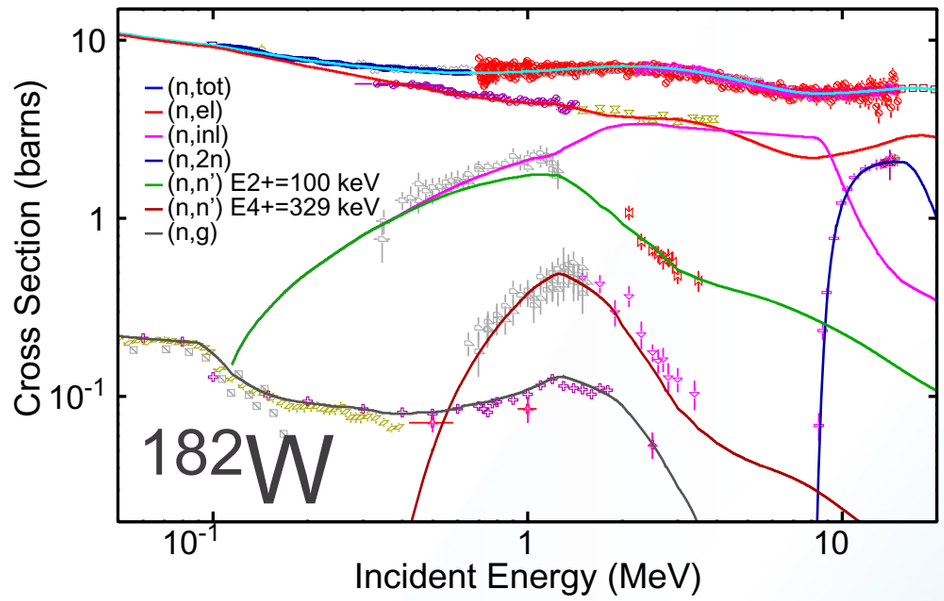
References 3118

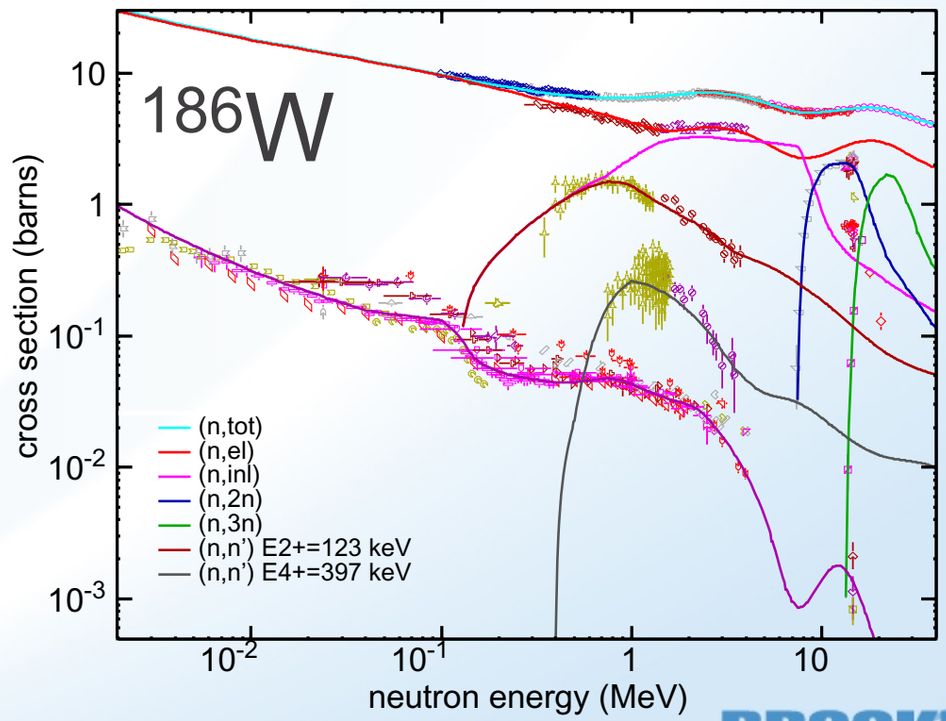
I. INTRODUCTION

In the early days of nuclear technology the designers were relying on experimental mockups to test new con-

*Corresponding author: r.capotenoy@iaea.org

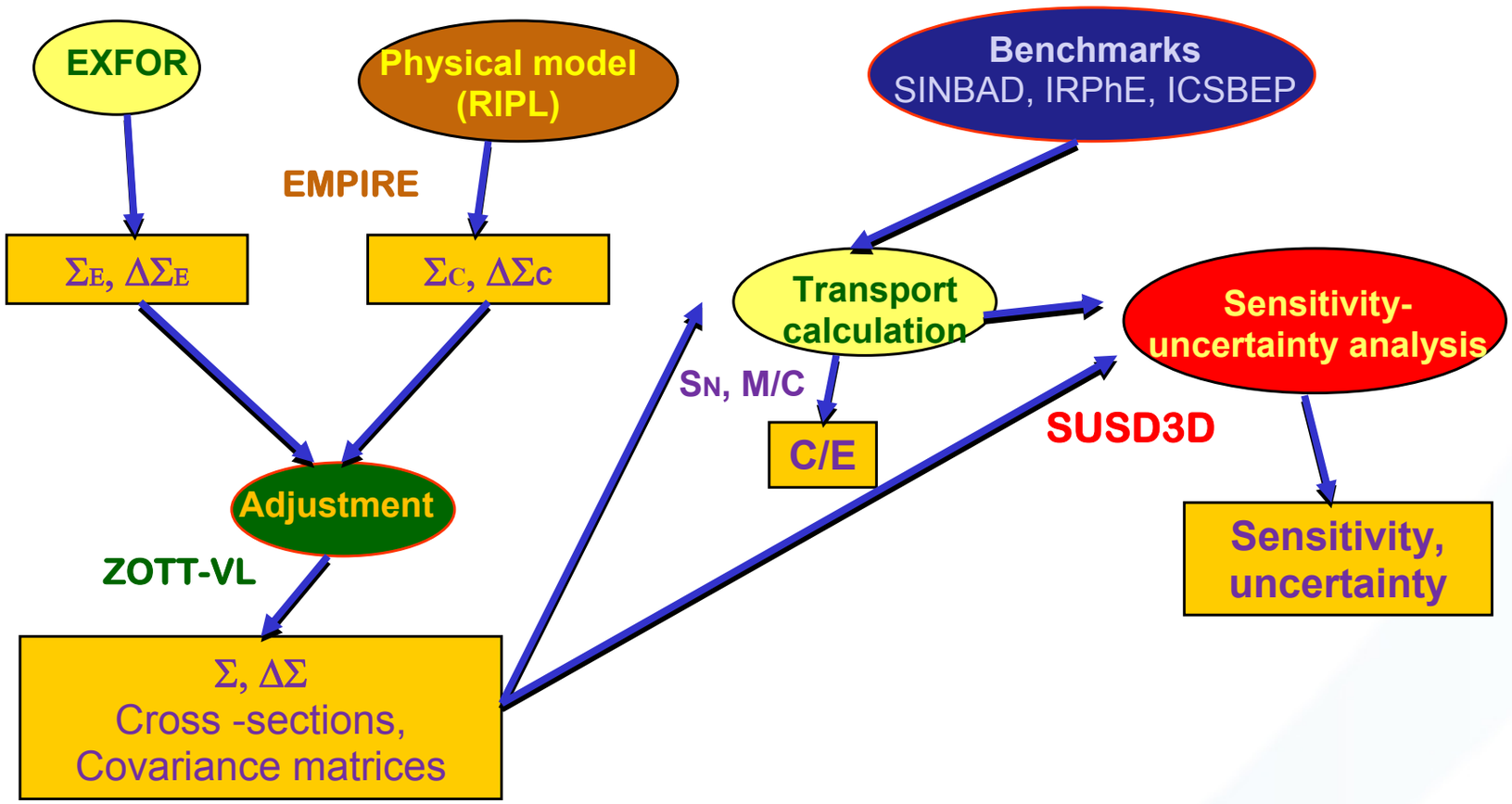
doi:10.1016/j.nds.2011.11.007





A. Trkov, R. Capote, E. Soukhovitskii, et al., "Covariances of Evaluated Nuclear Cross Section Data for 232Th, 180,182,183,184,186W and 55Mn", Nuclear Data Sheets, 112(12): 3098-3119 (2011).

EMPIRE+GANDR system is a hybrid

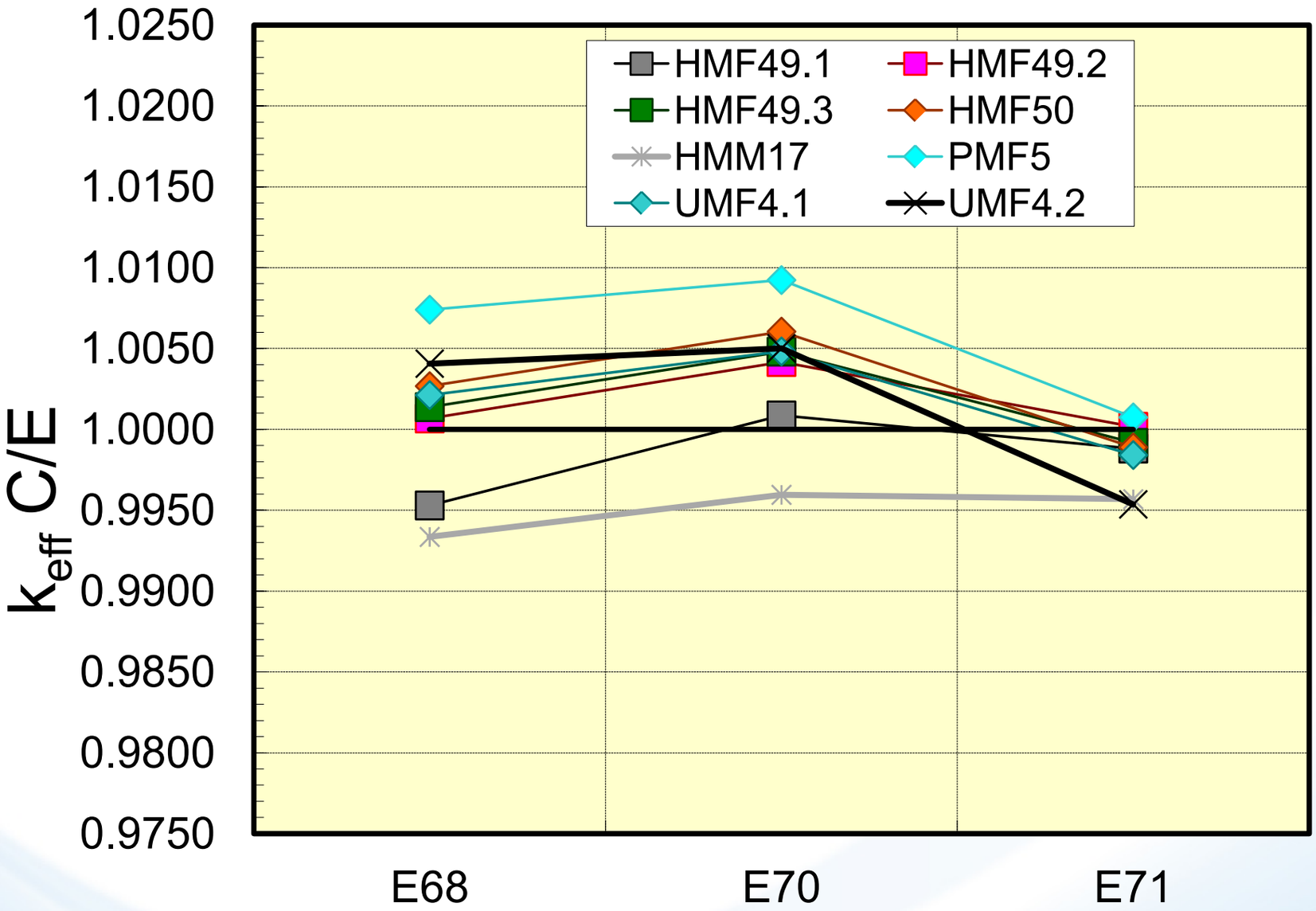


D.W. Muir, ***GANDR*** *project (IAEA),* Online at www-nds.iaea.org/gandr/.

A. Trkov and R. Capote, "Cross-Section Covariance Data", Th-232 evaluation for ENDF/B-VII.0 (MAT=9040 MF=1 MT=451); Pa-231 and Pa-233 evaluations for ENDF/B-VII.0 (MAT=9133 and 9137 MF=1 MT=451), National Nuclear Data Center, BNL (http://www.nndc.bnl.gov), 15 December 2006.

Slide from R. Capote

Benchmarks with W are significantly improved



E71 Calculated Eigenvalue Spread is significantly reduced compared to E70 or E68.

Revised W evaluations were contributed to the ENDF/B community by the IAEA.

An overview of the library

ENDF B-VII.1

Fission Products and Other Evaluations

1. ^{95}Mo
2. ^{92}Mo
3. ^{99}Tc
4. ^{103}Rh
5. ^{109}Ag
6. ^{133}Cs
7. ^{143}Nd
8. ^{145}Nd
9. ^{147}Nd
10. ^{147}Sm
11. ^{149}Sm
12. ^{152}Sm
13. ^{153}Eu
14. ^{58}Co
15. ^{62}Ni
16. Zr
17. ^{113}Cd
18. ^{157}Gd

Structural Material Evaluations

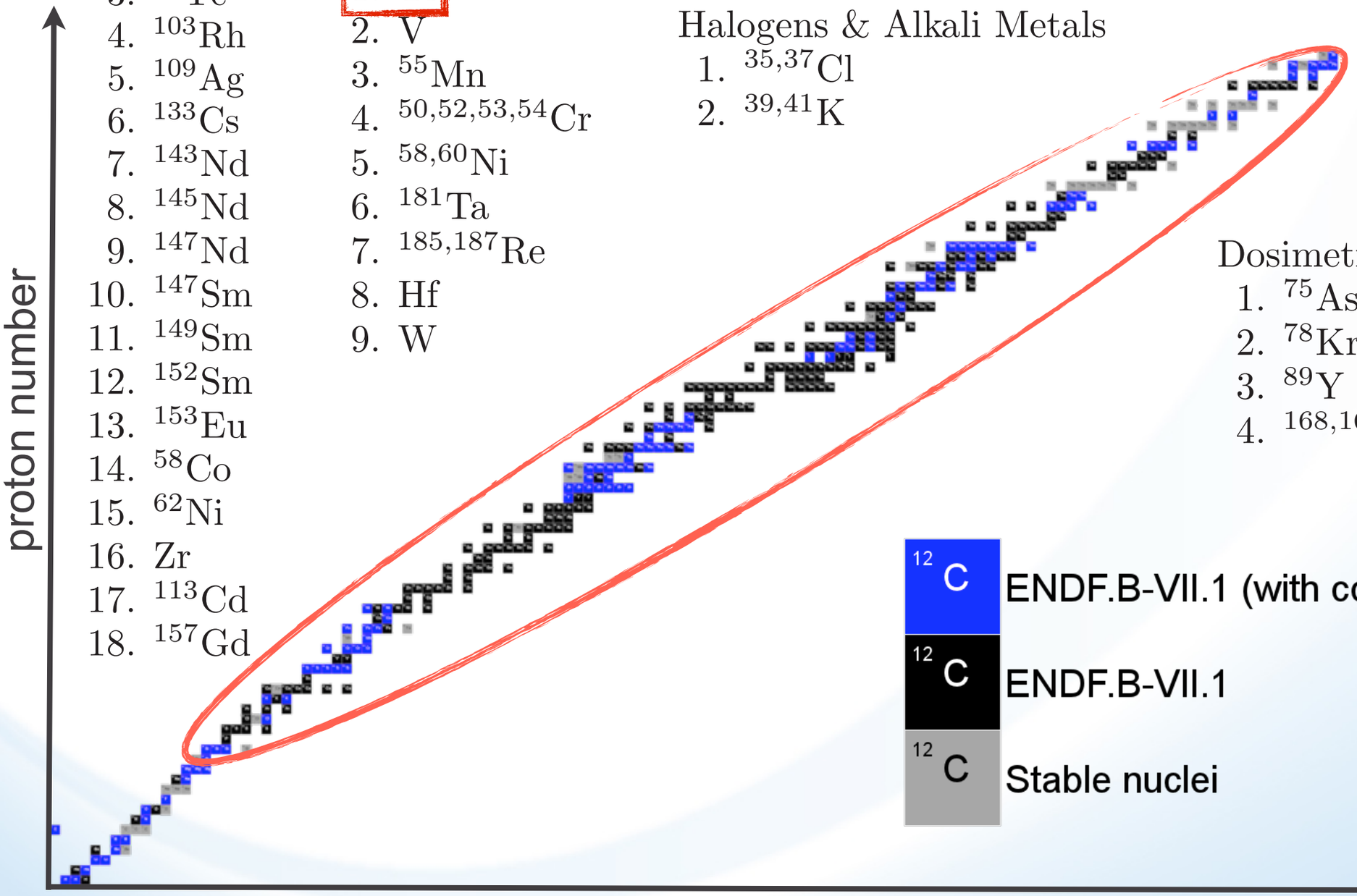
1. Ti
2. V
3. ^{55}Mn
4. ^{50,52,53,54}Cr
5. ^{58,60}Ni
6. ^{181}Ta
7. ^{185,187}Re
8. Hf
9. W

Halogens & Alkali Metals

1. ^{35,37}Cl
2. ^{39,41}K

Dosimetry cross sections

1. ^{75}As
2. ^{78}Kr
3. ^{89}Y
4. ^{168,169,170}Tm and ^{203,205}Tl



^{12}C ENDF.B-VII.1 (with covariance data)

^{12}C ENDF.B-VII.1

^{12}C Stable nuclei

New RRR for Ti;
Revert (n,el) angular dist. to E6.8

ENDF B-VII.1

TABLE XI: Thermal cross sections and their uncertainties for ^{48}Ti+n in barns.

Isotope	Cross Section	VII.1	VII.0	Atlas
^{48}Ti	Capture	8.32±0.23	7.84	8.32±0.16
	Total	12.35±0.30	12.16	12.42±0.25
	Scattering	4.03±0.17	4.32	4.10±0.20

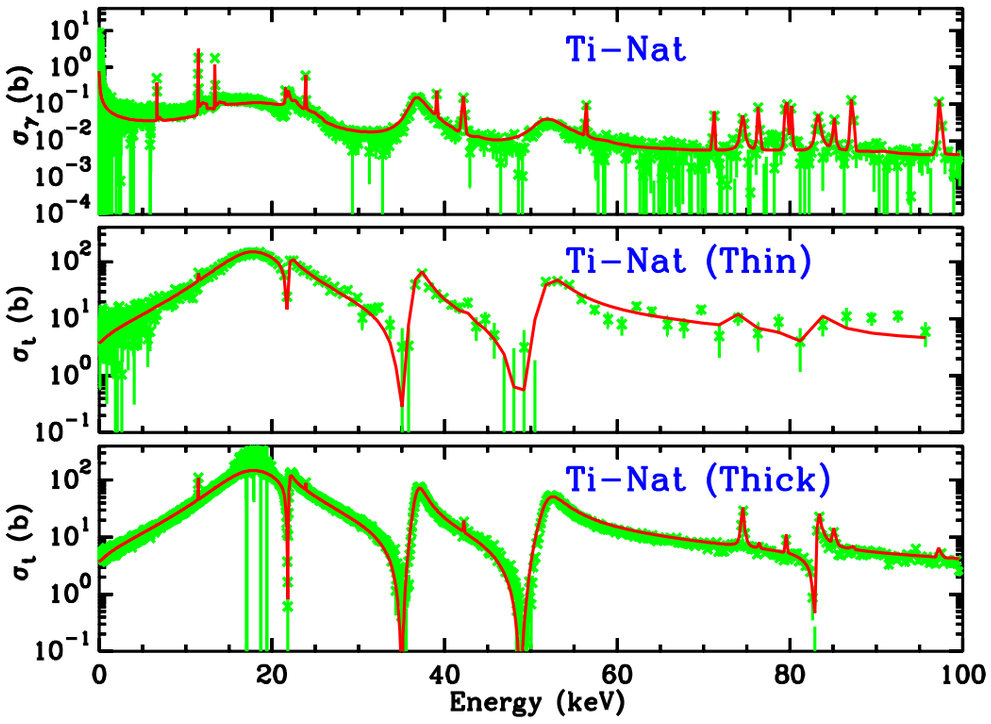
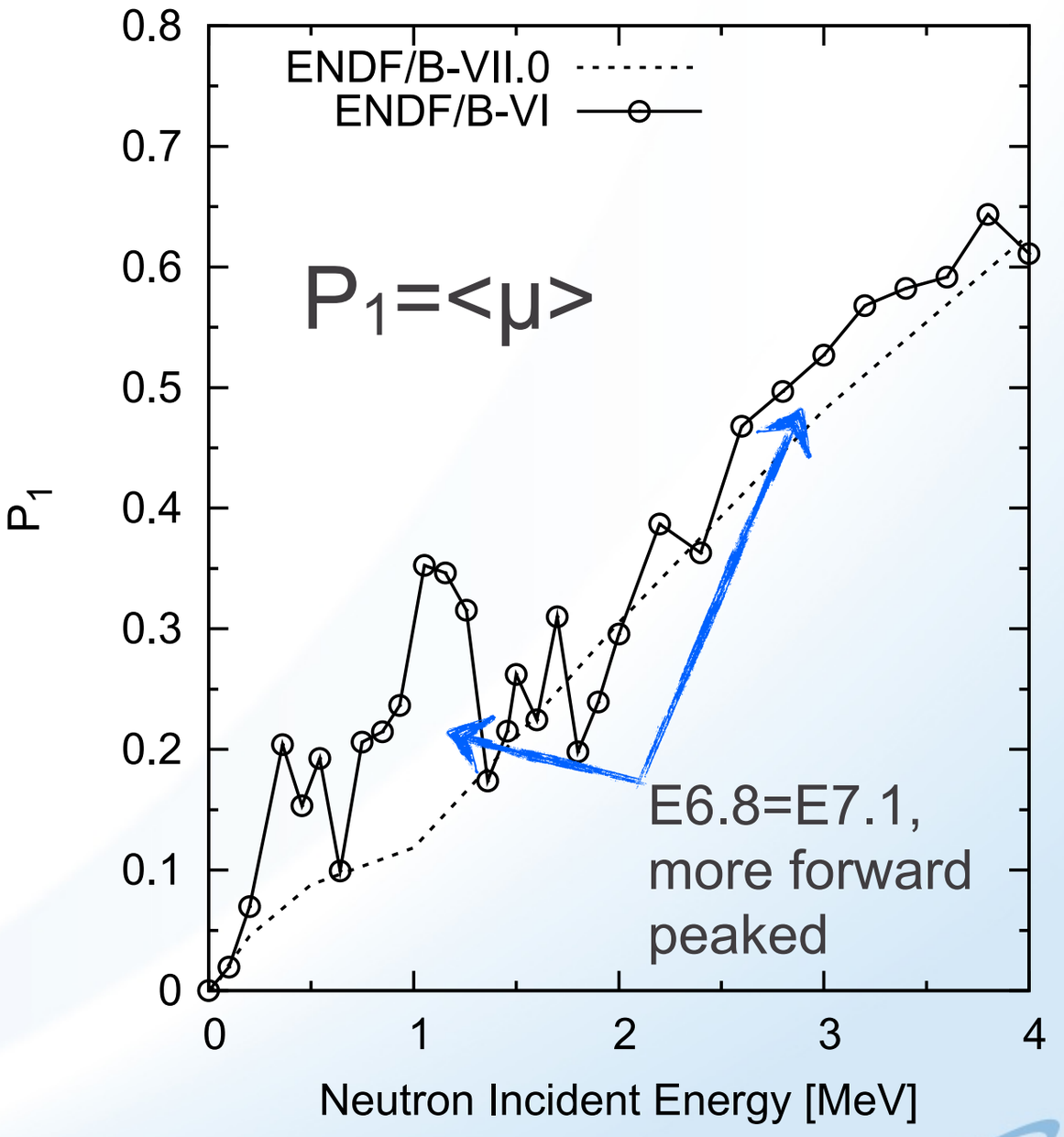
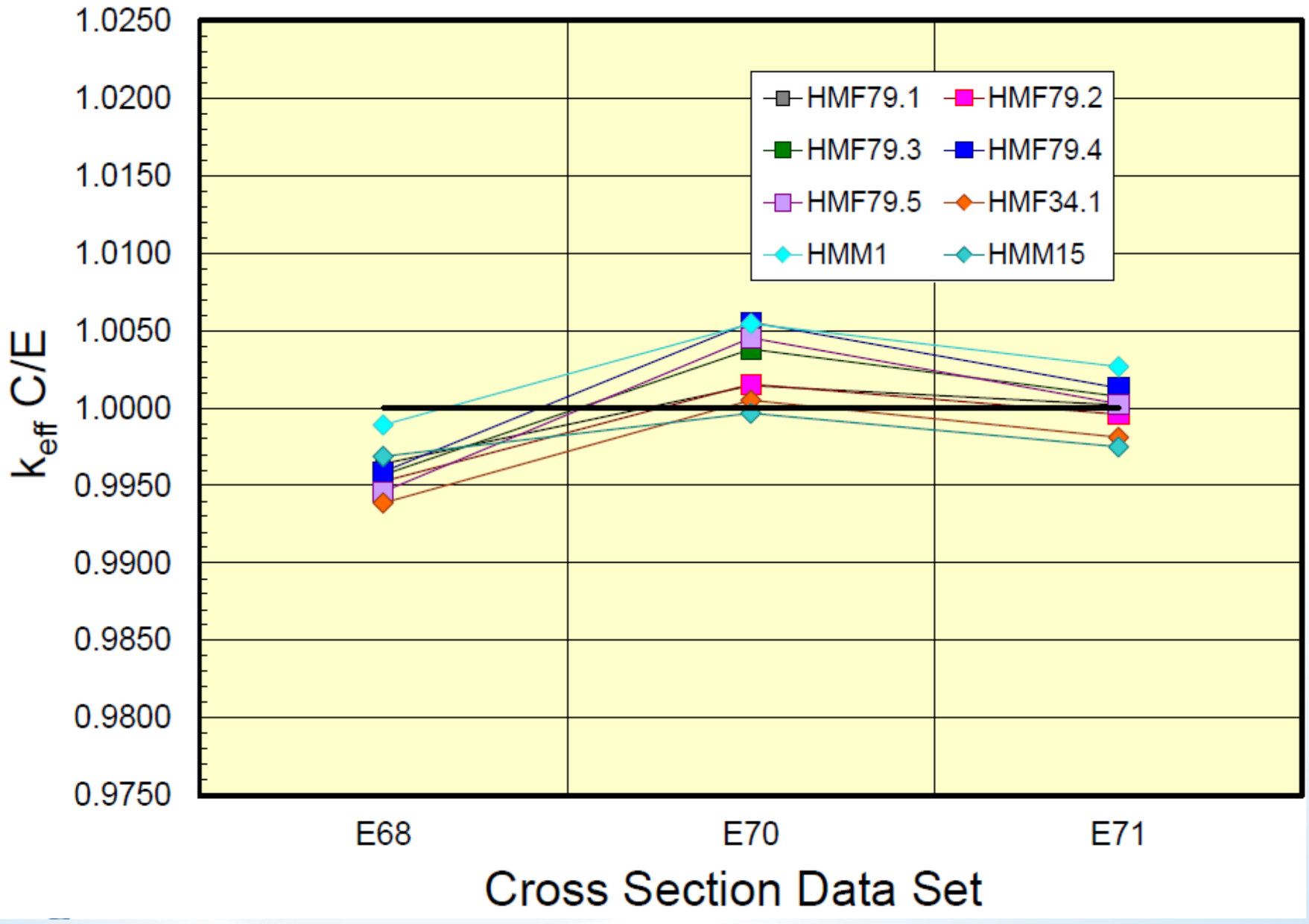


FIG. 13: Comparisons of SAMMY calculations with the resonance parameters of the total and capture cross-sections of natural titanium in the energy region 10 eV to 100 keV.



These changes pushed Ti into the sweet spot



Ti bearing assemblies

ENDF/B-VI.8 is “too cold”

ENDF/B-VII.0 is “too hot”

ENDF/B-VII.1 is “just right”!

An overview of the library

ENDF B-VII.1

Fission Products and Other Evaluations

1. ^{95}Mo
2. ^{92}Mo
3. ^{99}Tc
4. ^{103}Rh
5. ^{109}Ag
6. ^{133}Cs
7. ^{143}Nd
8. ^{145}Nd
9. ^{147}Nd
10. ^{147}Sm
11. ^{149}Sm
12. ^{152}Sm
13. ^{153}Eu
14. ^{58}Co
15. ^{62}Ni
16. Zr
17. ^{113}Cd
18. ^{157}Gd

Structural Material Evaluations

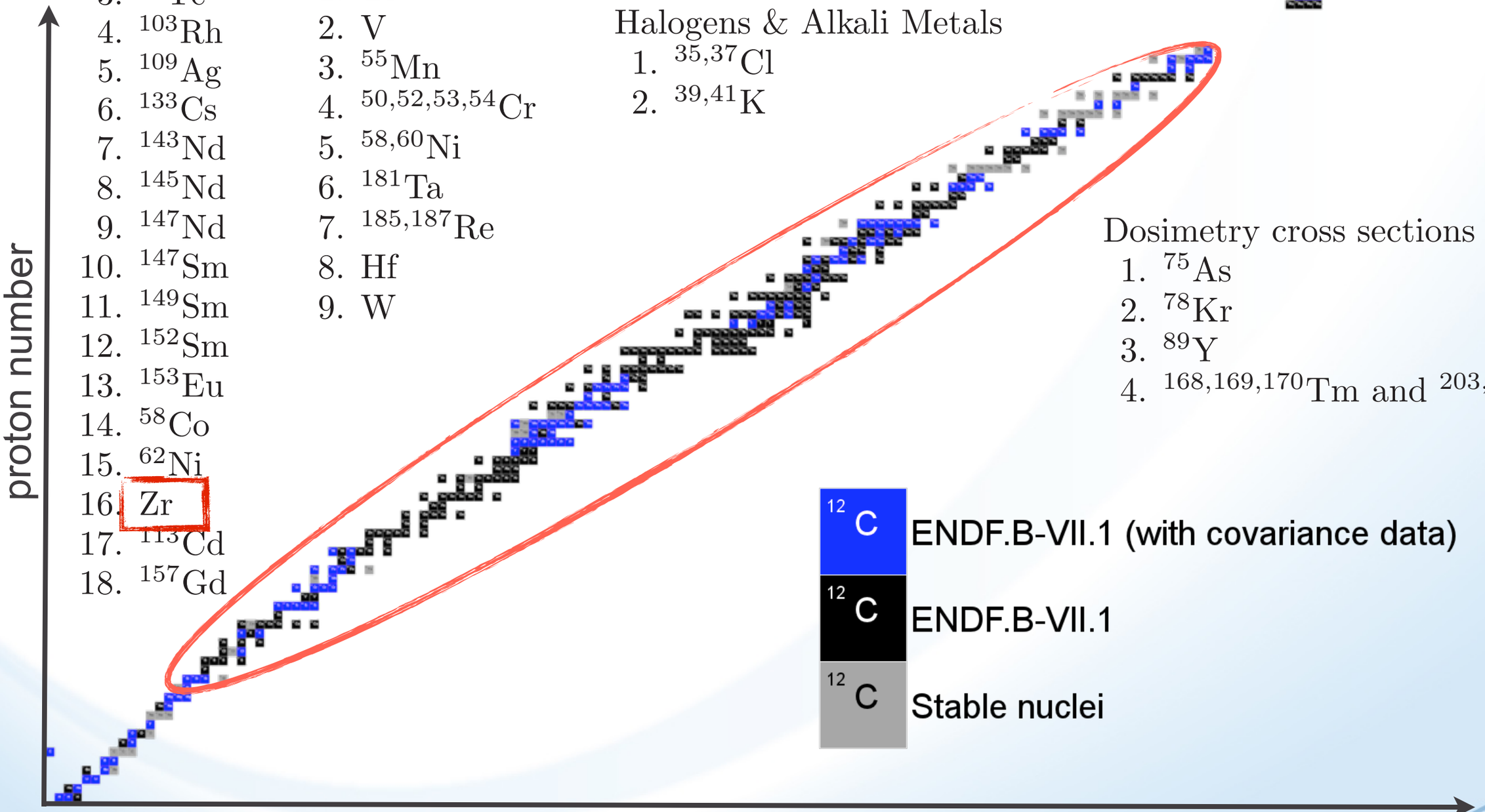
1. Ti
2. V
3. ^{55}Mn
4. ^{50,52,53,54}Cr
5. ^{58,60}Ni
6. ^{181}Ta
7. ^{185,187}Re
8. Hf
9. W

Halogens & Alkali Metals

1. ^{35,37}Cl
2. ^{39,41}K

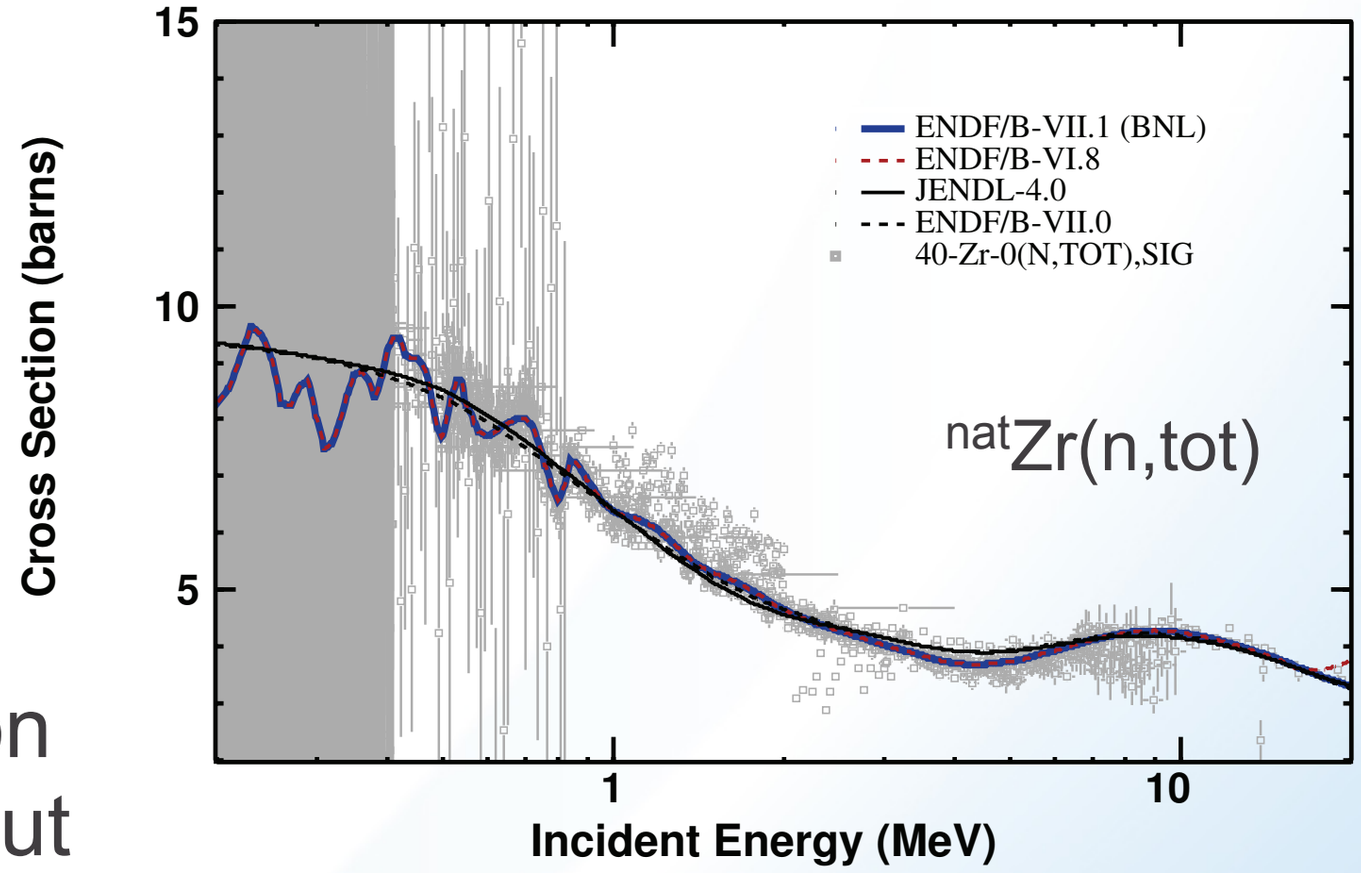
Dosimetry cross sections

1. ^{75}As
2. ^{78}Kr
3. ^{89}Y
4. ^{168,169,170}Tm and ^{203,205}Tl



Zr needed to be reworked for ENDF/B-VII.1

- ENDF/B-VI.8 fitted ^{nat}Zr(n,tot), but missed outgoing dists.
- ENDF/B-VII.0 is EMPIRE evaluation, but not fitted
- Attempted re-evaluation for ENDF/B-VII beta, but that version tested poorly
  - Leakage problems (not leaky enough!)
  - Suspected problem (n,el) angular distributions
  - Lead evaluator had health issues that prevented him from fixing evaluation



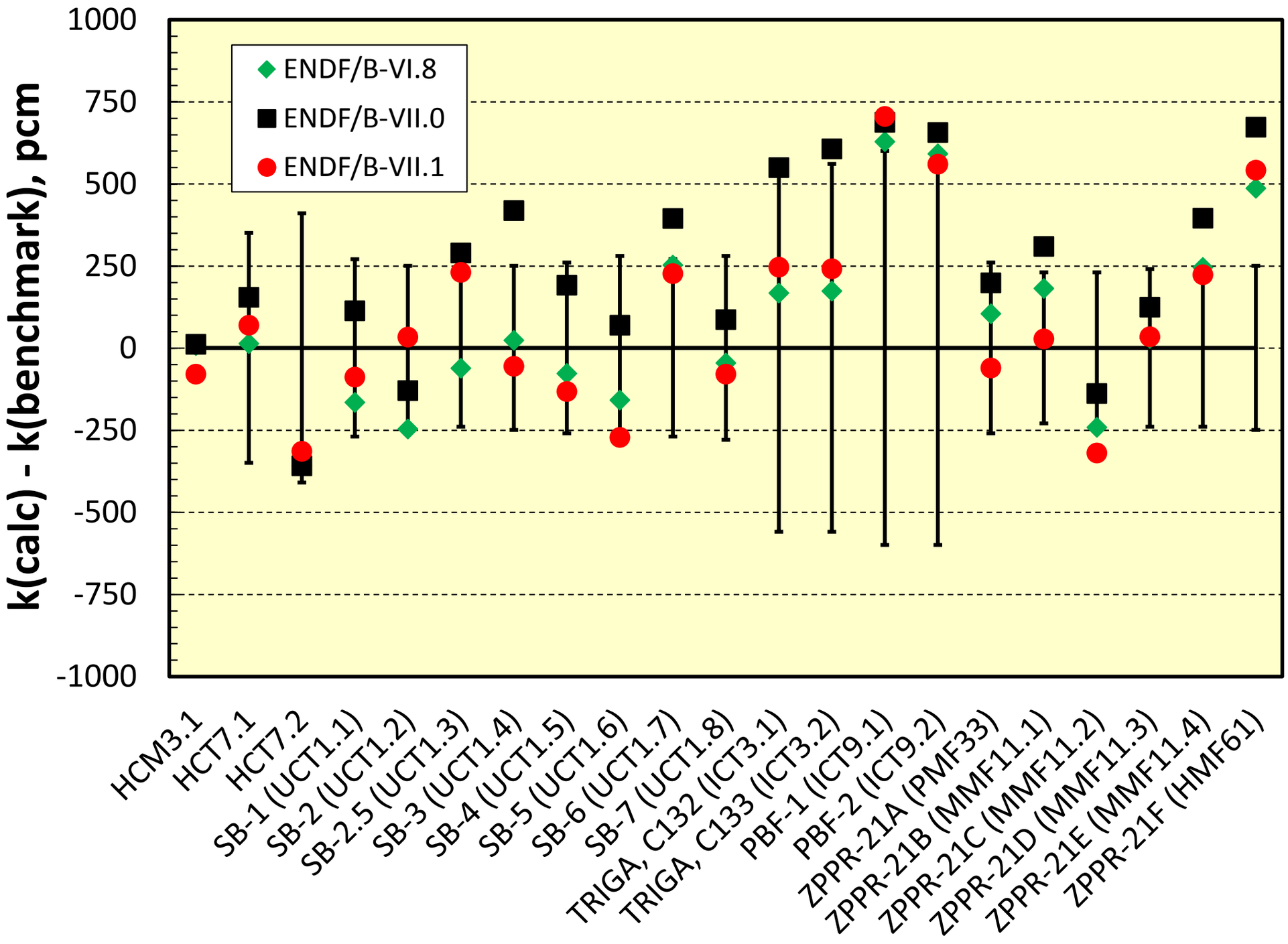
We took over the evaluation and made a few key changes

ENDF B-VII.1

- Found backward peaked low energy neutron dists. - now patched using JENDL-4
- S. Mughabghab reevaluated the RRR:
  - ^{90}Zr all new
  - ^{91}Zr first pass at fixes

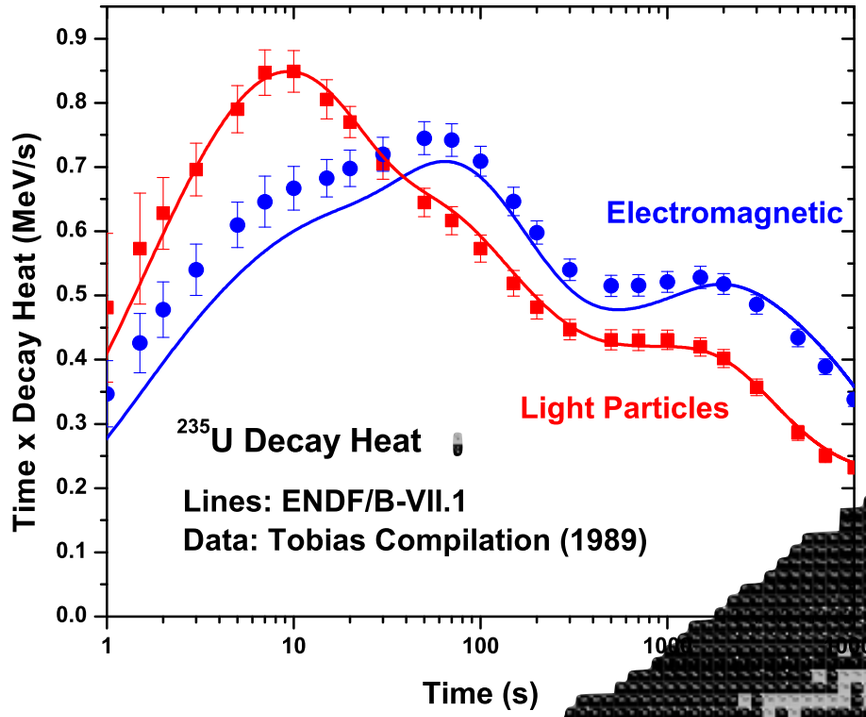
Reaction	^{90}Zr σ_T (barn)	^{90}Zr I_γ (barn)	^{91}Zr σ_T (barn)	^{91}Zr I_γ (barn)
Total	5.50762	-	11.0729	-
Elastic	5.49765	-	9.85728	-
Capture	9.97256×10^{-3}	0.132506	1.21566	6.0062

New Zr evaluations perform well in TRIGA and ZPR assemblies



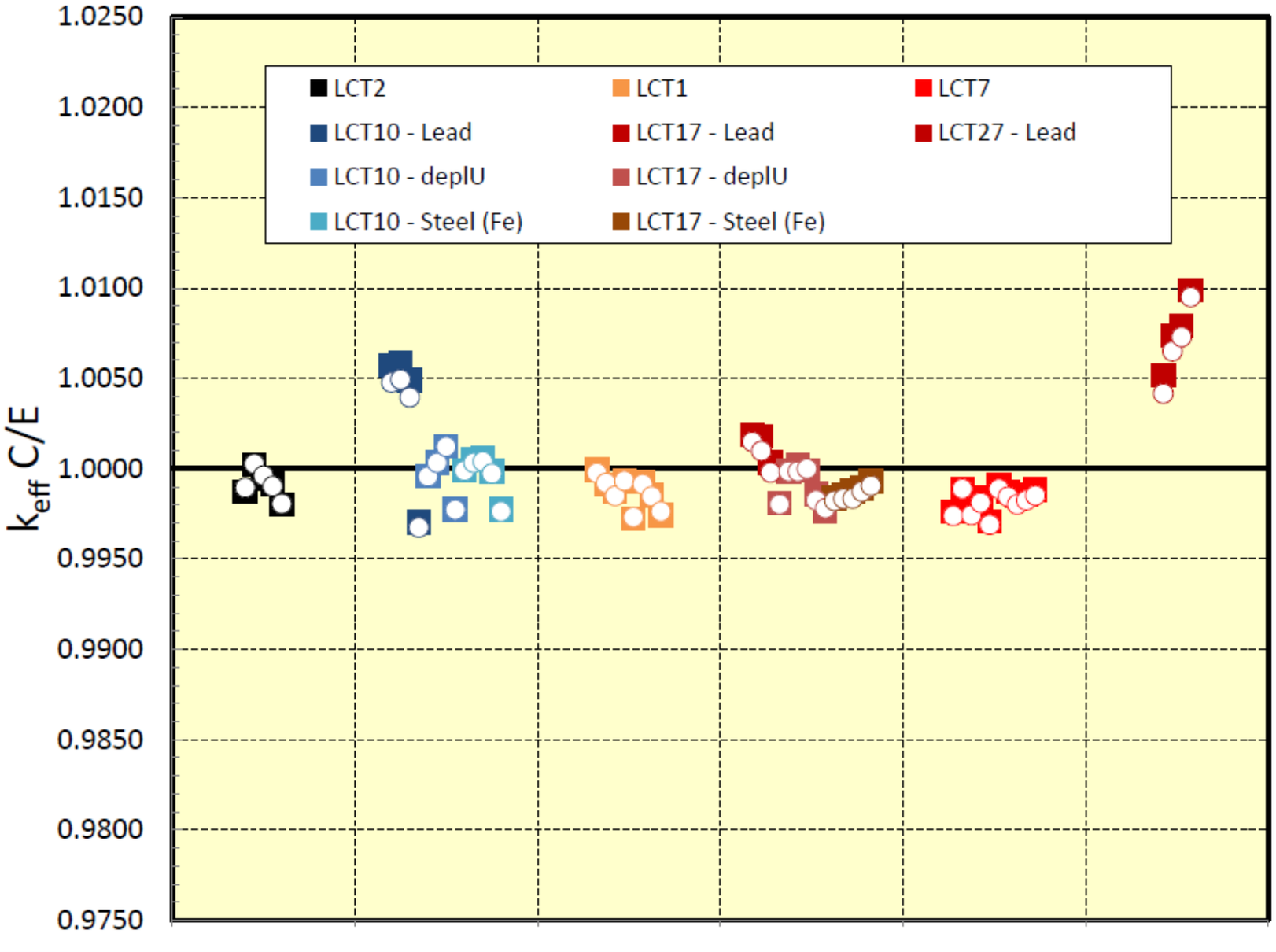
New decay sublibrary enables more accurate decay heat calculations

ENDF B-VII.1



Despite all these improvements, there is still work to be done: Pb

ENDF B-VII.1



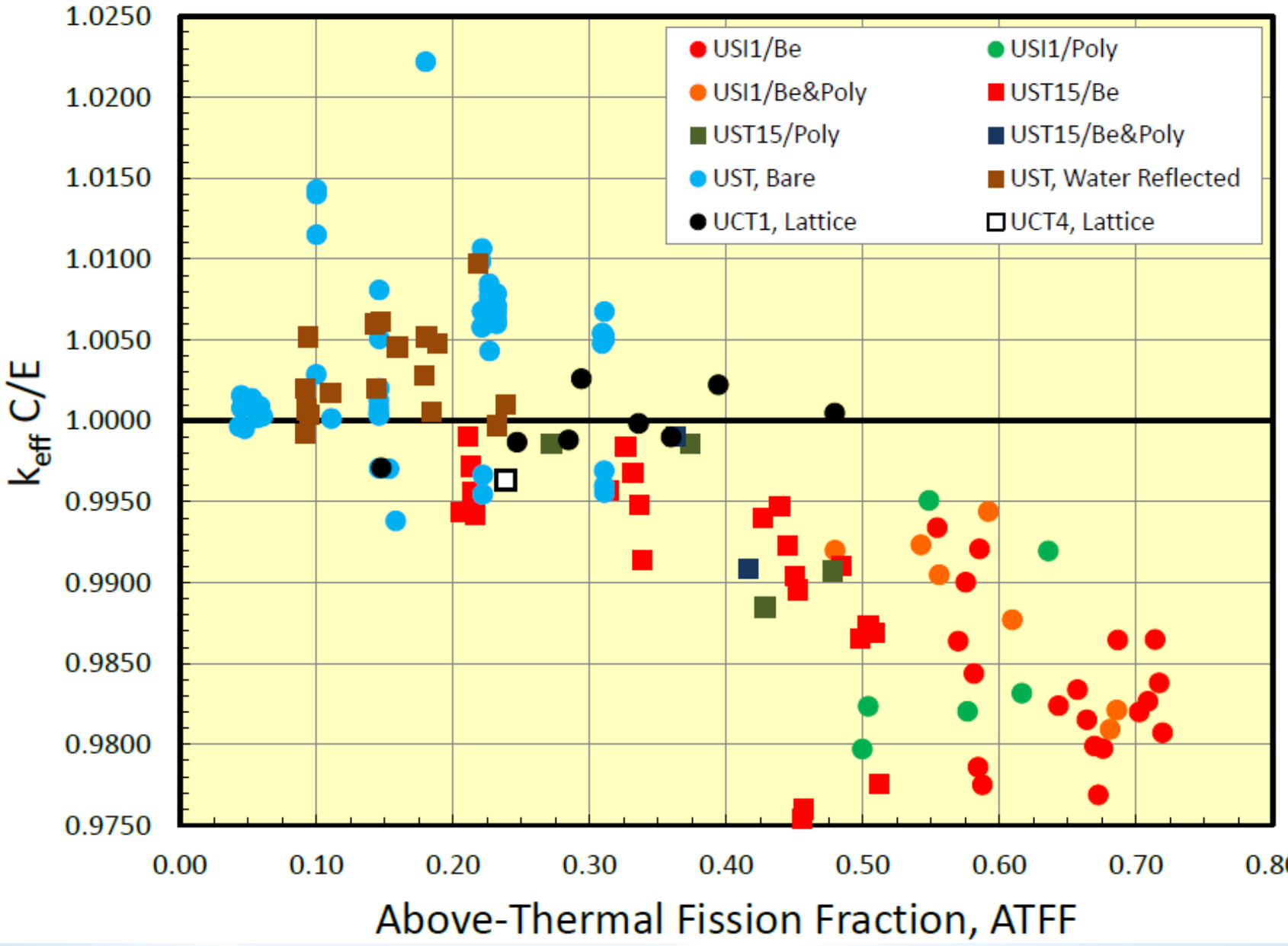
Water moderated attice systems with and without metal reflectors.

Steel (Fe) and ^{depl}U results are good; Pb results are poor.

HMF with Pb is also poorly predicted.

Slide from S. Kahler

^{233}U solution assemblies also indicate a problem



A long-standing bias in calculated eigenvalues; little change in E71 results.

Black circles are UCT (LWBR) related; a successful though little publicized NR program); were we lucky?

Slide from S. Kahler

Every evaluation needs to be checked and we humans can't seem to do it right

ENDF B-VII.1

- **The Problem:**
  - No evaluator remembers to run basic checks (CHECKR, FIZCON) on the evaluations
  - We should not have rely on Skip and Ramon to tell us if NJOY barfed...
- **A Solution:** "continuous integration", a common practice in software development. Every commit or every hour (you pick), retest any evaluation that changed.
- As a result, bugs are discovered ***as soon as data is committed***

ADVANCE: Online Data Verification System (*A*utomated *D*ata *V*erification and *A*ssurance for *N*uclear *C*alculations *E*nhancement)

Prototype ADVANCE system was invaluable in preparing ENDF/B-VII.1

ENDF/B-VII.1/neutrons/Ta

status	isotope	abundance	svn log	ENDF (orig. file)	STANEF (log)	STANEF (output diff)	CHECKR (log)	FIZCON (log)	PSYCHE (log)	fudge (warnings log)	reactionSuite (gnd file)	covarianceSuite (gnd file)	NJOY (log)	AMPX (log)
	^{180}Ta	0.012 +/- 0.002 %				Files identical			CORE	No file		No file	No file	No file
✓	^{181}Ta	99.988 +/- 0.002 %				Files identical			(28 URR dens. (a))	(1 skip total, 1 redun URR (a))		No file	No file	No file
✓	^{182}Ta	0.0 %				Files identical			(1 iffy Q)	(2 xtra interp, 1 skip total, 1 redun URR (a))		No file	No file	No file

What do the messages mean?

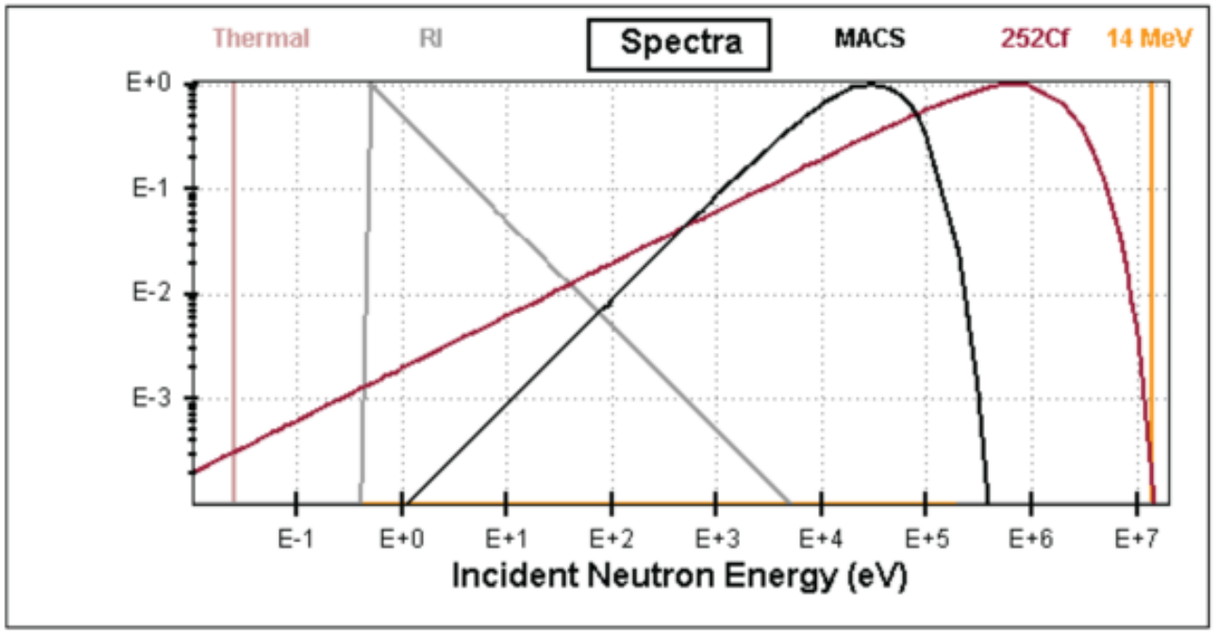
1. **fudge** info "redun URR (a)": Redundant data in URR
2. **fudge** info "xtra interp": Multple interpolation regions in a file where there didn't need to be that many.
3. **fudge** unimplimented "skip total": Fudge currently ignores the total cross section.
4. **psyche** unknown "URR dens. (a)": Level density in URR not in agreement with PSYCHE's, possibly misguided, expectations
5. **psyche** unknown "iffy Q": Non-threshold reaction with Q value differing from PSYCHE's, possibly misguided, expectations

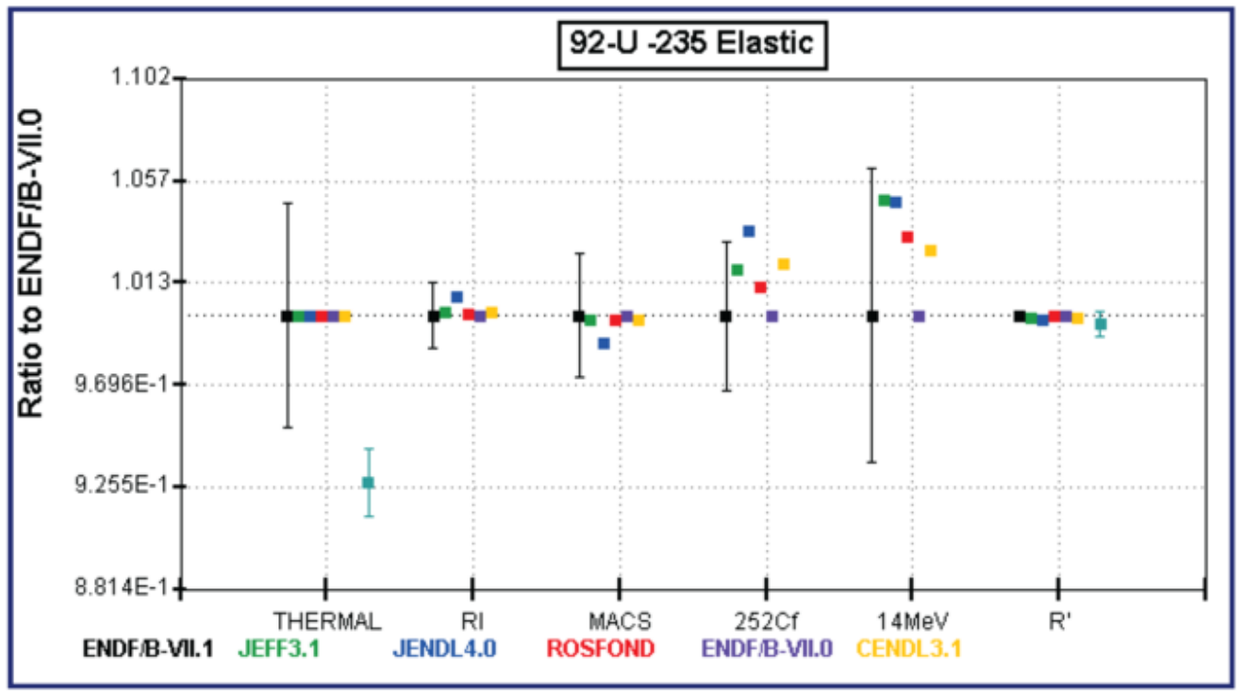
Page generated at 2011-11-08 10:57:48.143028
BNL and/or NNDC boilerplate here

ADVANCE will be expanded & should be ready for general use by the end of FY12

ENDF B-VII.1

- Use CruiseControl for test management
- Integrate current report generator
  - NNDC codes
  - NJOY output
  - fudge output
- Integrate covariance QA system
  - MACS, other spectrum average plots
  - plots of cross sections
- Ground work for general evaluation review system





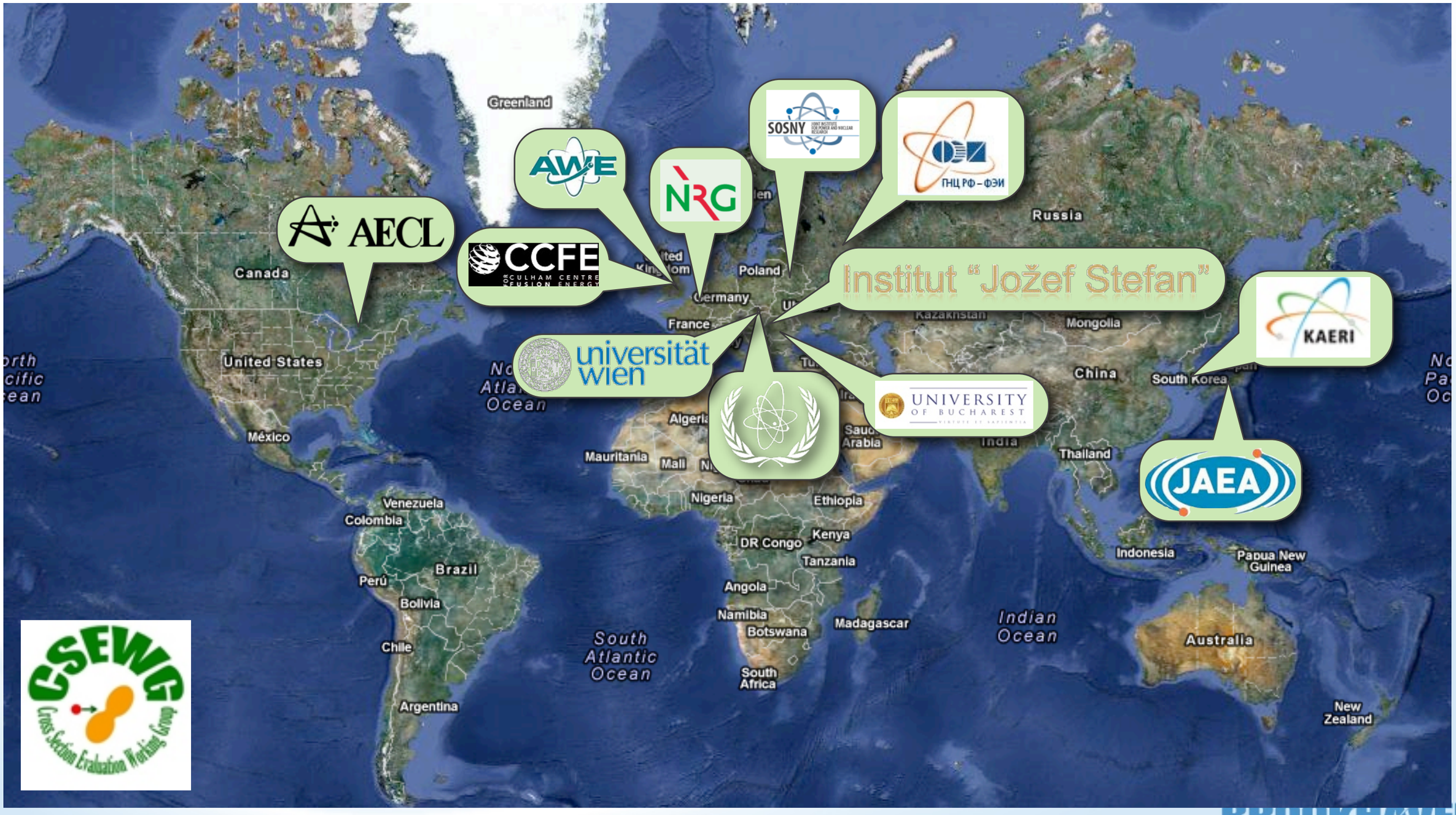
Other longer term changes are in the works

- **New data:**
  - Activation/dosimetry reactions ?
  - Expanded charged particle library (porting ENDL2011 charged particle sublibrary)
  - Filling holes in reaction networks
  - Eliminate last elemental evaluation from transport library: ^{nat}C
- **New format:**
  - Most likely based on Generalized Nuclear Data format
  - USNDP/CSEWG actively participating
  - WPEC hopefully to form to collect international input
- **Investigating possibility of international, unified evaluated nuclear data library**

ENDF/B-VII.1 was the combined effort of collaborators from across the US...

... and the world.

ENDF B-VII.1



Sheraton New York Hotel & Towers
811 7th Avenue
New York, NY 10019, USA

ND2013

Local Organizing Committee

Michal Herman (co-chair),
Alejandro Sonzogni (co-chair),
Yvette Malavet-Blum (secretary),

Ramon Arcilla, David Brown,
Sam Hoblit, Tim Johnson,
Elizabeth McCutchan, Said Mughabghab,
Gustavo Nobre, Analia Palumbo,
Boris Pritychenko, Jagdish Tuli

INTERNATIONAL CONFERENCE ON NUCLEAR DATA FOR SCIENCE & TECHNOLOGY

March 4-8, 2013

www.bnl.gov/nd2013

Important Dates	
Aug. 1, 2012	Abstracts for oral/poster presentations due.
Sept. 1, 2012	Program is announced.
Feb. 10, 2013	Deadline to reserve rooms at the Sheraton at conference rates.
Mar. 4, 2013	Conference begins.
Mar. 8, 2013	Deadline for article submission.

Topics

- Nuclear reaction data
- Nuclear structure and decay data
- Delayed neutrons
- Fission yields
- Atomic masses
- Experimental facilities and detection techniques
- Nuclear data measurements and analysis
- Nuclear theories, models and data evaluation
- Uncertainty quantification and covariances
- Evaluated nuclear data libraries
- Nuclear data processing
- Nuclear data adjustment
- Validation of evaluated data
- Integral experiments
- Cross section and decay standards,
- Data dissemination and international collaboration
- Nuclear Fission (75th anniversary)
- Nuclear data for reactors
- Nuclear decay heat
- Dosimetry and shielding
- Safeguards and security
- Criticality safety
- Homeland security and safety
- Accelerator related applications
- Fusion technology
- Space, cosmic-rays, radiation effects on electronics
- Astrophysics and cosmology
- Medical and environmental applications
- Nuclear physics education

Sponsors & Co-sponsors

BROOKHAVEN NATIONAL LABORATORY · U.S. DEPARTMENT OF ENERGY · Office of Science · NNDC · AEN NEA · Los Alamos NATIONAL LABORATORY

Prospects for Full-Core Monte Carlo Simulation including Multiphysics Feedback

PHYSOR12 Workshop
Advanced Monte Carlo for Reactor Physics Core Analysis

April 15, 2012

Bill Martin
Nuclear Engineering and Radiological Sciences
University of Michigan
wrm@umich.edu

Acknowledgements

- **This presentation is based on discussions with a number of reactor methods developers and Monte Carlo specialists and their recent papers and presentations. See the list of references.**
- **Specific thanks to Forrest Brown (LANL), Kord Smith (MIT), Dave Griesheimer (Bettis), John Wagner (ORNL), Tom Sutton (KAPL), Eduard Hoogenboom (Delft), Bojan Petrovic (Ga Tech), and Han Joo (SNU) for helpful and informative discussions. I have also "borrowed" selected overheads from their presentations and extracted results from their papers.**

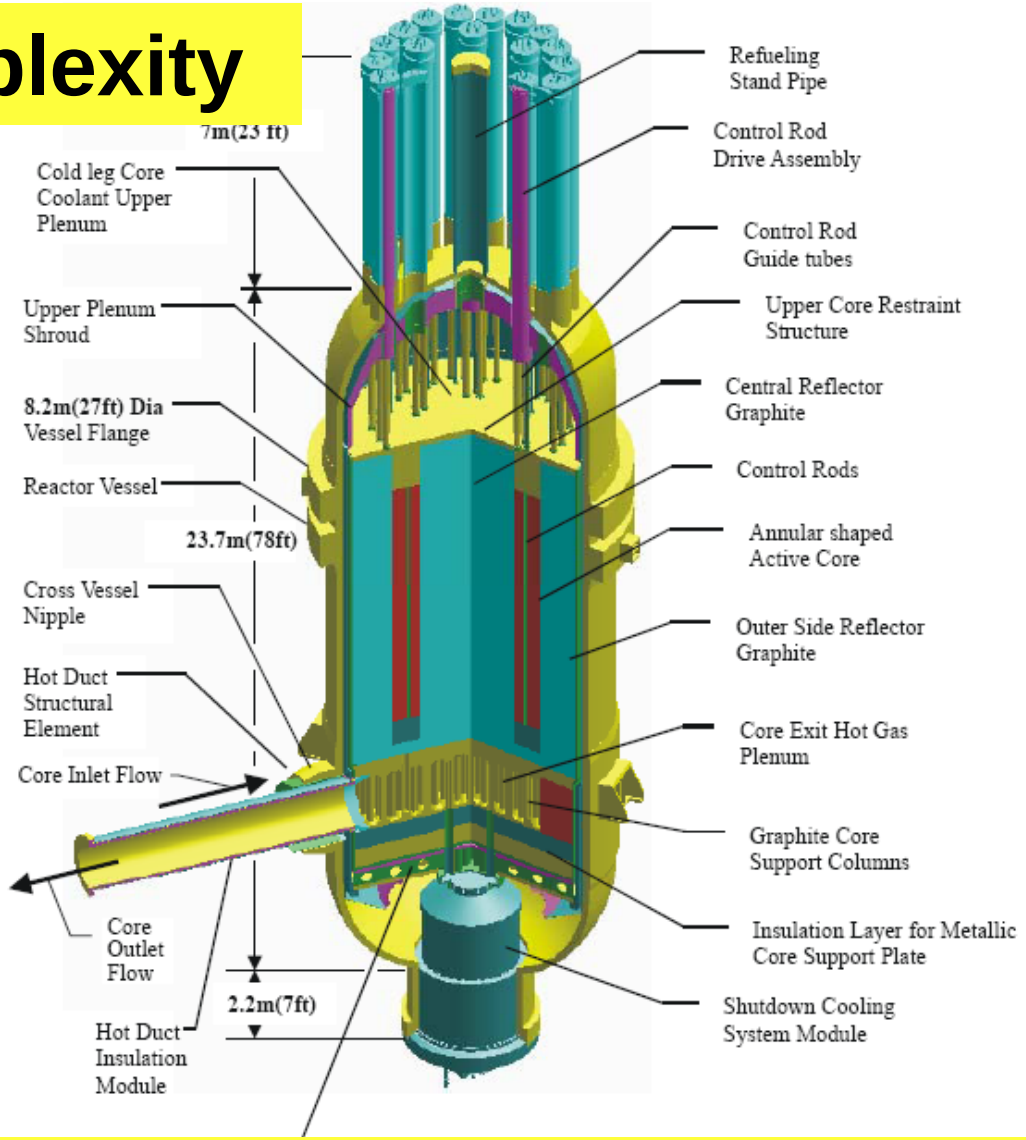
Outline of talk

- **Why do we want Monte Carlo for routine design/analysis of full-core reactor configurations?**
- **What are the challenges to achieving this goal?**
- **How are we doing?**
- **Prospects for the future**

Advantages of Monte Carlo

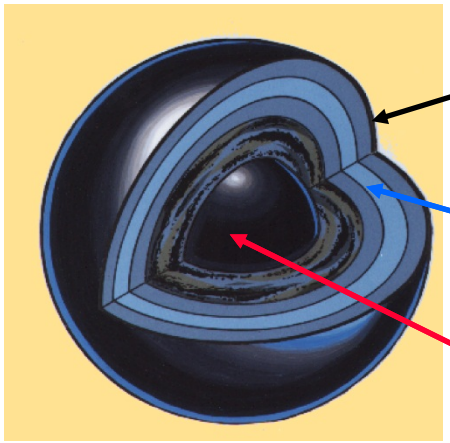
- **Monte Carlo can analyze neutronic configurations with arbitrary geometrical complexity and arbitrary physics complexity.**
- **For continuous energy Monte Carlo, there is no "operator split" step associated with generating multigroup cross sections, a key step in the overall calculational sequence which introduces errors that are difficult to quantify.**
- **Monte Carlo is known to perform efficiently (parallelization efficiency) on all known (production) computer architectures, perhaps with substantial changes to the code and to the underlying algorithm and data structures**

Geometric complexity



Very high temperature gas reactor

Geometric complexity – from TRISO microspheres to full core



Coated microsphere: TRISO fuel (< 1 mm dia)

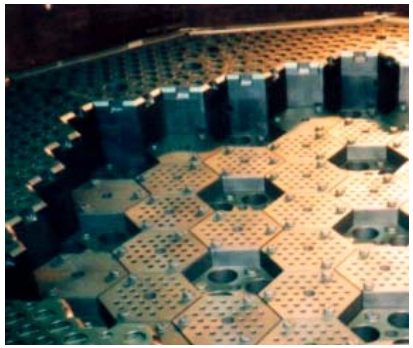
Ceramic coatings (4)

Fuel kernel

PARTICLES

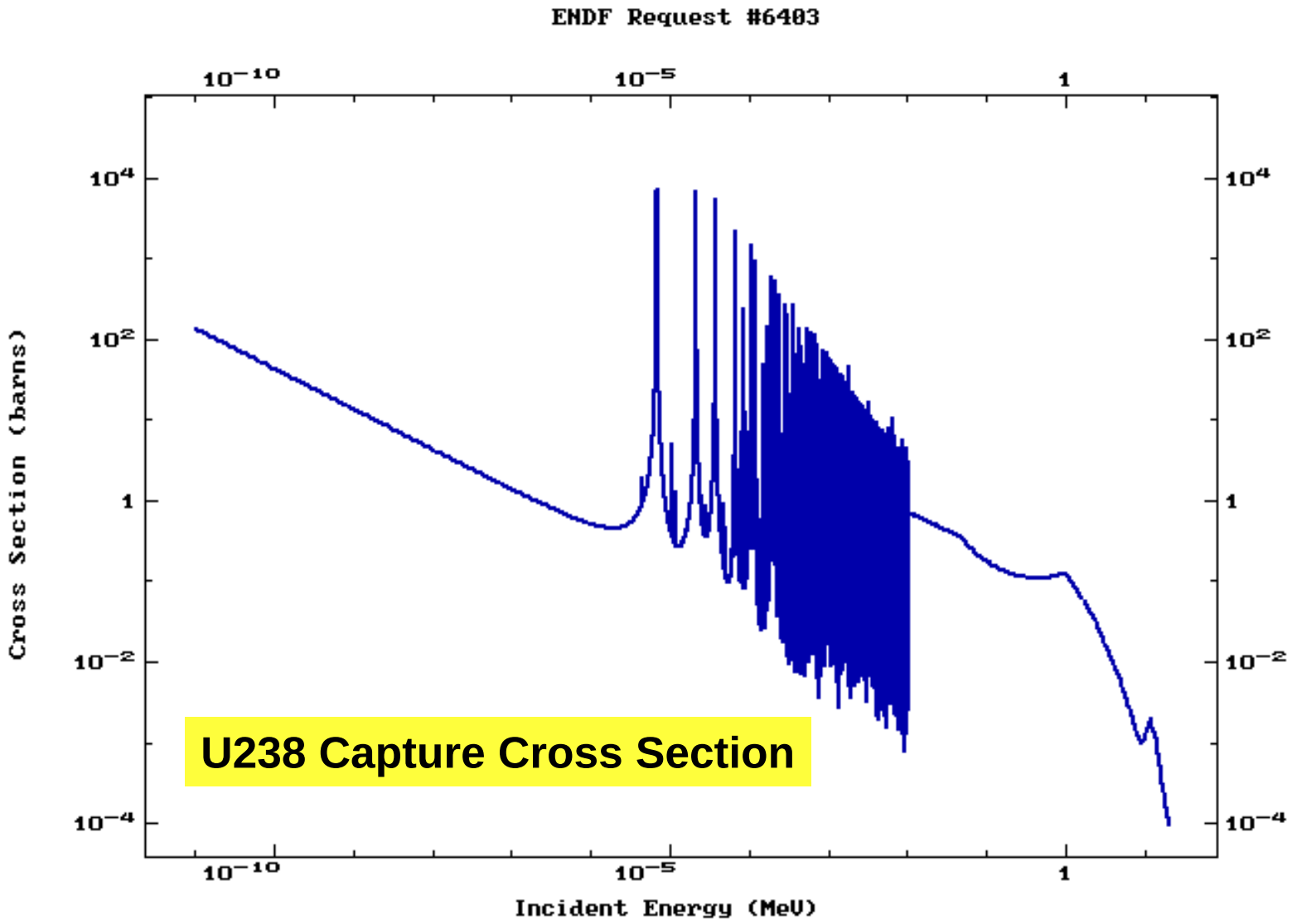
COMPACT

FUEL BLOCK



VHTR CORE

Physics complexity



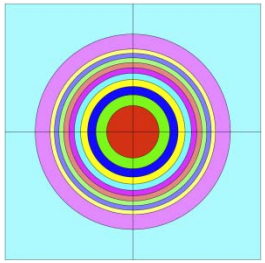
The push for full-core Monte Carlo

- **Monte Carlo offers the potential for high fidelity simulation of complex reactor configurations. However, the impetus for developing full-core Monte Carlo as a routine design/analysis tool goes well beyond high fidelity.**
- **Full-core Monte Carlo with depletion and multiphysics feedback enables a sea change to the workflow for nuclear reactor analysis. Pin cell and assembly calculations are not needed. Color sets and restarts are not needed. The following overhead from John Wagner illustrates the current workflow.**

Current State-of-the-Art in Reactor Analysis

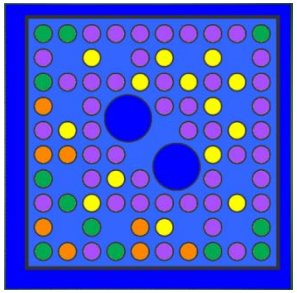
General Electric ESBWR

pin cell



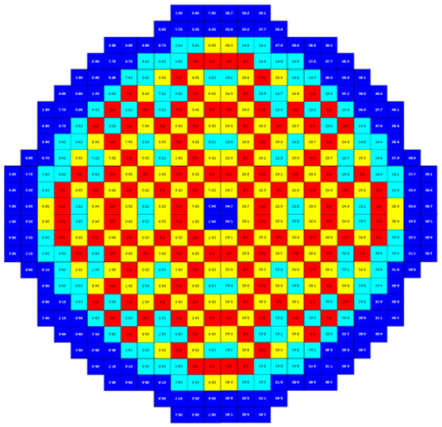
- 1-D transport (high-order)
- High energy fidelity (> 200 groups)
- Approximate state and BCs

lattice cell



- 2-D transport
- Moderate energy fidelity (30-50 groups)
- Approximate state and BCs
- Depletion with spectral corrections
- Spatial homogenization

core



- 3-D diffusion (low-order)
- Low energy fidelity (2-4 groups)
- Homogeneous lattice cells
- Heterogeneous flux reconstruction
- Coupled physics

The push for full-core Monte Carlo (2)

- **A number of experienced groups are pushing hard to develop this capability. Consider the following excerpts from the 4 speakers at the MCD Computational Roundtable at the Summer 2011 ANS Meeting in Florida.**

Monte Carlo Methods in Reactor Physics:

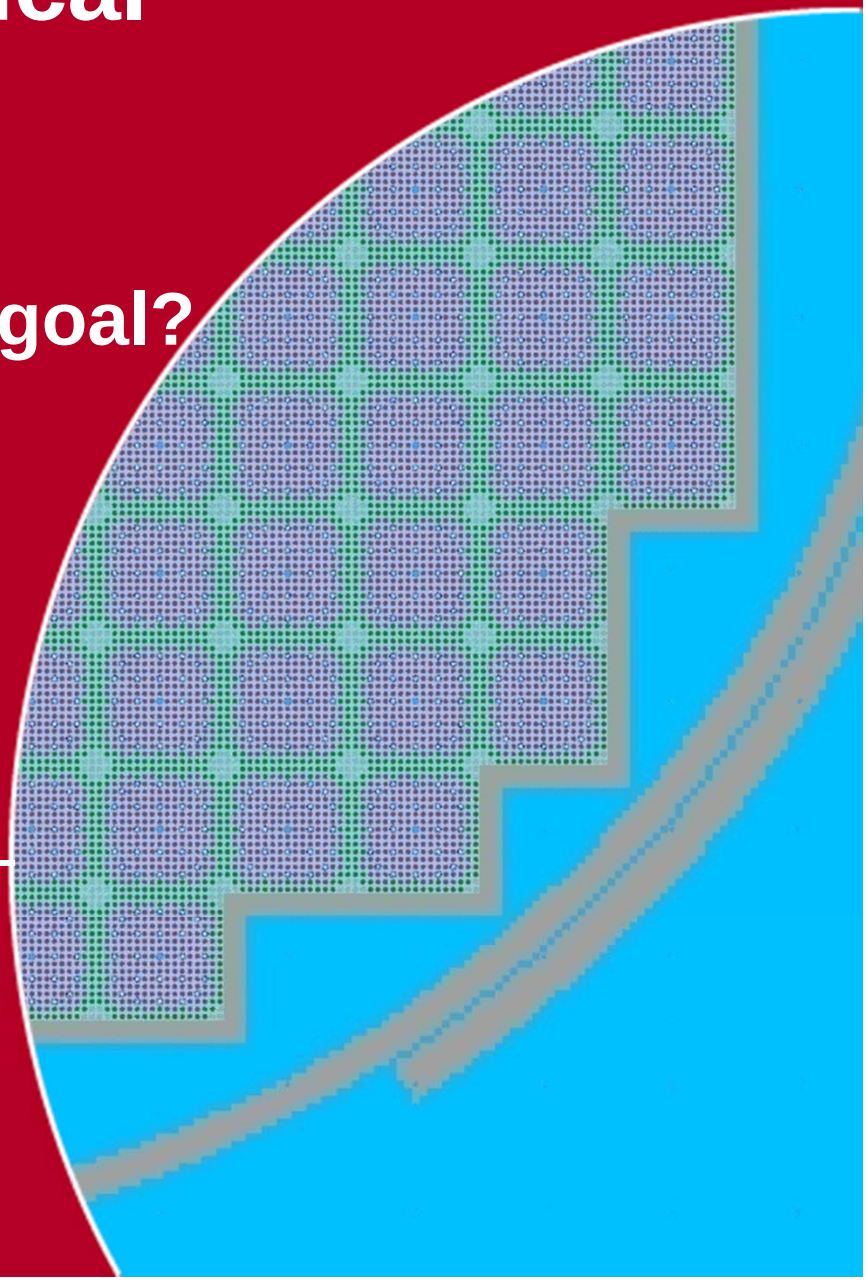
Current Status & Future Prospects

Organizer: Anil Prinja (U. New Mexico)
Chair: Forrest Brown (LANL)

Panel: Forrest Brown (LANL / UNM)
Kord Smith (Studsvik / MIT)
John Wagner (ORNL)
David Griesheimer (Bettis)

Monte Carlo for Practical LWR Analysis:

what's needed to get to the goal?



Kord S. Smith

June 27, 2011

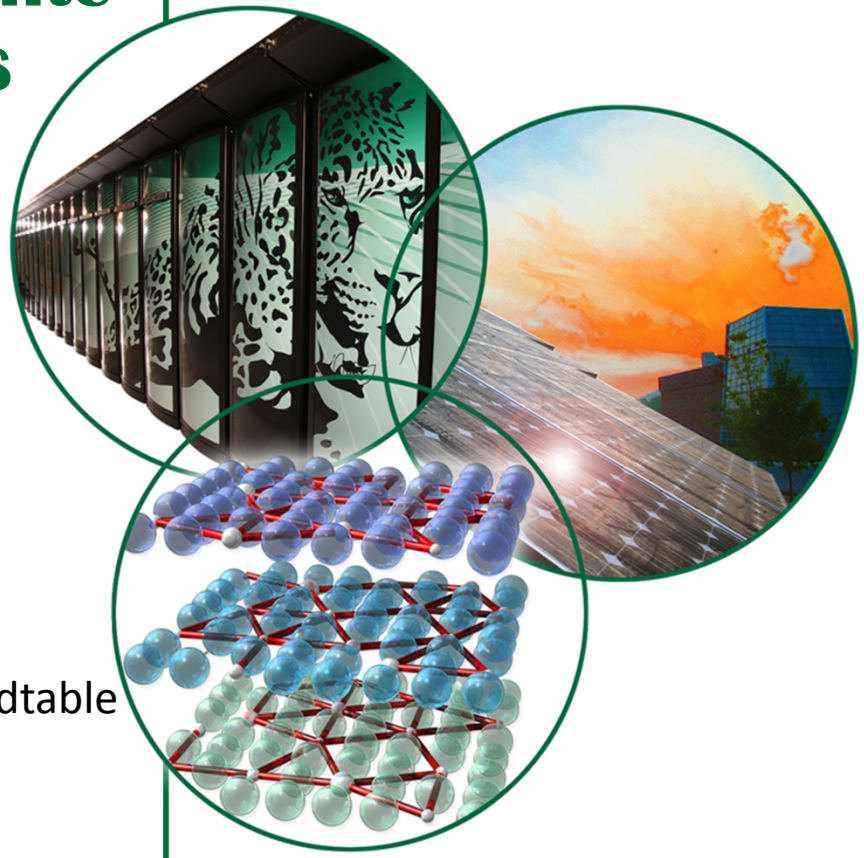
kord.smith@studsvik.com

kord@mit.edu

Hybrid and Parallel Domain-Decomposition Methods Development to Enable Monte Carlo for Reactor Analyses

Presenter: John Wagner

Contributors: Scott Mosher, Tom Evans, Douglas Peplow, Brenden Mervin, Nicholas Sly, Ahmad Ibrahim



Current Issues in Computational Methods – Roundtable

Monte Carlo Methods in Reactor Physics: Current Status and Future Prospects

ANS Annual Meeting, June 27, 2011

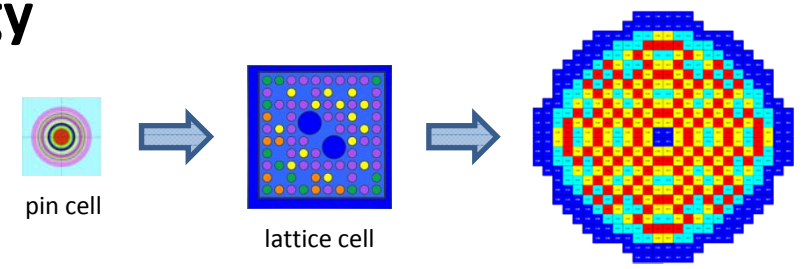
U.S. DEPARTMENT OF ENERGY

OAK RIDGE NATIONAL LABORATORY

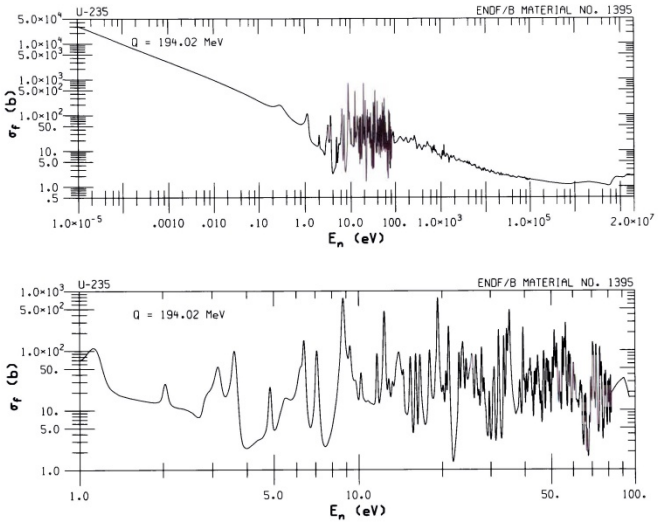
MANAGED BY UT-BATTELLE FOR THE DEPARTMENT OF ENERGY

Our goal is to enable efficient full-core Monte Carlo reactor simulations on HPC platforms

- **Current state-of-the-art methodology**
  - Based on nodal framework (late 1970's)
  - High-order transport at small scale, diffusion at large scale
  - Single workstation paradigm



- **Continuous-energy Monte Carlo (MC)**
  - Explicit geometric, angular and nuclear data representation – **highly accurate**
  - Avoids problem-dependent multigroup xs processing – **easy to use**
  - Computationally intensive – **considered prohibitive for "real" reactor analyses**



U-235 fission cross section

B-T-3875

Monte Carlo Methods in Reactor Physics: Current Status and Future Prospects -- In-Line Feedback Effects

June 27, 2011

D.P. Griesheimer

Bechtel Marine Propulsion Corporation
Bettis Atomic Power Laboratory

Tom Sutton presented the following talk at the University of Michigan last October, detailing the plans for development of MC21, arguably the most advanced of the Monte Carlo codes for attaining full-core capability as well as multiphysics feedback.

Progress in Monte Carlo for Reactor Design and Analysis

October 6, 2011

Thomas M. Sutton
Bechtel Marine Propulsion Corp.
Knolls Atomic Power Lab.

With contributions by members of the MC21 development and user teams:
D. P. Griesheimer, P. S. Dobreff, D. J. Kelly, T. H. Trumbull, T. J. Donovan,
B. R. Nease, D. F. Gill, D. C. Carpenter, B. E. Toth, D. L. Millman, P. K. Romano,
R. N. Slaybaugh, R. R. Gouw, E. Caro, H. Joo, S. L. Brown, W. E. Kerrick,
L. J. Tyburski

Challenges to be overcome in order to achieve the capability for routine full-core Monte Carlo

- **Sheer size of the problem to be solved: prohibitive computational time and memory demand**
- **Slow source convergence**
- **Apparent versus true variance**
- **Accommodating multiphysics coupling**
- **Adapting to future architectures – opportunity or challenge?**

Challenges for Full-Core Monte Carlo

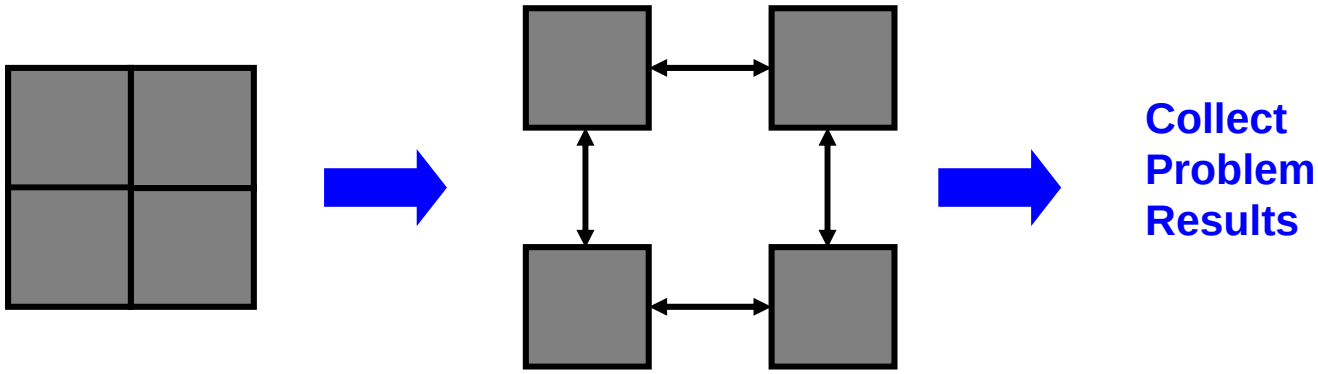
- **Sheer size of the problem to be solved: prohibitive computational time and memory demand**
- **Slow source convergence**
- **Apparent versus true variance**
- **Accommodating multiphysics coupling**
- **Adapting to future architectures – opportunity or challenge?**

Sheer size of the simulation

- **Issue: geometry information, cross section data, and tally data too large to contain in memory for single CPU.**
- **Remedies:**
  - **Domain decomposition**
  - **Data decomposition**
  - **Wait awhile ……**

Remedy 1: Domain Decomposition

If a Monte Carlo problem is too large to fit into memory of a single processor



- **Need periodic synchronization to interchange particles among nodes**
- **Use message-passing (MPI) to interchange particles**

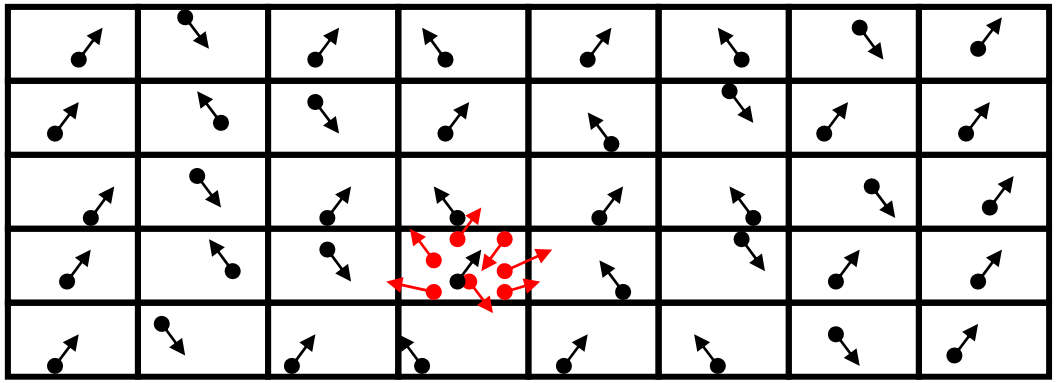
➲ **Domain decomposition is often used when the entire problem will not fit in the memory of a single SMP node (e.g. Mercury at LLNL)**

Domain decomposition may not scale

- **Inherent parallelism is on <u>particles</u>**
  - Scales well for all problems
- **Domain decomposition**
  - Spatial domains on different processors
  - Scales OK for Keff or α calculations,

  where particle distribution among domains is roughly uniform
  - Does **not** scale for time-dependent problems

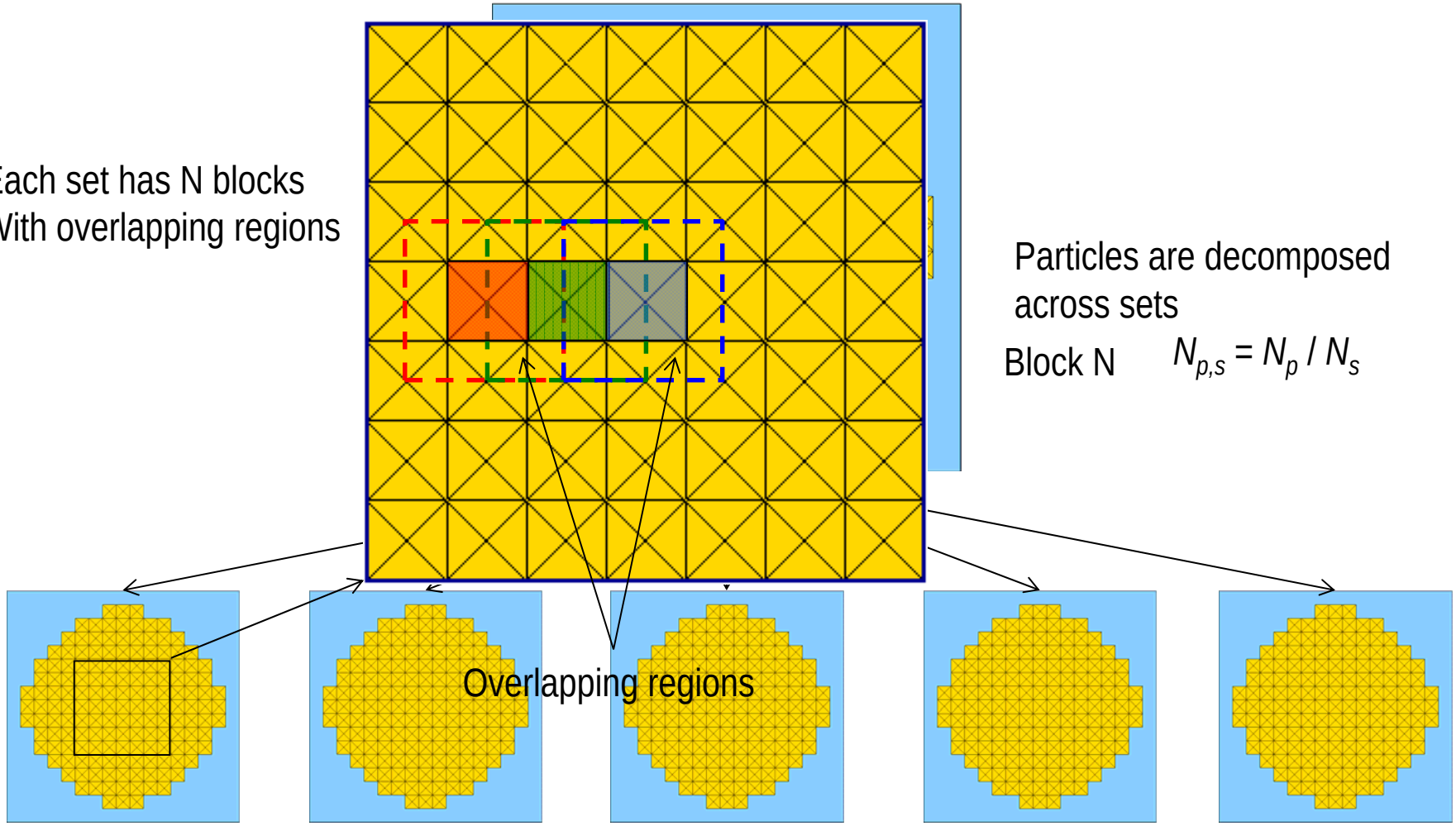
  due to severe load imbalances among domains
- **Domain decomposition - scaling with N processors**
  - **Best: performance ~ N (uniform distribution of particles)**
  - **Worst: performance ~ 1 (localized distribution of particles)**



ORNL has been exploring an overlapping domain decomposition scheme. The following overhead is taken (with minor changes for readability) from John Wagner's Roundtable presentation in Florida

A novel MSOD domain-decomposition algorithm

Each set has N blocks
With overlapping regions



Particles are decomposed across sets

Block N $N_{p,s} = N_p / N_s$

- The multiset/block decomposition allows variance to be estimated by statistical averaging across sets.
- Load-balancing and machine-level communication is amortized by reducing communication across entire geometry.

Remedy 2: Data decomposition

Data is distributed by domain decomposition, but parallelism is on particles. Maybe reverse this:

Parallel on particles + distributed data

- **Basic idea:**
  - **Existing parallel algorithm for particles**
  - **Distribute data among processor nodes (data decomposition)**
  - **Fetch the data to the particles as needed (dynamic)**

- **Essentially same approach as used many years ago for CDC (LCM) or CRAY (SSD) machines**
- **Scales well for all problems (but slower)**
- **Forrest Brown (LANL), Paul Romano (PhD student, MIT), and Ben Forget (MIT)**

Depletion adds to the computational time and memory burden

- **There are many MC depletion codes out there. Many couple existing depletion codes (e.g., Origen or Cinder) with existing MC codes, creating codes such as MOCUP, Monteburns, MCODE, etc. Typically done with a script.**
- **A few MC codes have integrated depletion capabilities:**
  - **Serpent**
  - **Vesta-Moret**
  - **MCNP6**
  - **MC21**
- **Depletion adds considerable demand on memory and computational time.**
- **Depletion complicates uncertainty quantification and propagation of error.**

Remedy 3: Wait awhile ….

- **Domain decomposition complicates the coding and may have workload issues.**
- **Data decomposition is promising but will require substantial changes to MC codes**
- **Alternative: wait until the vendors offer a large enough multicore node with sufficient memory. Nodes are actually SMPs with memory that scales with the number of cores.**
- **Example – the T-H group (Annalisa Manera) in Nuclear Engineering at Michigan purchased a dual-hex (12 cores) Dell node (Xeon) with 192 GB of memory.**
- **No need to change existing parallel MC codes.**
- **Procrastination sometimes has its virtues.**

How can we measure progress towards overcoming CPU and memory constraints?

- **The Kord Smith Challenge**
- **Modified Kord Smith Challenge**
- **NEA benchmark**
- **Reported results**
- **Anticipated achievement of the Kord Smith Challenge**

First, a little history …..

*The Kord Smith Challenge**

- **At the 2003 ANS M&C conference, Kord Smith formulated a challenge for Monte Carlo reactor calculations**
  - **Calculate the local power in 40 – 60 million tally regions**
  - **The standard deviation on the local power should be 1% or less**
  - **He estimated using Moore's law that it would be 2030 before this could be done in one hour on a single workstation**

borrowing heavily from Tom Sutton's MC21 presentation

The Modified Kord Smith Challenge

- **At the 2007 ANS M&C conference, Bill Martin revisited the challenge**
  - **The number of tallies was reduced by a factor of 10**
- **Multi-core processors were allowed**
- **Estimated that the calculation could be accomplished in 2019 using a 1500-core processor (a desktop "workstation")**

Institutionalized as an NEA Benchmark

- **At the 2009 M&C conference, Bill Martin and Eduard Hoogenboom proposed a large PWR benchmark model to aid in monitoring the progress being made towards practical large-scale Monte Carlo reactor calculations**
- **At the PHYSOR 2010 conference, Dan Kelly presented MC21 results for the (original) benchmark problem**
  - **10 billion histories**
  - **18 hours on 400 cores**
  - **95% of the local powers had standard deviations less than 3%**

MC21 Results (PHYSOR 10)

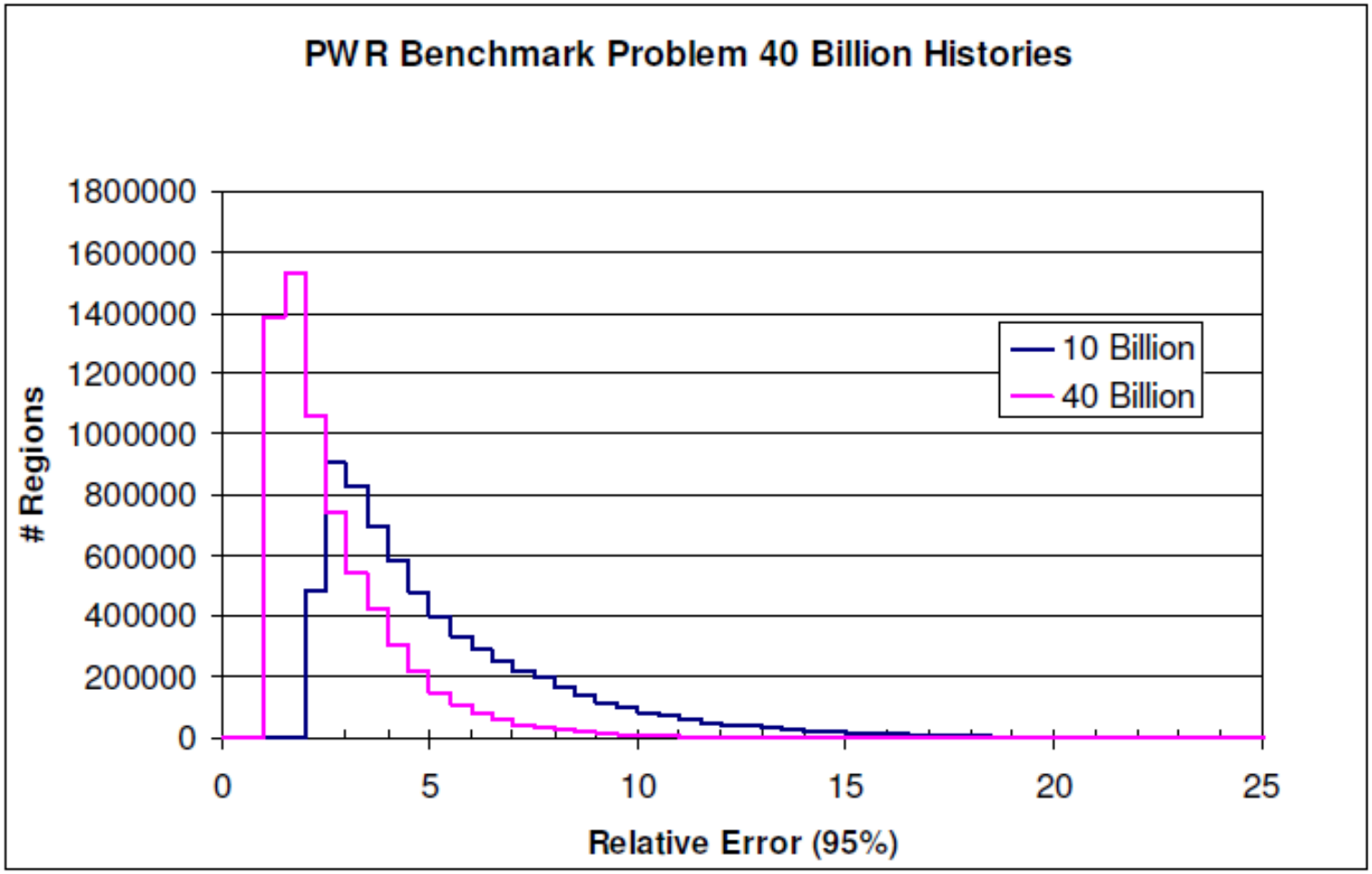


Figure 8. Number of Regions versus Relative Error with 40 Billion Histories

NEA Benchmark (2)

- **At the 2010 SNA + MC conference, Jaakko Leppänen presented Serpent results**
  - **100 billion histories**
  - **21 days on 7 CPUs**
  - **90% of the local powers had std devs less than 2%**
- **Rumor has it that more MC21 results are to be reported this week and that the Kord Smith Challenge will have been met.**
- **If true, the Kord Smith Challenge may be achieved 7-18 years earlier than predicted!! Stay tuned!!**

Challenges for Full-Core Monte Carlo

- Sheer size of the problem to be solved: prohibitive computational time and memory demand
- **Slow source convergence**
- Apparent versus true variance
- Accommodating multiphysics coupling
- Adapting to future architectures – opportunity or challenge?

Slow source convergence

- **Power iteration very slow for high dominance ratio problems characteristic of large power reactors**
- **Shannon entropy can help diagnose convergence but cannot speed it up**
- **Two hybrid (MC/deterministic) approaches are having success accelerating MC source convergence**
  - **Acceleration of MC with low-order operator**
    - **Functional Monte Carlo (FMC)**
    - **Coarse mesh finite difference (CMFD) acceleration**
  - **Acceleration of Monte Carlo with adjoint-based weight windows (FW-CADIS)**

Generalized Hybrid Monte Carlo-CMFD Methods for Fission Source Convergence

Emily R. Wolters, Edward W. Larsen, William R. Martin
Department of Nuclear Engineering & Radiological Sciences
University of Michigan, Ann Arbor, Michigan, USA

MC 2011 CONFERENCE - RIO DE JANEIRO, BRAZIL - MAY 8-12, 2011

REVIEW OF CMFD-ACCELERATED MC

CMFD-Accelerated Monte Carlo: proposed by M.J. Lee, K. Smith, H.G. Joo and D.J. Lee (2009) to accelerate Monte Carlo source convergence.

We now briefly describe this method beginning with the 1D, 1G transport equation:

$$\mu \frac{\partial}{\partial x}\psi(x,\mu) + \Sigma_t(x)\psi(x,\mu) = \frac{1}{2}\left[\Sigma_s(x) + \frac{\nu\Sigma_f(x)}{k_{eff}}\right]\int_{-1}^{1}\psi(x,\mu)d\mu', \qquad -1 \le \mu \le 1, \qquad 0 \le x \le X$$

$$\psi(0,\mu) = \psi^L(\mu), \qquad 0 < \mu \le 1$$

$$\psi(X,\mu) = \psi^R(\mu), \qquad -1 \le \mu < 0$$

Define angular flux moments: $\phi_n(x) = \int_{-1}^{1} P_n(\mu)\psi(x,\mu)d\mu, \quad n \ge 0$

1. Apply $\int_{-1}^{1}\int_{x_{k-1/2}}^{x_{k+1/2}}(\cdot)\,d\mu dx$ to transport equation to obtain *balance equation*:

$$\phi_{1,k+1/2} - \phi_{1,k-1/2} + \Sigma_{a,k}h_k\phi_{0,k} = \frac{\nu\Sigma_{f,k}h_k}{k_{eff}}\phi_{0,k}$$

CMFD-ACCELERATED MC (CONT'D)

2. Introduce a transport-corrected "Fick's Law":

$$\phi_{1,k+1/2} = -\tilde{D}_{k+1/2}\left(\phi_{0,k+1} - \phi_{0,k}\right) + \hat{D}_{k+1/2}\left(\phi_{0,k+1} + \phi_{0,k}\right)$$

Fick's Law — Correction Term

$$\tilde{D}_{k+1/2} = \frac{D_{k+1/2}}{h_{k+1/2}}$$

= dimensionless diffusion coefficient

3. This expression defines the "correction factor" or "HCMFD nonlinear functional":

$$\hat{D}_{k+1/2} = \frac{\phi_{1,k+1/2} + \tilde{D}_{k+1/2}\left(\phi_{0,k+1} - \phi_{0,k}\right)}{\phi_{0,k+1} + \phi_{0,k}}$$

← Estimate these nonlinear functionals in Monte Carlo

4. System of algebraic (HCMFD) equations for the scalar flux and eigenvalue:

$$-\tilde{D}_{k+1/2}\left(\phi_{0,k+1} - \phi_{0,k}\right) + \tilde{D}_{k-1/2}\left(\phi_{0,k} - \phi_{0,k-1}\right) + \Sigma_{a,k} h_k \phi_{0,k}$$
$$= \frac{\nu\Sigma_{f,k} h_k}{k_{eff}} \phi_{0,k} - \hat{D}_{k+1/2}\left(\phi_{0,k+1} + \phi_{0,k}\right) + \hat{D}_{k-1/2}\left(\phi_{0,k} + \phi_{0,k-1}\right)$$

Low-order (diffusion-like) deterministic equations

The solution to the HCMFD equations converges MUCH more quickly than the MC solution!

GENERALIZED METHODS

1. Apply $\int_{-1}^{1}\int_{x_{k-1/2}}^{x_{k+3/2}} f_{k+1/2}(x)P_1(\mu)(\cdot)\,d\mu dx$ to transport equation. Integrate by parts to obtain the following balance equation:

   f(x) is to-be-specified

$$f_{k+1/2}(x)\phi_2(x)\Big|_{x_{k-1/2}}^{x_{k+3/2}} - \int_{x_{k-1/2}}^{x_{k+3/2}} \frac{df_{k+1/2}}{dx}\phi_2(x)dx + \int_{x_{k-1/2}}^{x_{k+3/2}} f_{k+1/2}(x)\Sigma_t(x)\phi_1(x)dx = 0$$

2. Divide this equation by $\int_{x_{k-1/2}}^{x_{k+3/2}} f_{k+1/2}(x)\Sigma_t(x)dx$ to formulate an identity with a term resembling the current:

$$F_{k+1/2} \equiv \frac{f_{k+1/2}(x)\phi_2(x)\Big|_{x_{k-1/2}}^{x_{k+3/2}} - \int_{x_{k-1/2}}^{x_{k+3/2}} f'_{k+1/2}(x)\phi_2(x)dx}{\int_{x_{k-1/2}}^{x_{k+3/2}} f_{k+1/2}(x)\Sigma_t(x)dx} + \frac{\int_{x_{k-1/2}}^{x_{k+3/2}} f_{k+1/2}(x)\Sigma_t(x)\phi_1(x)dx}{\int_{x_{k-1/2}}^{x_{k+3/2}} f_{k+1/2}(x)\Sigma_t(x)dx} = 0$$

$F_{k+1/2}$ = identically zero when the exact transport solution is used to evaluate it. (Not necessarily zero when Monte Carlo estimates of the transport solution are used to evaluate it.)

GENERALIZED METHODS (CONT'D)

3. Subtract $F_{k+1/2}$ from the numerator of the HCMFD-I nonlinear functional:

$$\hat{D}_{k+1/2}^{NEW} = \frac{\phi_{1,k+1/2} - F_{k+1/2} + \tilde{D}_{k+1/2}\left(\phi_{0,k+1} - \phi_{0,k}\right)}{\phi_{0,k+1} + \phi_{0,k}}$$

Rationale: $\phi_{1,k+1/2}$ and $\dfrac{\int_{x_{k-1/2}}^{x_{k+3/2}} f_{k+1/2}(x)\Sigma_t(x)\phi_1(x)dx}{\int_{x_{k-1/2}}^{x_{k+3/2}} f_{k+1/2}(x)\Sigma_t(x)dx}$ will cancel (to some degree) and reduce errors in the functional!

4. Consider three definitions of $f_{k+1/2}$:

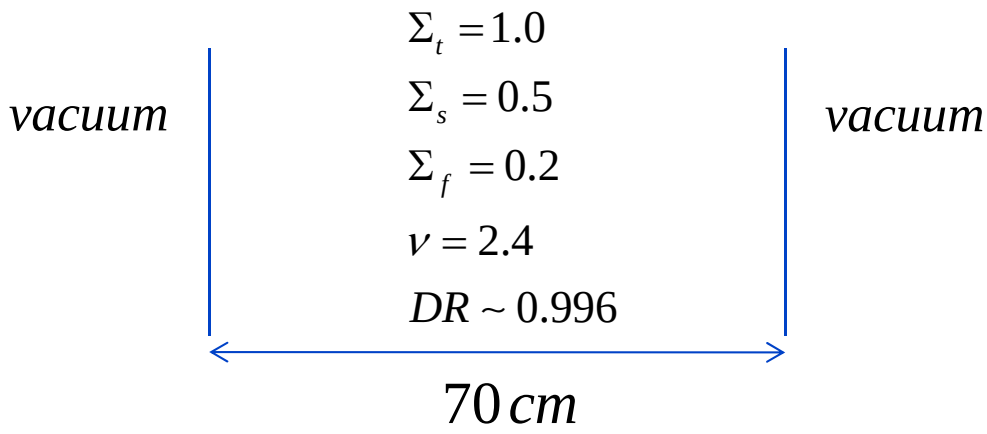
HCMFD-I $\quad f_{k+1/2}(x) = 0$ (HCMFD-I is simply CMFD-Accelerated Monte Carlo.)

HCMFD-II $\quad f_{k+1/2}(x) = 1$

HCMFD-III $\quad f_{k+1/2}(x) = \text{tent function} = \begin{cases} \dfrac{1}{h_{k+1}}\left(x_{k+3/2} - x\right) & x_{k+1/2} \le x \le x_{k+3/2} \\ \dfrac{1}{h_k}\left(x - x_{k-1/2}\right) & x_{k-1/2} \le x \le x_{k+1/2} \end{cases}$

HOMOGENEOUS 1G SLAB

Again, the main idea: HCMFD-x eigenfunction (x=I,II,or III) converges MUCH more quickly than the Monte Carlo eigenfunction. Use it after each cycle to obtain a more accurate and stable MC fission source.



Histories/Cycle (N)	Inactive Cycles (NI)	Active Cycles (NA)	Fine Grid [cm]	CMFD Grid [cm]
100,000	200	200	0.5	0.5

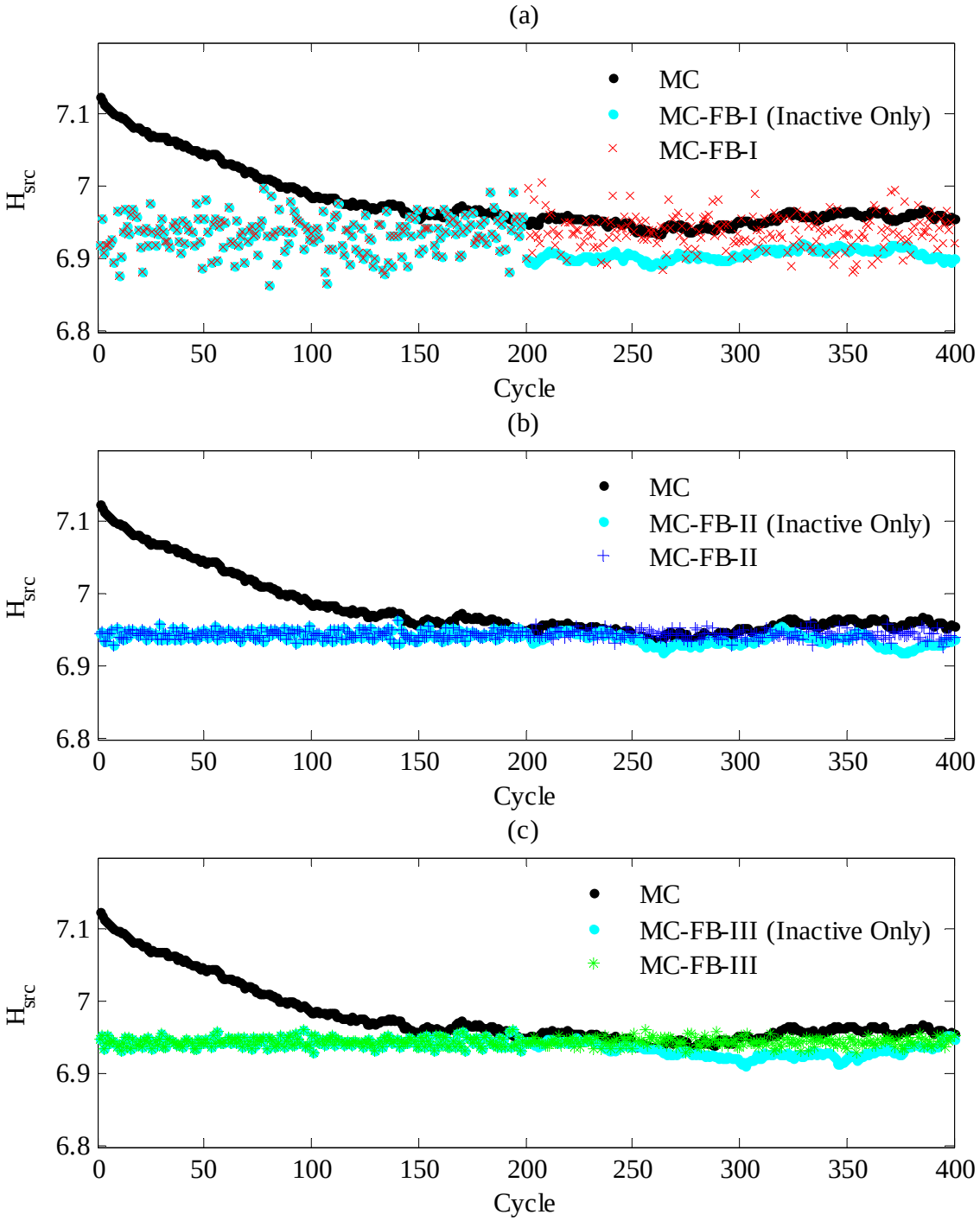


Figure 1. Effect of feedback on Monte Carlo fission source convergence.

Legend:

MC = standard MC

MC-FB-x (Inactive only) = HCMFD-x feedback applied during inactive cycles only

MC-FB-x = HCMFD-x feedback applied during all cycles

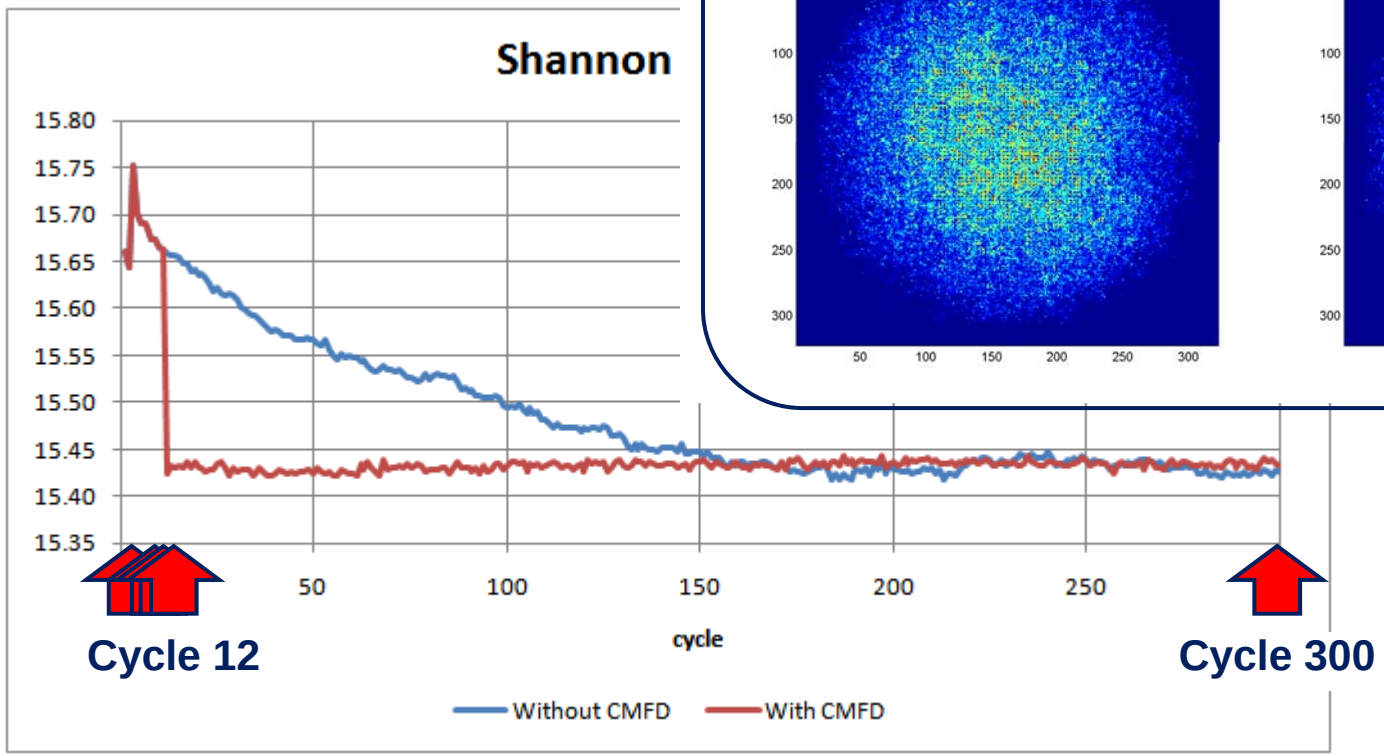
Observations

- Standard MC requires 200 inactive cycles for convergence
- MC w/ feedback converges immediately and stays converged as long as feedback is applied
- Inactive cycles can almost be eliminated (cost savings)
- Methods II and III better than I

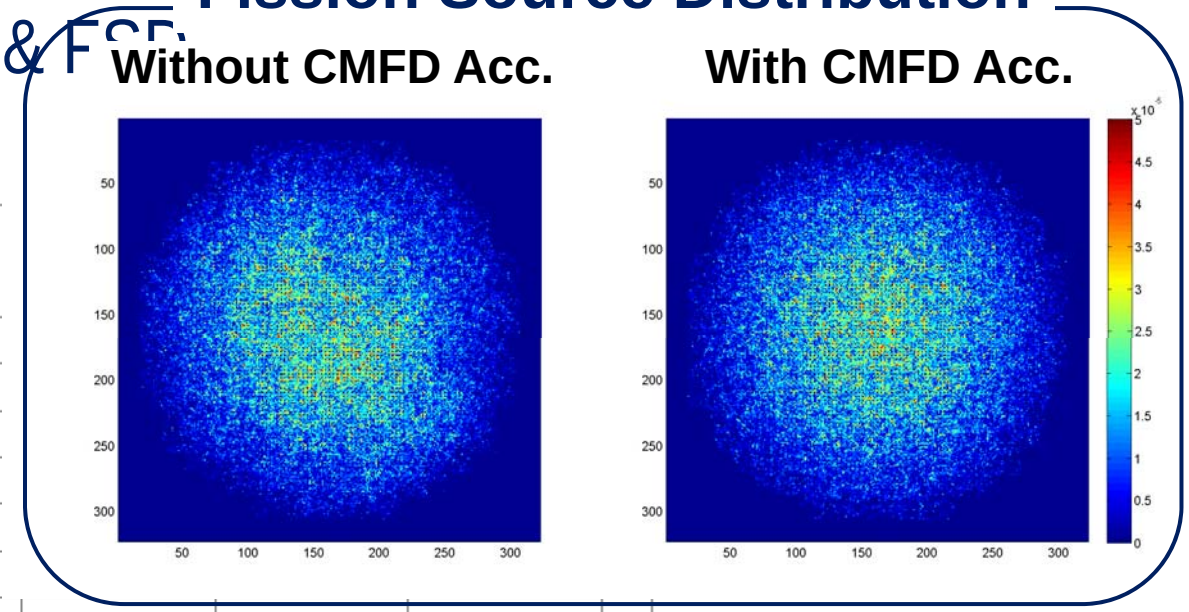
Similar results have been obtained for more realistic reactor configurations. For example, these results were presented by Lee et al. (SNU) at SNA+MC2010 in Tokyo.

Improved Convergence with CMFD Acceleration

- Shannon Entropy & FSD

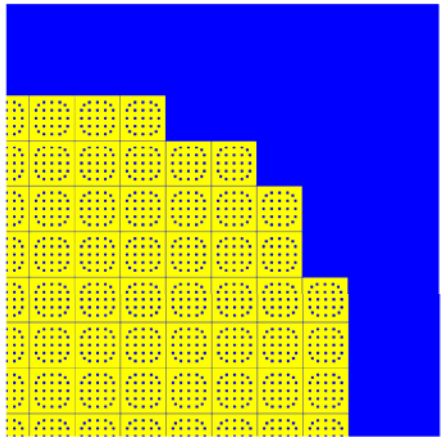


Fission Source Distribution

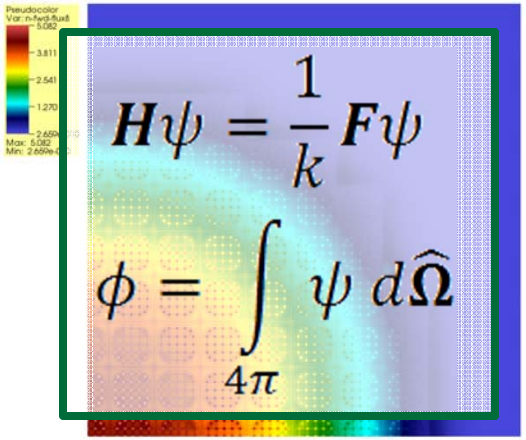


A more traditional "hybrid" Monte Carlo method is the work of John Wagner to use deterministic transport to calculated weighting factors to bias the Monte Carlo run. This method is called FW-CADIS (forward-weighted consistent adjoint method).

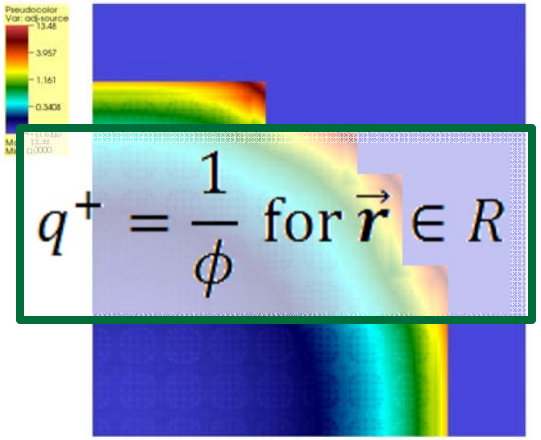
We extended the FW-CADIS method to reactor eigenvalue problems



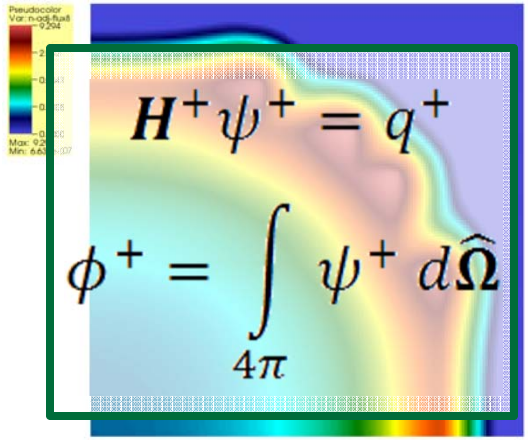
1: construct DX model



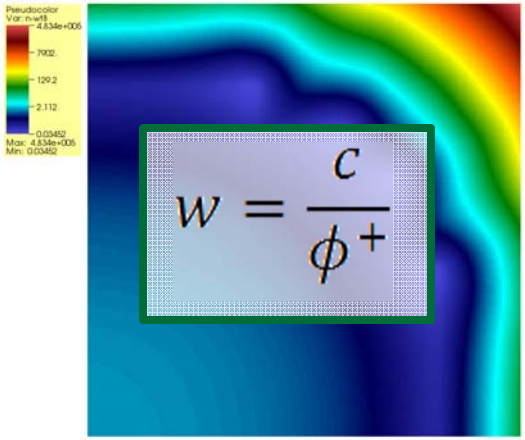
2: solve DX eigenvalue equation



3: construct adjoint source



4: solve DX fixed-source adjoint eqn



5: construct weight windows

Summary of the FW-CADIS method

- **The method weights the adjoint source with the inverse of the forward flux/response**
  - Where the forward flux/response is low, the adjoint importance will be high, and vise versa
- **Once the importance function is determined, the CADIS equations for calculating weight targets**
  - Hence, we refer to the method as ***Forward-Weighted CADIS***
- **The method requires:**
  - A forward solution (for adjoint source weighting)
  - An adjoint solution (for determining biasing parameters)
  - Both can be automated

Challenges for Full-Core Monte Carlo

- Sheer size of the problem to be solved: prohibitive computational time and memory demand
- Slow source convergence
- **Apparent versus true variance**
- Accommodating multiphysics coupling
- Adapting to future architectures – opportunity or challenge?

Apparent vs true variance

- **Forrest Brown at MC2009 (Saratoga Springs) noted that the apparent variance could differ substantially from the true variance in a keff calculation. This factor could be substantial, on the order of 5-10.**
- **The next overhead is taken from the MC21 presentation made at PHYSOR 10. The true variance is clearly larger than the apparent variance.**

MC21 Results (PHYSOR 10)

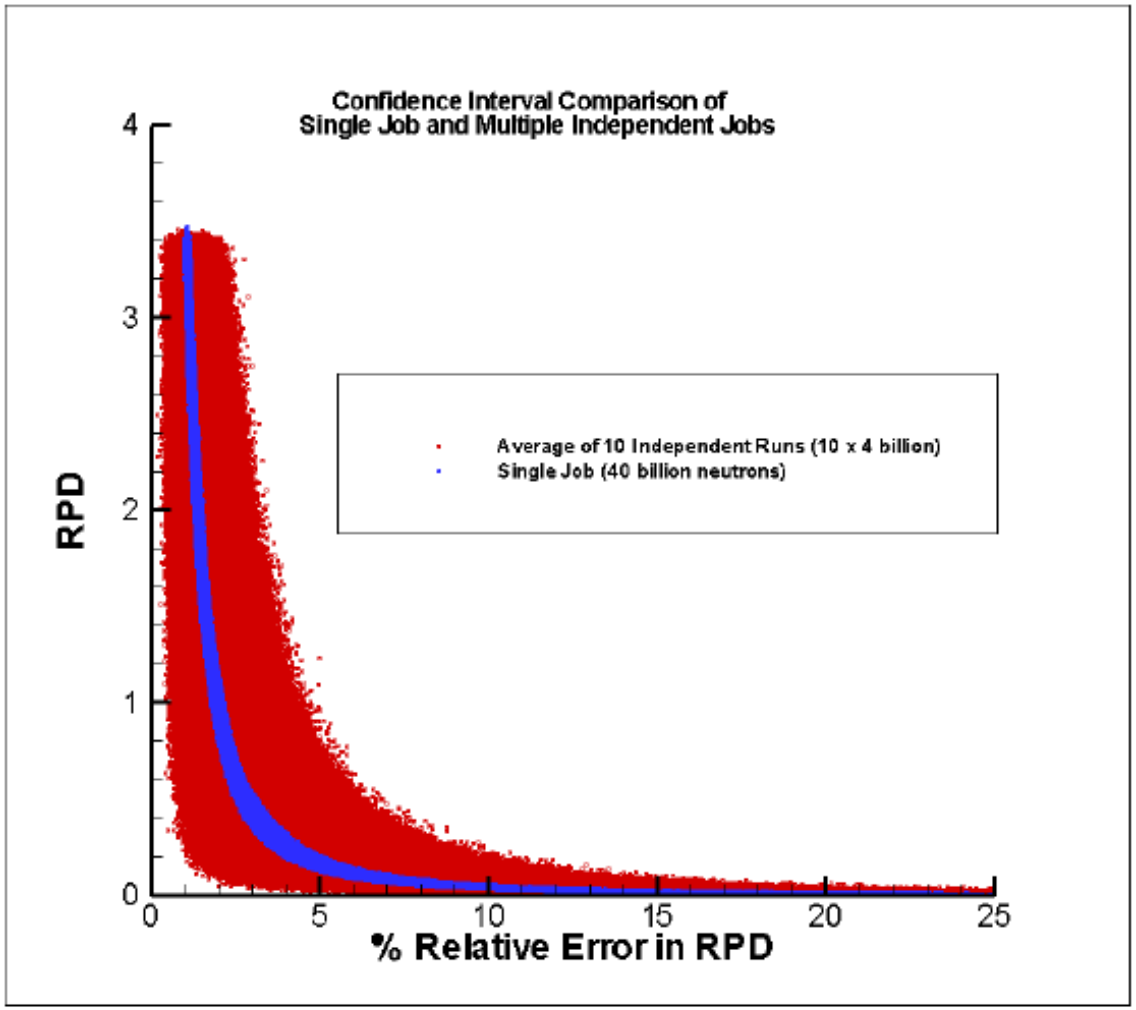
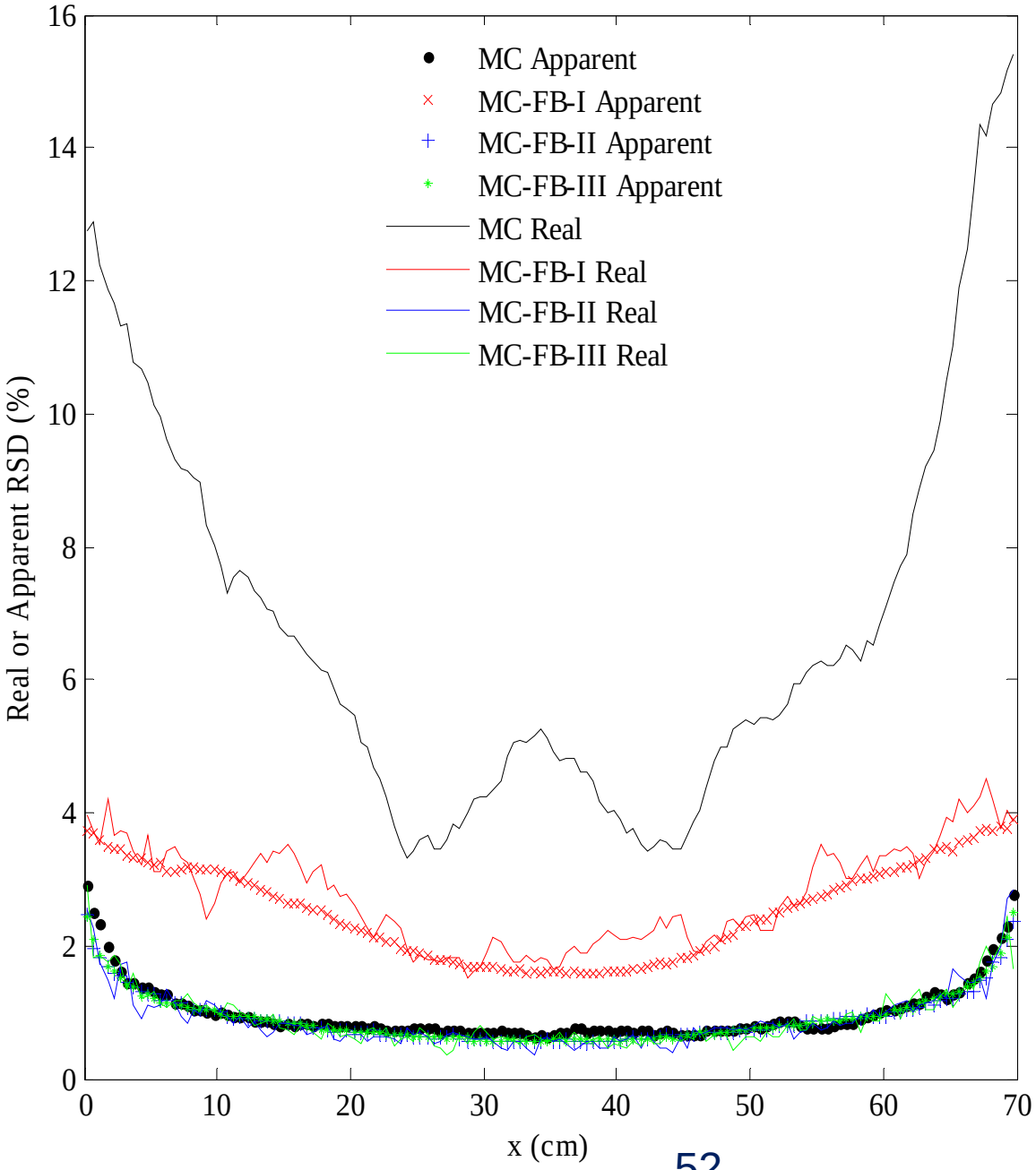


Figure 15. Comparison of Confidence Intervals between a Single Large Run and Ten Independent Runs

Apparent vs true variance for CMFD/FMC

- **The next two overheads are taken from the FMC-accelerated Monte Carlo method developed by Emily Wolters (PhD UM 2010, now at Argonne) and reported at M&C2011 (Rio).**

Figure 4. Real and apparent errors



52

Thin solid lines: real error (over 25 independent calculations)
Markers: apparent error (from single calculation)

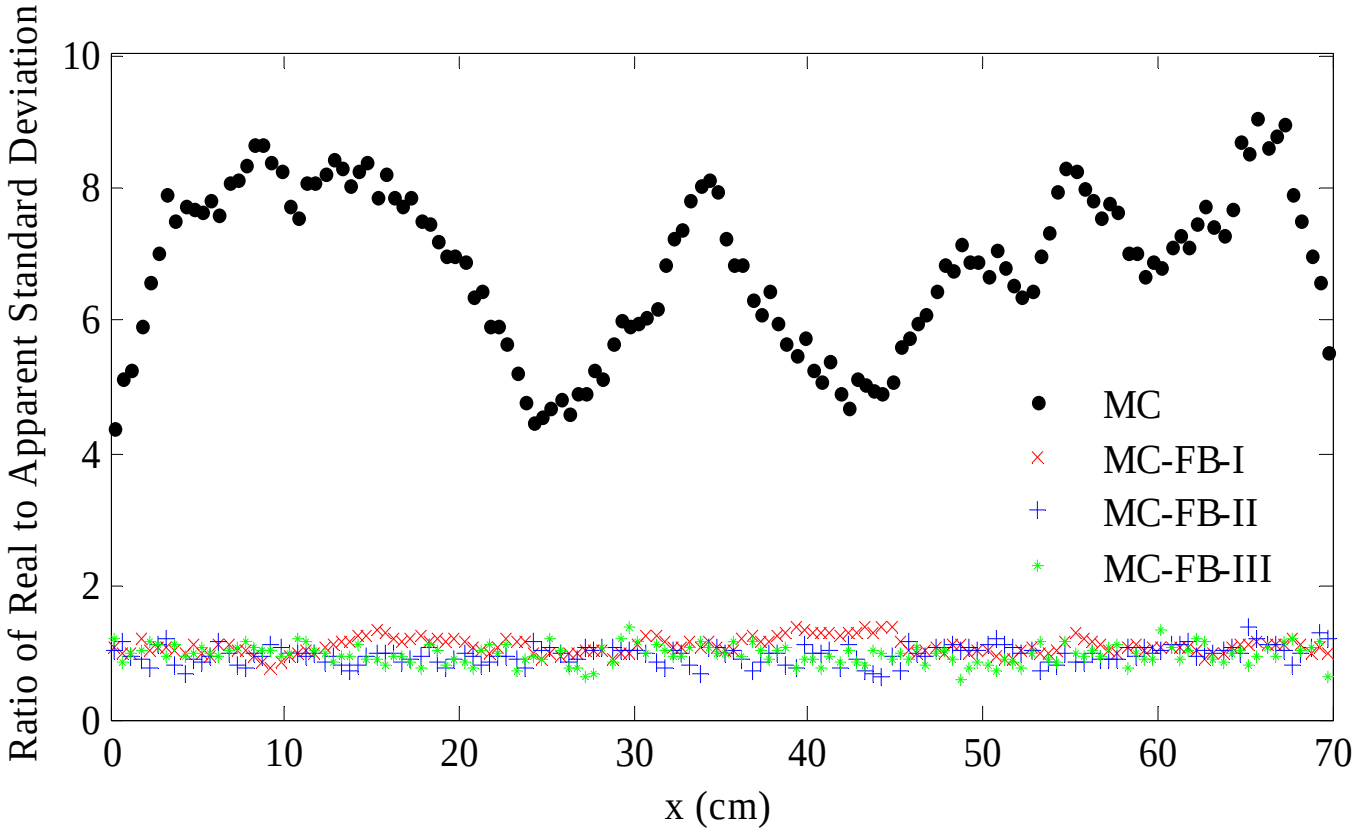
Real error:

- With feedback, real error is 5 to 6 times less than standard Monte Carlo real error for Methods II, III
- Real error 3 times less for Method I
- Applying HCMFD-II or –III feedback for this problem reduces active cycles by a factor of >25

Apparent error:

- "Apparent" error in MC underestimates "real" error
- With feedback, "apparent" error almost equal to the real error: ***excellent estimation of real error from a single calculation when feedback is applied***

Figure 5. Ratio of real to apparent error when feedback is applied.



The real error (over many independent simulations) is well-estimated by the apparent error in a single simulation (when feedback is applied).

53

Apparent vs true variance for CMFD

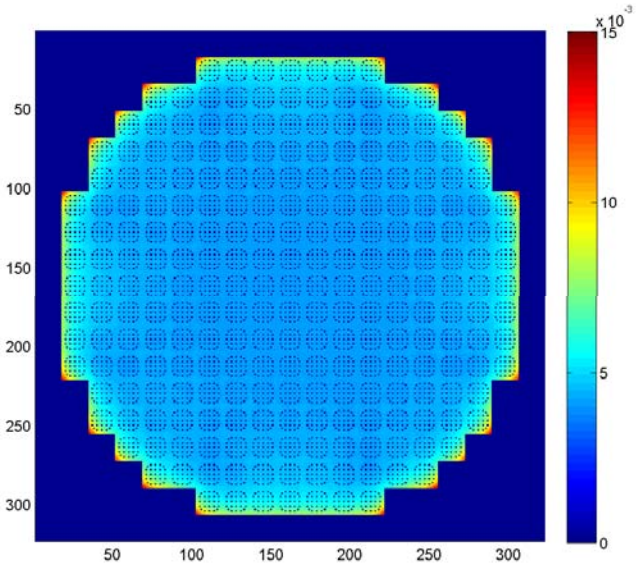
- **Min-Jae Lee, Han Gyu Joo, Deokjung Lee and Kord Smith (SNA + MC2010, Tokyo) reported that CMFD acceleration reduced the discrepancy between the apparent and true variances. The next two overheads are taken from their presentation.**

An Example of Underestimation of Variance

☐ Standard Deviation of Pin Power

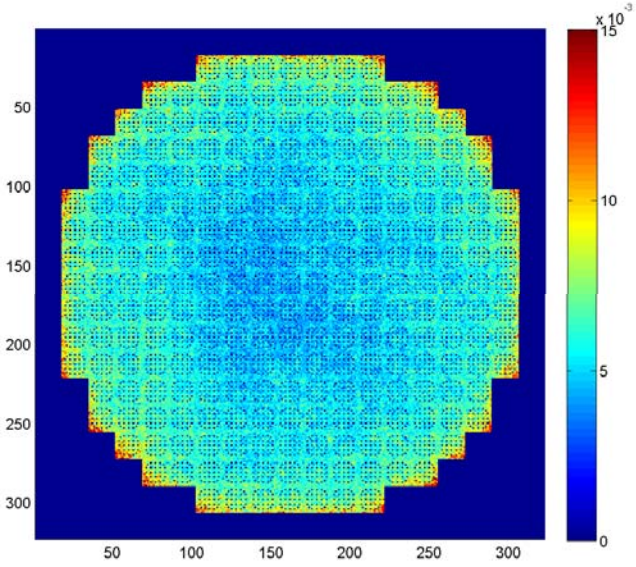
- From 25 independent MC simulation
- 100,000 histories/cycle x 1,000 active cycles

Apparent Standard Deviation



With CMFD Acceleration

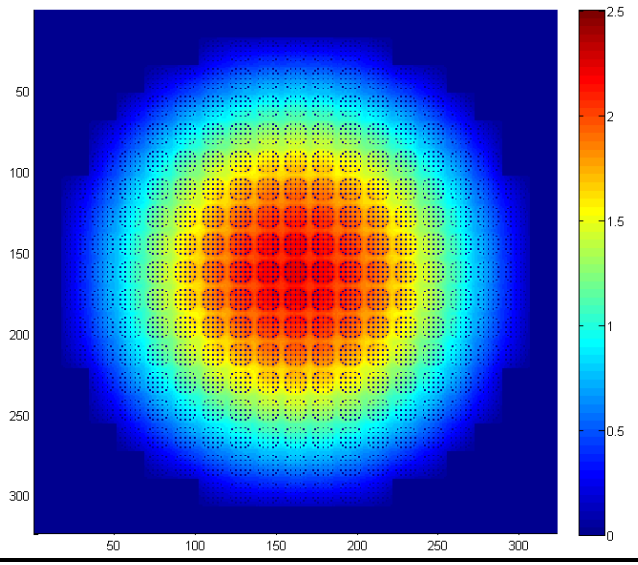
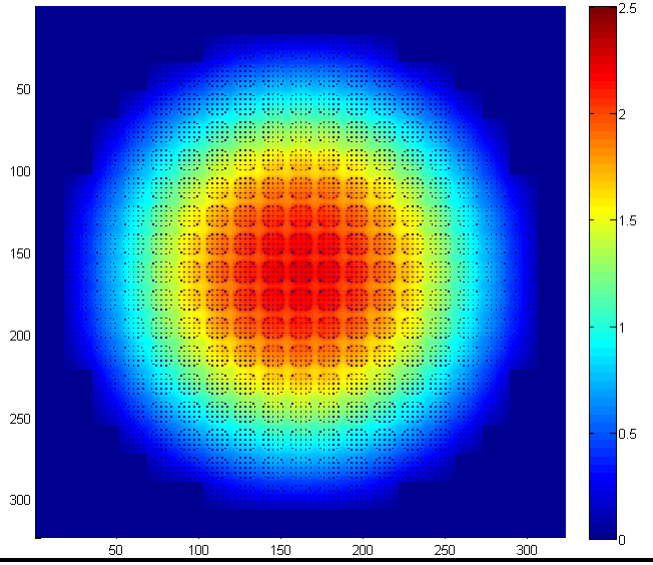
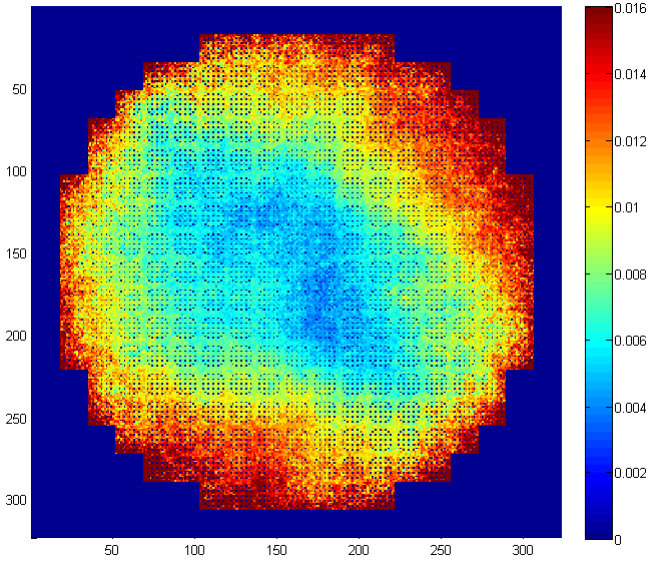
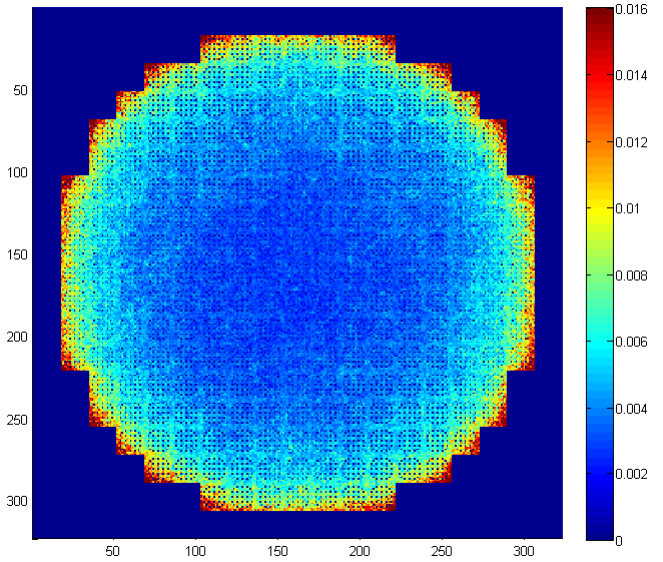
Real Standard Deviation



The main objective of this research is

to reduce real standard deviation in MC simulation !

Results – Pin Power Distribution

	Without CMFD acceleration	With CMFD acceleration
Pin Power Distribution		
Real Standard Deviation		

Discrepancy reduced with CMFD acceleration

- **The CMFD acceleration not only improved source convergence (i.e, reduced the number of inactive cycles) but also reduced the variance during the active cycles.**
- **By renormalizing the MC source distribution with the low-order fission source distribution, CMFD acceleration was effectively "pinning" the fission source distribution to the low-order solution (which had limited local detail).**

Validity of estimate of the variance

- **Dilemma – changing the fission source distribution during the active cycles makes the estimate of variance suspect because the samples are no longer independent identically distributed (IID) observations.**
- **One solution is to run multiple (e.g., 25) simulations and compute the variance from the results. This was done by Lee et al but may be inconvenient to implement.**
- **Another solution is reported by Tom Sutton is based on an old idea by Prael and Gelbard – accumulate statistics from a batch of cycles, say 100 cycles, noting that the serial correlations from one 100 cycle batch to the next might be negligible.**
- **Need more theoretical analysis.**

Challenges for Full-Core Monte Carlo

- Sheer size of the problem to be solved: prohibitive computational time and memory demand
- Slow source convergence
- Apparent versus true variance
- **Accommodating multiphysics coupling**
- Adapting to future architectures – opportunity or challenge?

Issues associated with multiphysics coupling with Monte Carlo

- **Histogram solutions with MC**
- **Temperature dependence of cross sections**
- **Disparate meshes**
- **Propagation of statistical error**
- **Moving away from operator splitting**
- **Effect of statistical error on convergence of the multiphysics feedback iterations**

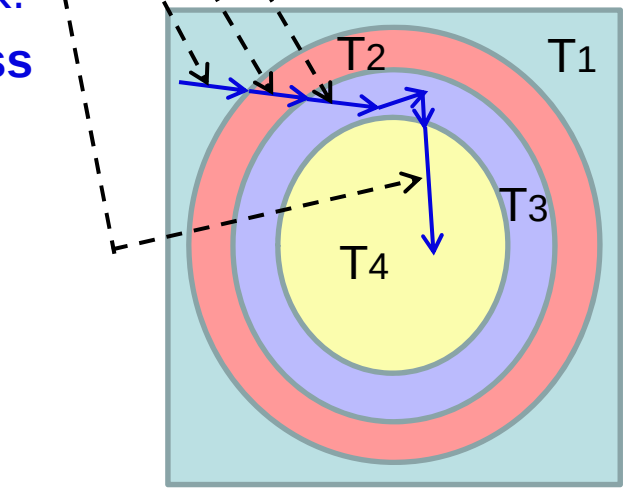
Potential approaches for multiphysics

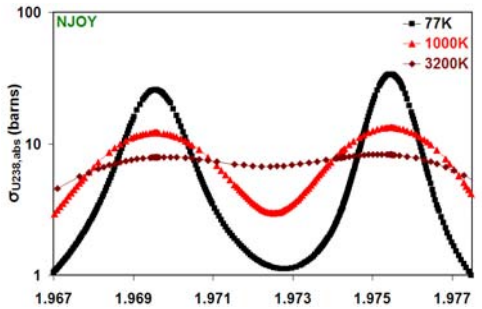
- Use continuous tallies instead of histograms
  - Functional expansion tallies (D. Griesheimer)
  - Kernel density estimator (K. Banerjee)
- Use “On-the-fly” Doppler Broadening (G.Yesilyurt)
- Use delta tracking to allow collision processing with only 0K cross sections (Viitanen and Leppanen, PHYSOR12)
- Use kernel density estimators (K. Banerjee) for the MC solution (mesh-free estimation)
- JFNK coupling for multiphysics feedback
- Need more analysis and numerical experience to understand impact of statistical errors on convergence

On-the-Fly Doppler Broadening (Gokhan Yesilyurt, UM and Argonne)

- Broadened cross sections are determined **during the random walk** in current region at temperature T.
- **Up to 17-termTaylor/asymptotic expansion** for all T in the range 77K-3200K.
- Regressed against the **exact Doppler cross section** (Cullen) to obtain the unknown coefficients as a function of T and neutron energy E.
- **No cross sections are needed** -- only the expansion coefficients for all T, isotopes, and energy grid points.
- **Agrees with NJOY** (within 0.1% for all T).
- **Negligible** computational cost (!!)

$$\sigma^{x}(T) = \sum_{n=1}^{6} \frac{f_n}{T^{n/2}} + c + \sum_{n=1}^{6} g_n T^{n/2}$$





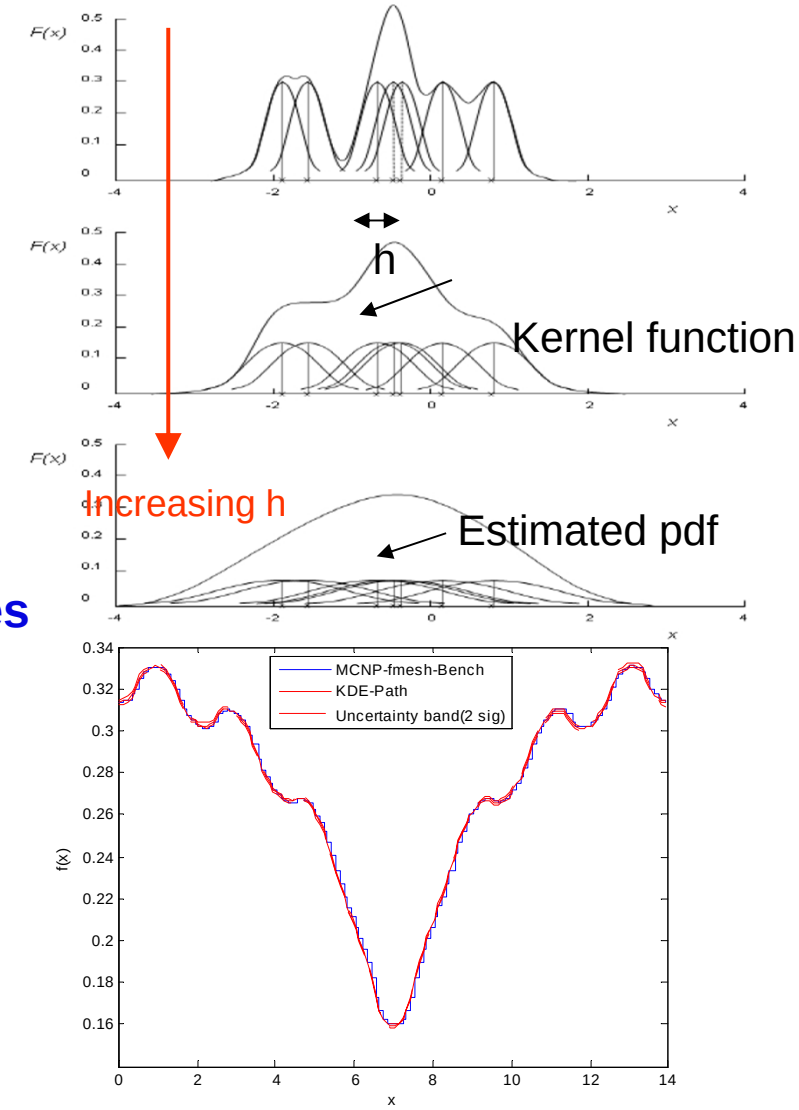
Implemented in MCNP6 (Forrest Brown talk at this workshop)

Kernel Density Estimator (Kaushik Banerjee, UM and Holtec Intl)

- $X_1, X_2, \ldots, X_N$ are N real observations from a density function f(x). f(x) can be formally estimated as

$$\hat{f}(x) = \frac{1}{Nh}\sum_{i=1}^{N} k\left(\frac{x - X_i}{h}\right)$$

- Conventional collision and track length estimators can be evaluated with KDE. These estimators are mesh-free.
- KDE yields continuous, functional estimates of the tallies and their variances (like FET).
- Continuous and mesh-free tallies might be useful for multiphysics coupling
- Aside: KDE can be used to estimate the surface flux estimator (F2) and the point detector estimator (F5) in a scattering region, with bounded variance and no bias.



Challenges for Full-Core Monte Carlo

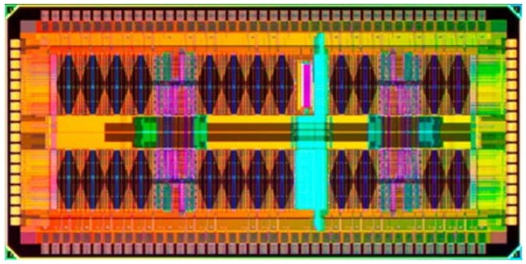
- **Sheer size of the problem to be solved: prohibitive computational time and memory demand**
- **Slow source convergence**
- **Apparent versus true variance**
- **Accommodating multiphysics coupling**
- **Adapting to future architectures – opportunity or challenge?**

Adapting to new computer architectures

- **To stay on the Moore's Law performance curve, Monte Carlo codes must be adapted to run efficiently on new architectures.**
- **To date, Monte Carlo scales well on all architectures:**
  - **Random walks are inherently parallel within a fission source cycle or within a timestep. Parallelizing across particles is natural and allows efficient load balancing without *a priori* knowledge of the solution.**
    - **MCNP5 – history-based parallelization with MPI and OpenMP**
  - **For vector architectures, the history-based random walk algorithm can be turned inside out to yield an event-based (or its stack-driven variant) algorithm that results in excellent speedups on vector and parallel-vector architectures**
    - **RACER – KAPL (event-based)**
    - **MVP – JAERI (stack-driven)**

What about multi-core processors?

- **Dual quad core processors are in wide use today. The trend by the chip manufacturers is multi-N-core where N is increasing rapidly.**
  - **Dual hexa-cores are available (Apple, Dell, ….)**
  - **Intel has developed a 80-core processor (Polaris)**
  - **Xeon nodes available up to dual 10-cores**



IBM (Wii U)

- **Monte Carlo codes which use OpenMP, or "threaded" across histories, can take immediate advantage of multi-core processors: MCNP5 is threaded and uses MPI.**

What about GPU processors?

- **GPU processors are essentially attached SIMD processors that function like vector processors.**
- **The IBM Roadrunner at LANL consists of conventional multi-core processors with attached cell (similar to GPU) processors.**
- **Monte Carlo may scale well on GPU processors but only if the code has already been "vectorized."**
- **Estimate: many tens (if not 100s!) of person-years to vectorize a conventional Monte Carlo code such as MCNP. By then there will be a new computer architecture!**
- **If HPC architectures move exclusively down the GPU processor path (seems unlikely), this could be a limiting factor for using Monte Carlo for routine design/analysis of global reactor configurations.**

Summary and Conclusions
Prospects for Full-Core Monte Carlo

Summary: prospects for full-core Monte Carlo

- **Excessive memory demand – innovative decomposition schemes and the increasing capacity and decreasing cost of memory**
- **Prohibitive computational time – faster and cheaper multicore CPUs**
- **Slow source convergence – successfully applying CMFD and related low-order operators to accelerate source convergence AND pin down the fission source during the active cycles**

Prospects (2)

- **Apparent versus true variance – multiple realizations provide assurance that the estimated variance is OK but more analysis needed to avoid replication of runs for a reliable estimate of the variance.**
- **Accommodating multiphysics coupling – this area is just beginning to be explored. There are some ideas out there that need to be explored, including JFNK and KDE and OTF Doppler broadening.**
- **Adapting to future architectures – perhaps the most uncertain. The direction that computer architectures take is dependent on where the gaming industry and the transaction industry goes. Multicore is OK but GPUs would be problematical.**

References

- Daniel J. Kelly, Thomas M. Sutton, Timothy H. Trumbull, and Peter S. Dobreff, "MC21 Monte Carlo Analysis of the Hoogenboom-Martin Full-Core PWR Benchmark Problem," PHYSOR 10, Pittsburgh.
- Min-Jae Lee, Han Gyu Joo, Deokjung Lee, and Kord Smith, "Multigroup Monte Carlo Reactor Calculation with Coarse Mesh Finite Difference Formulation for Real Variance Reduction," SNA+MC2010, Tokyo.
- Forrest Brown, "Monte Carlo Methods in Reactor Physics: Current Status & Future Prospects," overheads of a talk presented at the M&C Division Computational Roundtable, American Nuclear Socieity Summer Meeting, Hollywood, FL (June 27, 2011).
- Kord Smith, "Monte Carlo for Practical LWR Analysis: what's needed to get to the goal?, overheads of a talk presented at the M&C Division Computational Roundtable, American Nuclear Socieity Summer Meeting, Hollywood, FL (June 27, 2011).
- John Wagner, "Hybrid and Parallel Domain-Decomposition Methods Development to Enable Monte Carlo for Reactor Analyses," overheads of a talk presented at the M&C Division Computational Roundtable, American Nuclear Socieity Summer Meeting, Hollywood, FL (June 27, 2011).
- Dave Griesheimer, "Monte Carlo Methods in Reactor Physics: Current Status and Future Prospects -- In-Line Feedback Effects," overheads of a talk presented at the M&C Division Computational Roundtable, American Nuclear Socieity Summer Meeting, Hollywood, FL (June 27, 2011).
- Emily R. Wolters, Edward W. Larsen, and William R. Martin, "Generalized Hybrid Monte Carlo – CMFD Methods for Fission Source Convergence," M&C2011, Rio de Janeiro.
- Tom Sutton, "Progress in Monte Carlo for Reactor Design and Analysis," overheads of a presentation given at the University of Michigan, 10-6-2011.
- Kaushik Banerjee and William R. Martin, "Kernel Density Estimation Method for Monte Carlo Global Flux Tallies," accepted for publication in Nuclear Science and Engineering, (2011).
- Gokhan Yesilyurt and William R. Martin, "On-the-Fly Doppler Broadening for Monte Carlo Codes," submitted to Nuclear Science and Engineering, (2011).

Any questions?

Advanced Monte Carlo for Reactor Physics Core Analysis -- In-Line Feedback Effects

April 15, 2012

D.P. Griesheimer

Bechtel Marine Propulsion Corporation
Bettis Atomic Power Laboratory

Monte Carlo Timeline

- Historical Applications of MC for Reactor Analysis
  - Neutron slowing-down / resonance capture integrals
  - Calculation of k_{eff}
  - Calculation of local reaction rates for static reactor conditions and fixed configuration (or small perturbations)

Current Research Areas

  - Depletion calculations
  - Incorporation of other non-linear feedback effects for quasi-static calculations
  - Time-dependent (kinetics) calculations
  - Time-dependent calculations including all non-linear feedback effects (FUTURE)

Current Status of Monte Carlo for Reactor Analysis

- 2D Power Distributions
  - Common calculation, practical for most reactor designs
  - Often used to “confirm” diffusion theory solutions
- 3D Power Distributions
  - Practical for small reactor designs
  - Use on large cores limited by computational cost
- Depletion Calculations
  - Same limitations as 3D power distributions
  - Use is increasing as computing power allows
- Other Non-Linear Feedback Effects
  - Active area of research; many prototype methods
  - Studies typically consider only one feedback effect at a time

Non-Linear Feedback Effects

- Importance of incorporating feedback effects in quasi-static calculations:
  - **Increased accuracy**: Local and global power distribution depend on feedback effects.
  - **Calculate new design products**: power defect, temperature defect, other sensitivities.
  - **Ease of use**: User does not have to guess at specific operating conditions, code will calculate conditions on the fly.

Non-Linear Feedback Effects

- We are NOT (yet) talking about full multiphysics
  - (First) Goal of feedback treatments is to improve the accuracy of quasi-static transport calculations.
  - Required accuracy of auxiliary feedback calculation depends on sensitivity of transport process to the parameter.

Important Feedback Effects for Quasi-Static Calculations

- **Depletion**
  - Xenon Feedback
- **Control Rod Motion**
  - Criticality search
- **Thermal Feedback**
  - Gamma Heating
  - In-Line Doppler
- **Mechanical Feedback**
  - Distortion (Thermal & Radiation Induced)

Deterministic Methods

- Deterministic methods (especially diffusion theory) have handled these non-linear feedback effects for many years
  - Typically handled through operator splitting
    - Transport solution
    - Auxiliary feedback calculation
    - Convergence determined by residual of flux solution between steps
  - Unclear if there is a “best” update sequence for converging multiple feedback effects simultaneously
  - Limited computer resources often forces a trade-off between fidelity and number of feedback effects

Monte Carlo Feedback

- To compete with deterministic tools for reactor analysis, MC codes must offer the same capabilities, including feedbacks
- Traditional (initial) MC approach to adding new capability:
  - Ignore statistical uncertainty, implement an analog of the deterministic method and hope for the best!
- Even so, handling feedback with MC is a difficult task
  - No standardized approach to feedback even for deterministic methods
  - Statistical uncertainty complicates tests for convergence
    - Often it is unclear what “converged” really means!
  - Brute-force iterative methods may be too expensive
    - MC solutions have a fixed cost (minimum number of histories to achieve reasonable answers); Deterministic methods can quickly reconverge from previous solution.

Monte Carlo Feedback

- Many approaches to MC feedback have been prototyped and tested, and research in this area has increased lately, but…
- More work is needed, especially in the areas of:
  - Propagation of statistical error
  - Convergence stability in the presence of statistical error
  - Convergence criteria for MC feedback calculations
  - Adaptive running strategies that minimize the number of neutron histories required for a given confidence interval on the final result
- A summary of some of our recent work on MC feedback follows…

Feedback Sequence

```
<TIMESTEP> 1
  timestep_length    100 hours
  power_level        3300 MW
  batches            1200
  discard            200
  histories          10000
{EXECUTE} thermal eqXe
  batches            550
  discard            50
  source_type        last
{EXECUTE} depletion
{EXECUTE} thermal
{EXECUTE} depletion
  batches            1050
{EXECUTE} spatial userTallies
<TIMESTEP> 2
...
```

Timestep

- Presently the calculation sequence is user defined
  - Simulations contain timesteps, which may include multiple in-line feedback calculations
  - User defines the number and sequence of each feedback calculation in the input
  - Job parameters can be changed between iterations.
- Issues:
  - No convergence metrics
  - User is responsible for defining the feedback sequence

In-Line Depletion

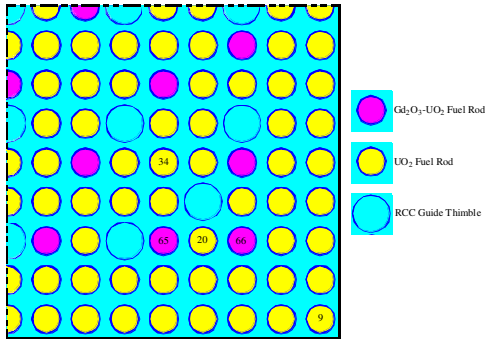
- Depletion calculations are performed in-line using an integrated depletion solver
- Four time differencing schemes have been considered for solving the depletion equations

- **Constant Flux**
- **Constant Power (*Cell2*)**
  - Initial constant flux depletion over timestep
  - Redeplete using converged reaction rates at timestep end
  - Report average number densities from the two depletions
- **Constant Power (Linear Rate)**
  - Initial constant flux depletion over timestep
  - Corrector depletions assume linear flux change over timestep
- **Constant Power (*Monteburns*)**
  - Initial constant flux depletion over ½ timestep.
  - Redeplete using converged reaction rates at timestep midpoint

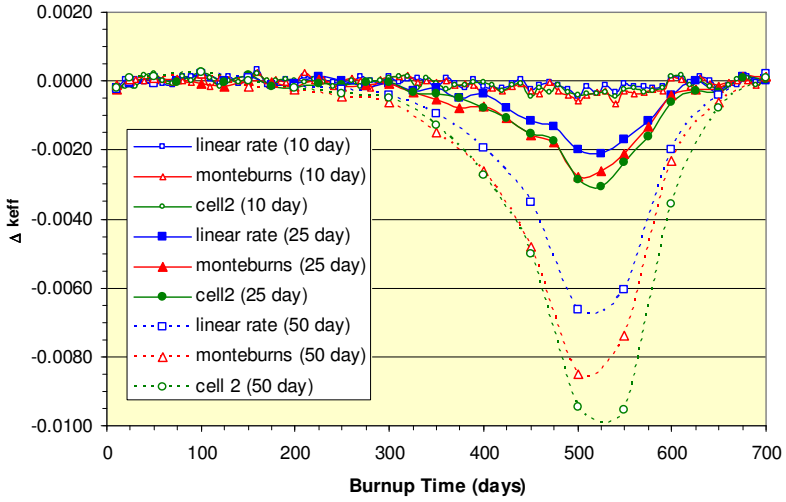
In-Line Depletion

- Depletion Issues
  - Selecting a running strategy (differencing scheme, timestep size, etc.)
  - Propagation of error through years of core operation
  - Calculating time integrated quantities (e.g. fluence) with a predictor-corrector method
  - Computational expense
    - Number of depletion regions
    - Number of fission products and reaction types to explicitly include in depletion chains

PWR Quarter Assembly with Gd-U Fuel Rods

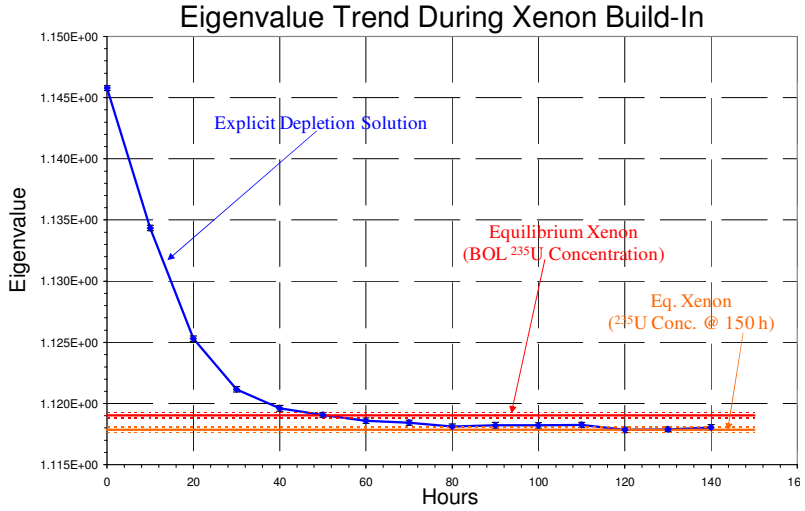


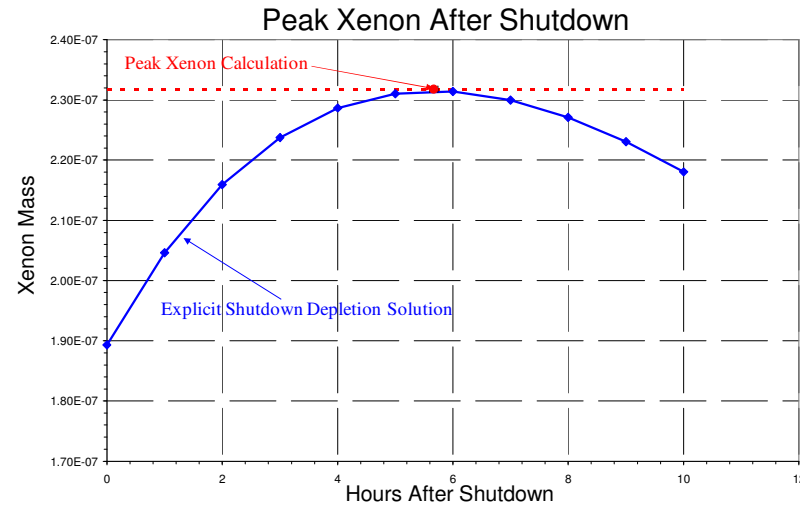
Eigenvalue Bias by Depletion Method



D.C. Carpenter, "A Comparison of Constant Power Depletion Algorithms," Proceedings of M&C 2009, Saratoga Springs, NY , May 3-7, 2009 (CD-ROM).

In-Line Xenon Feedback



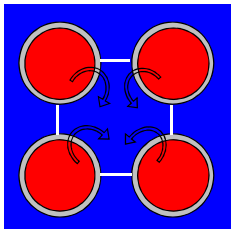


- Code converges to equilibrium Xe distribution during discard batches
- Avoids the need for small timestep depletion after power change
- In-line peak xenon calculation also available for shutdown calculations.
- **Issues**:
  - Understanding convergence behavior
    - Calculation affects convergence of fission source and Xe-135 distributions
  - Ensuring that depletion and xenon feedback modules can work together in a single calculation

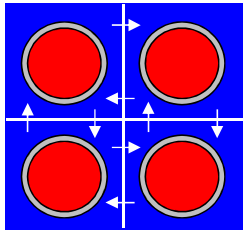
D.P. Griesheimer, "In-Line Xenon Convergence Algorithm for Monte Carlo Reactor Calculations," Proceedings of PHYSOR 2010, Pittsburgh, PA , May 9-14, 2010 (CD-ROM).

In-Line Thermal Feedback

Source-Sink
Heat Flow Map

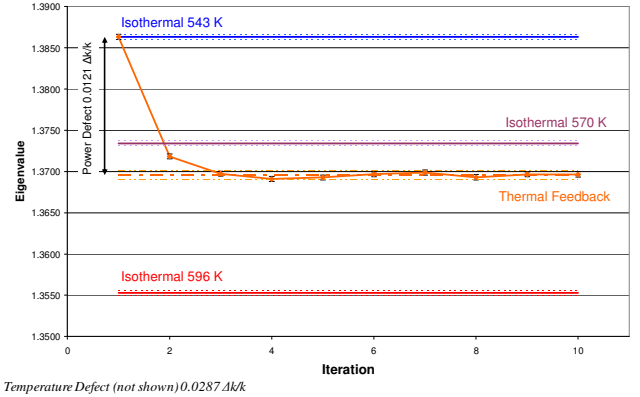


Sink-Sink
Coolant Flow Map



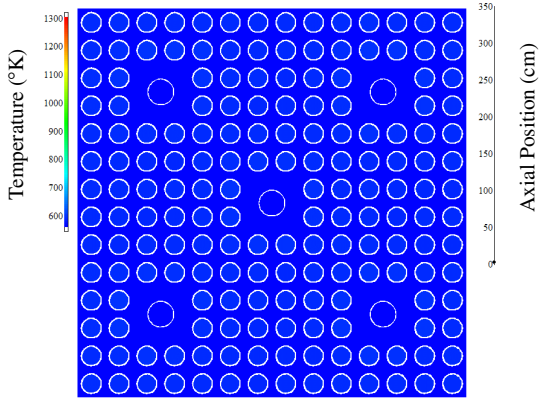
- Thermal feedback using a simple steady-state algorithm based on energy conservation
  - Users define heat sources and sinks in model, as well as flow paths between them
  - Code tallies fission energy deposition by sources and updates
    - Water properties (density) by sink region
    - Fuel temperature by source region

Eigenvalue Convergence with Thermal Feedback Iterations – PWR Fuel Pin



Temperature Defect (not shown) 0.0287 Δk/k

Axial Temperature Rise in PWR Assembly

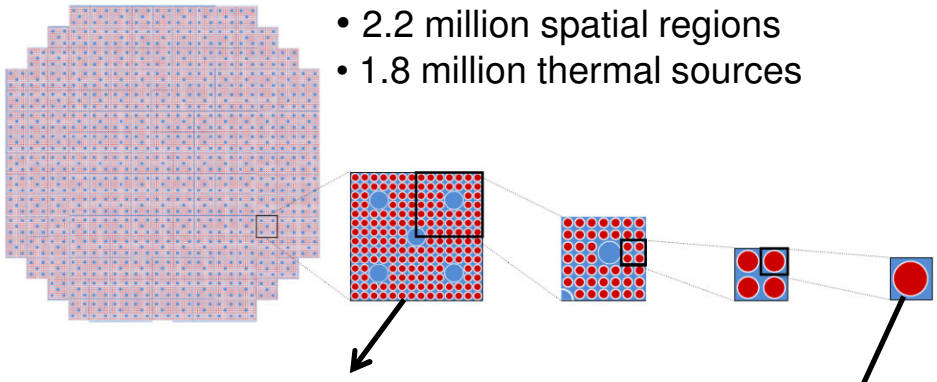


DP Griesheimer, DF Gill, JW Lane, DL Aumiller, "An Integrated Thermal Hydraulic Feedback Method for Monte Carlo Reactor Calculations," Proceedings of PHYSOR 2008, Interlaken, Switzerland, September 14-19, 2008 (CD-ROM).

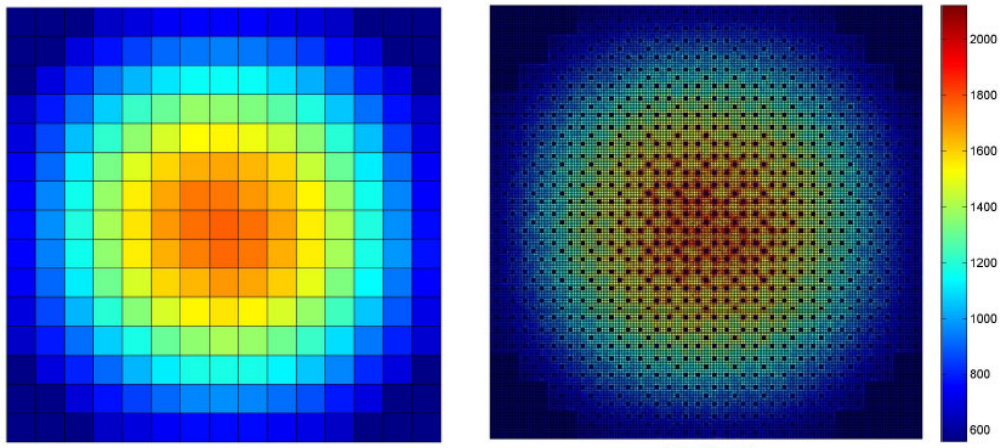
In-Line Thermal Feedback

Calvert Cliffs Thermal Homogenization Study

- 2.2 million spatial regions
- 1.8 million thermal sources



Average Fuel Temperature at Core Mid-plane

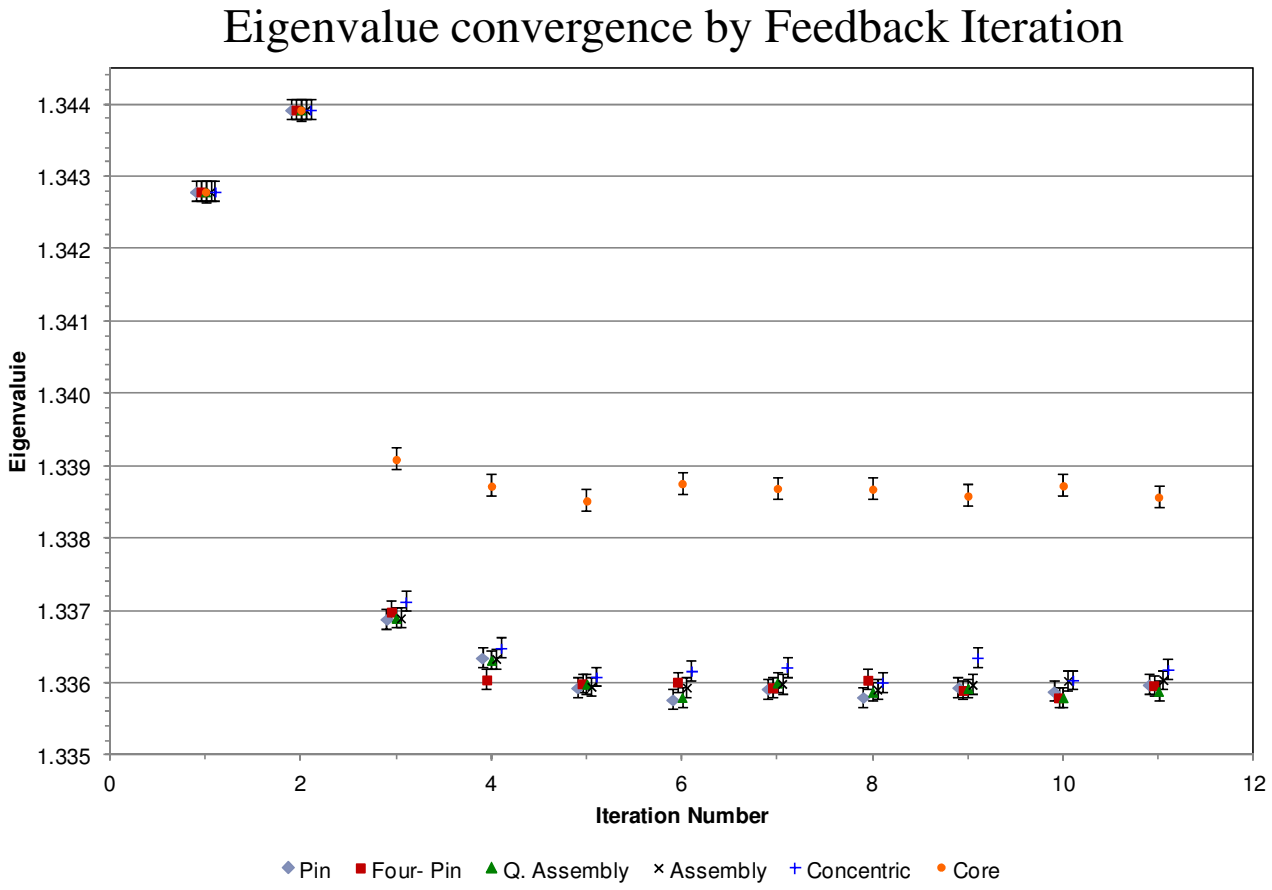


- Issues
  - Source/Sink homogenization
  - Convergence strategy
  - Model creation is labor intensive
  - Requires multi-temperature cross sections for fuel heating
  - Thermal conductivity of fuel/gap/clad changes with temperature and burnup

BR Hanna, "Spatial Homogenization Used in Thermal Hydraulic Feedback Method for Monte Carlo Reactor Calculations," Report for NucE 596, Pennsylvania State University (2011). Approved for public release as Bettis Report B-T-3865.

In-Line Thermal Feedback

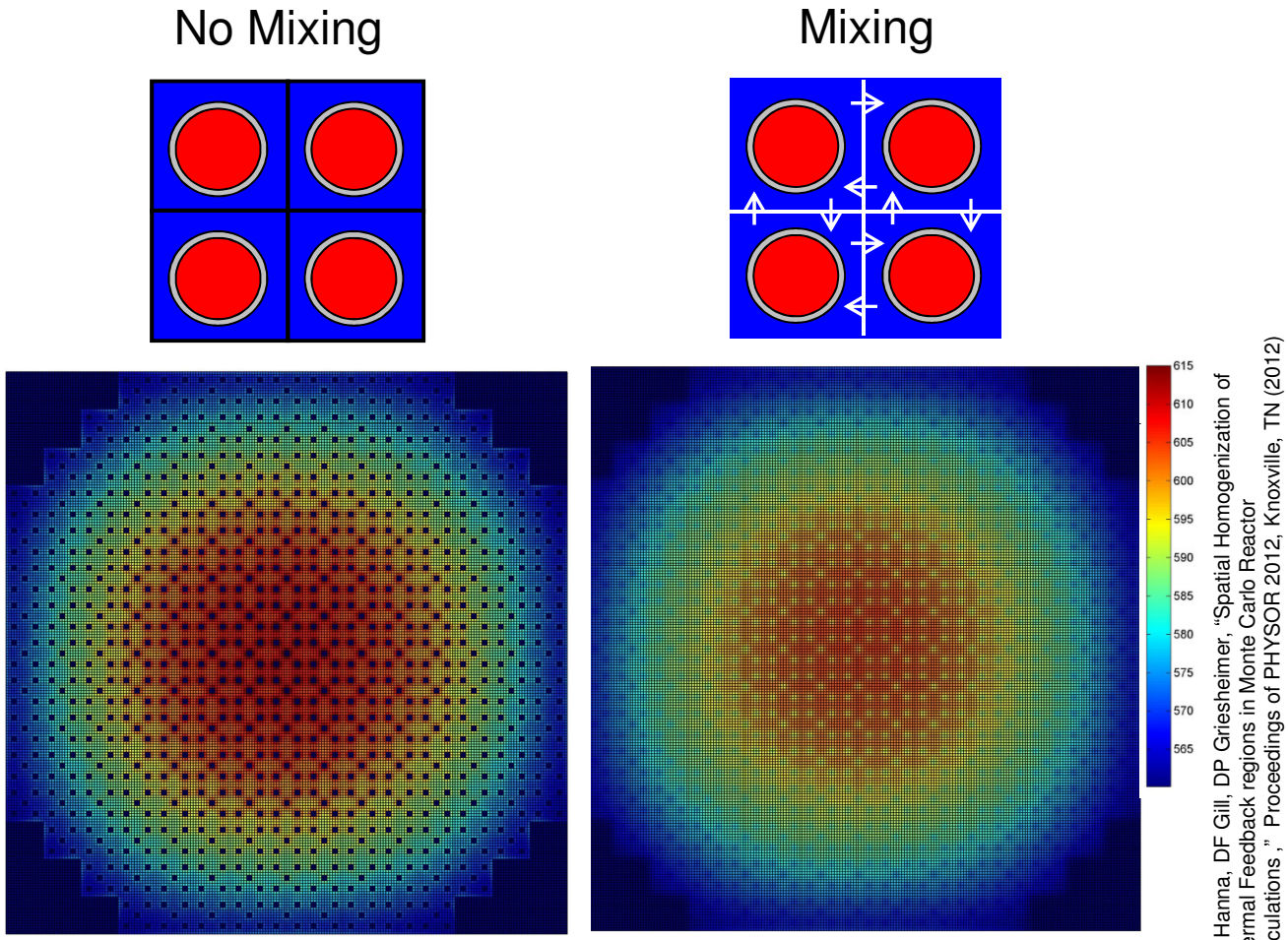
- k_{eff} Convergence
  - For Calvert Cliffs example, eigenvalue converges after 5 thermal feedback iterations (from isothermal initial condition)
  - Spatial homogenization of thermal regions did not show a large change in calculated eigenvalue



BR Hanna, DF Gill, DP Griesheimer, "Spatial Homogenization of Thermal Feedback regions in Monte Carlo Reactor Calculations ," Proceedings of PHYSOR 2012, Knoxville, TN (2012)

In-Line Thermal Feedback

- Effects of lateral coolant mixing
  - Explicitly modeled mixing of coolant between adjacent fuel pins
  - Assumed lateral mass flux rate was 1% of axial mass flux rate
  - Small increase in reactivity due to mixing of unheated coolant in control rod guide tubes.

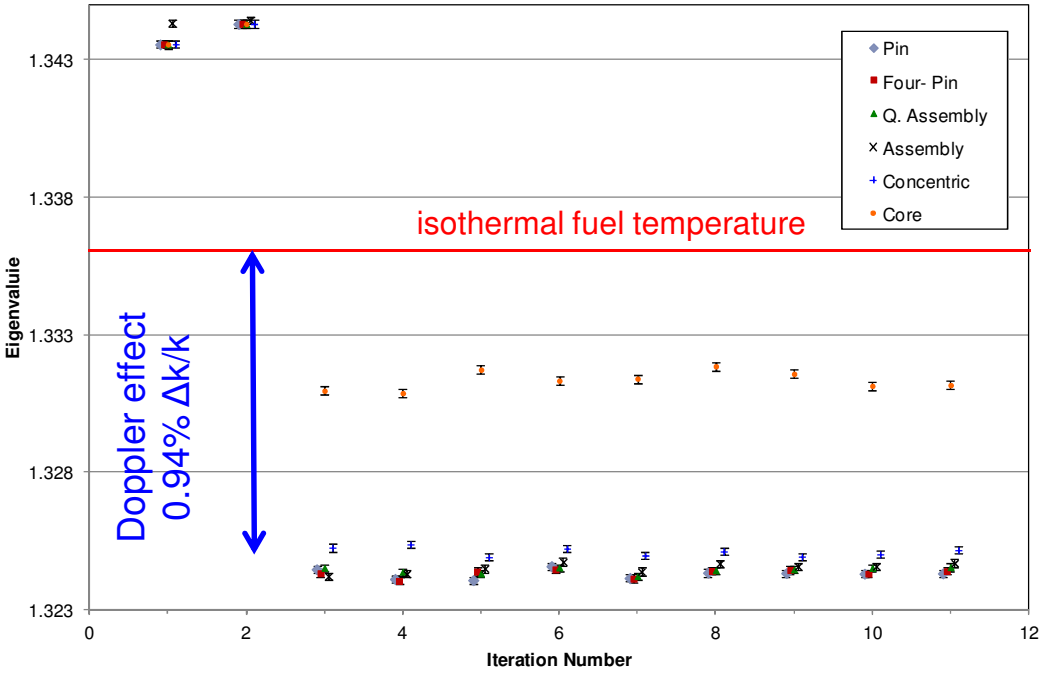


Coolant temperature (K) at top of core

BR Hanna, DF Gill, DP Griesheimer, "Spatial Homogenization of Thermal Feedback regions in Monte Carlo Reactor Calculations ," Proceedings of PHYSOR 2012, Knoxville, TN (2012)

In-Line Thermal Feedback

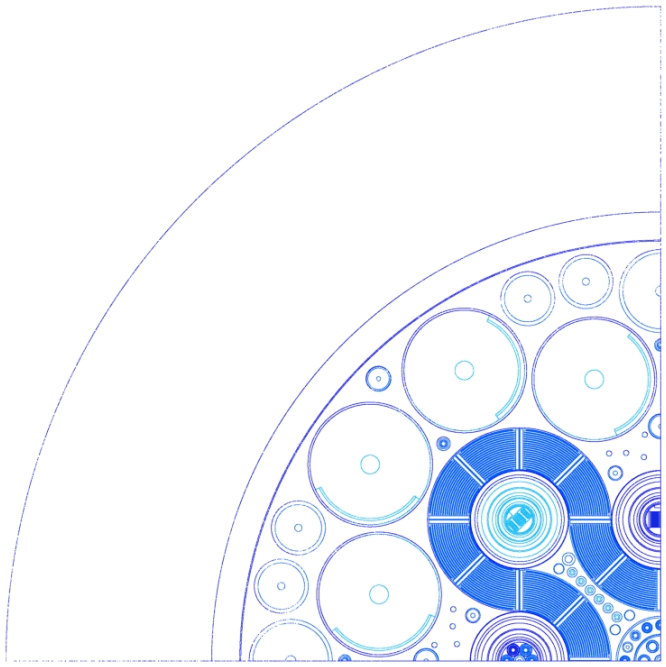
- Fuel Heating (Doppler Broadening)
  - Nuclear library created to include material cross sections at different temperatures.
  - Run-time statistical interpolation between specified temperatures to obtain cross section approximation.



Material	Cross Section Temperature (K)													
O-16	500	550	575	600	625	750	1000	1250	1500	1750	2000	2250	2500	2750
U-235, U-238	500	750	1000	1250	1500	1750	2000	2250	2500	2750				
H-H_2O	500	550	575	600	625									
ZR	500	600												

In-Line Movable Geometry

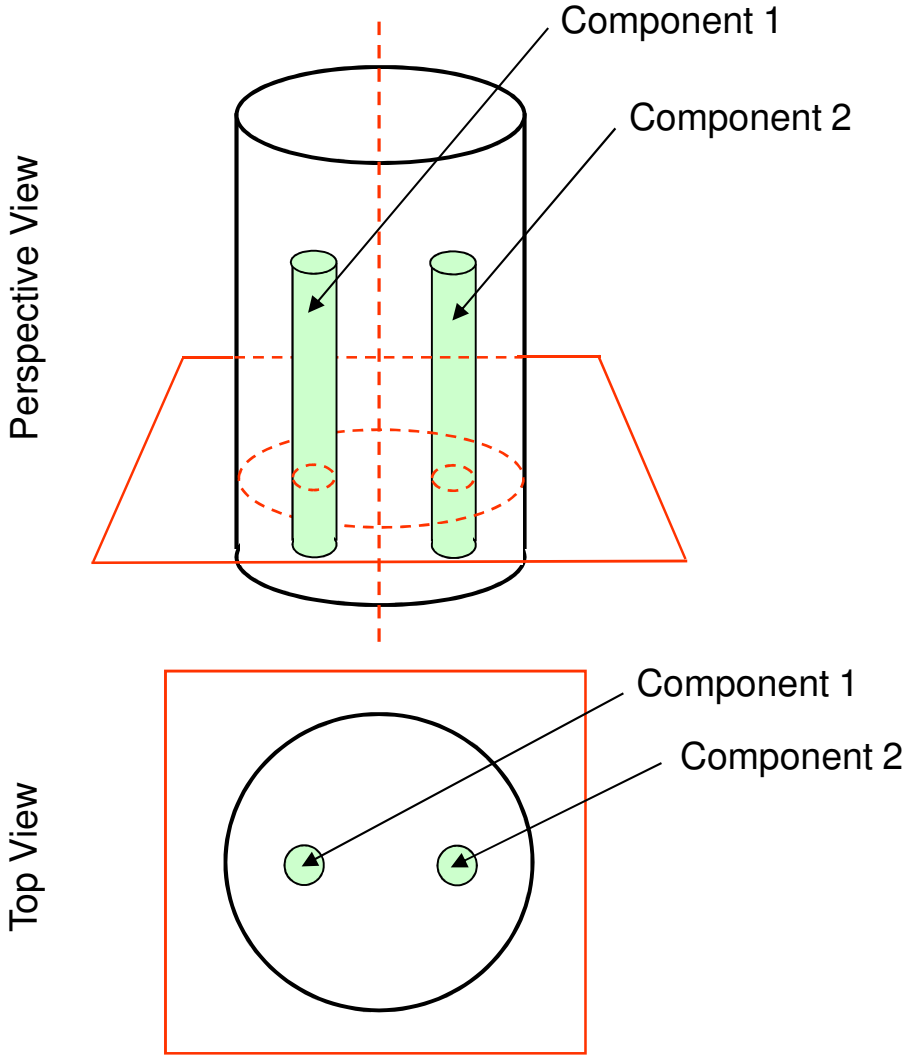
Animation of Rotating Control Drums in the Advanced Test Reactor (ATR)



Model courtesy of CM Rodenbush. Animation courtesy of BR Nease.

- Combinatorial geometry allows objects to be easily rotated and translated in space
  - Users select movement vectors for components during model construction
  - Ability to move components between any steps or iterations
- Issues:
  - Difficult to check for geometry conflicts after move.
  - Difficult/expensive to recalculate model volumes after move

In-Line Movable Geometry



Example Problem Setup

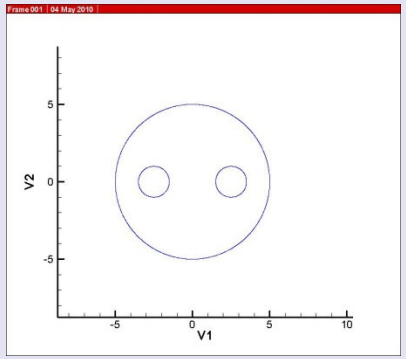
- **Component 1** – Rotation about central axis of parent cylinder.
- **Component 2** – Translation along z-axis.

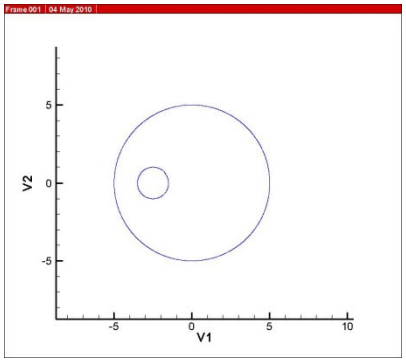
Example Control Sequence

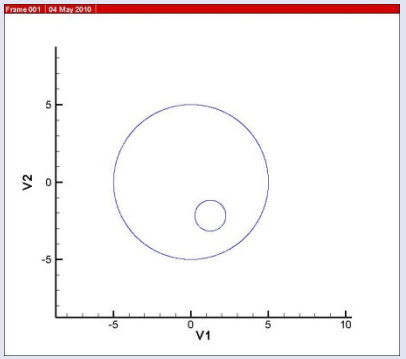
```
num_timesteps      4

<TIMESTEP>         1
{EXECUTE}       plot

<TIMESTEP>         2
move_group         2   current   10 cm
{EXECUTE}       plot

<TIMESTEP>         3
move_group         1   initial   120 degrees
{EXECUTE}       plot

<TIMESTEP>         4
move_group         1   initial   180 degrees
{EXECUTE}       plot
```

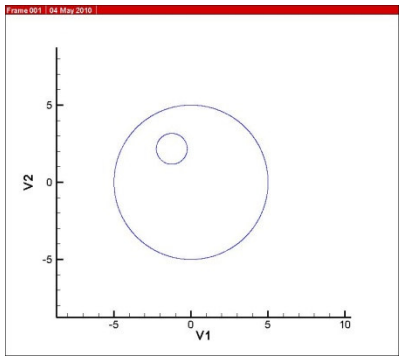
In-Line Movable Geometry

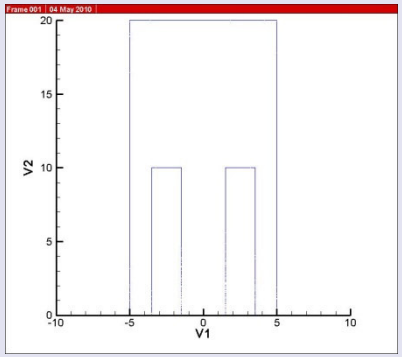
Timestep 1	Timestep 2	Timestep 3	Timestep 4
Initial setup	Translate group 2 by 10 cm along its direction vector	Rotate group 1 by 120 degrees around z-axis	Rotate group 1 by 180 degrees around z-axis

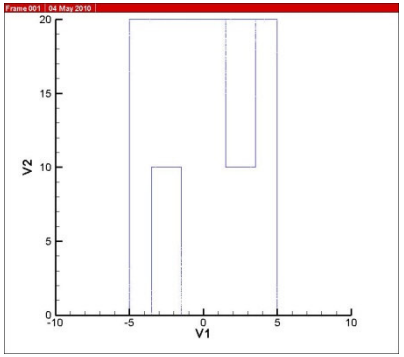








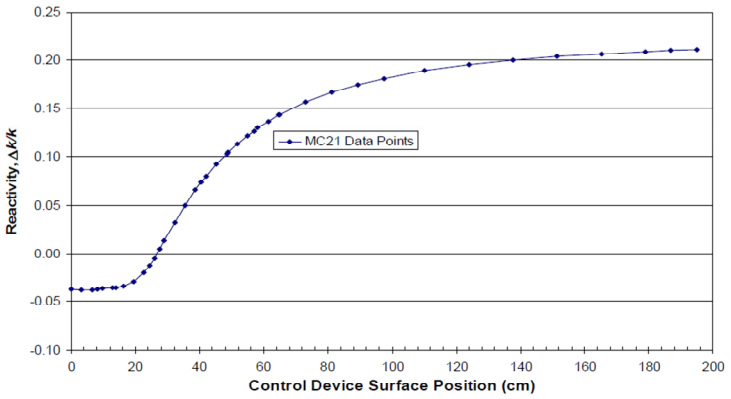




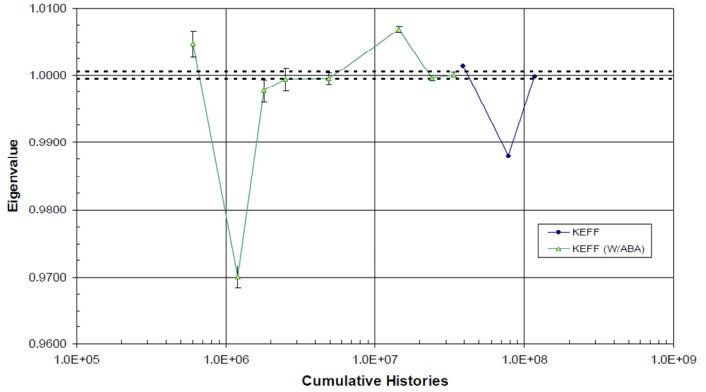
In-Line k_{eff} Search Capability

- Search algorithm automatically moves selected components to achieve a target eigenvalue
  - Adaptive batching algorithm (ABA) attempts to minimize run time
- Issues:
  - Incorporating statistical uncertainty when determining convergence
  - Development of fair adaptive-history termination strategies
  - Long run times

Rod Worth Curve for GE-9 Bundle Model



GE-9 Control Rod Search History

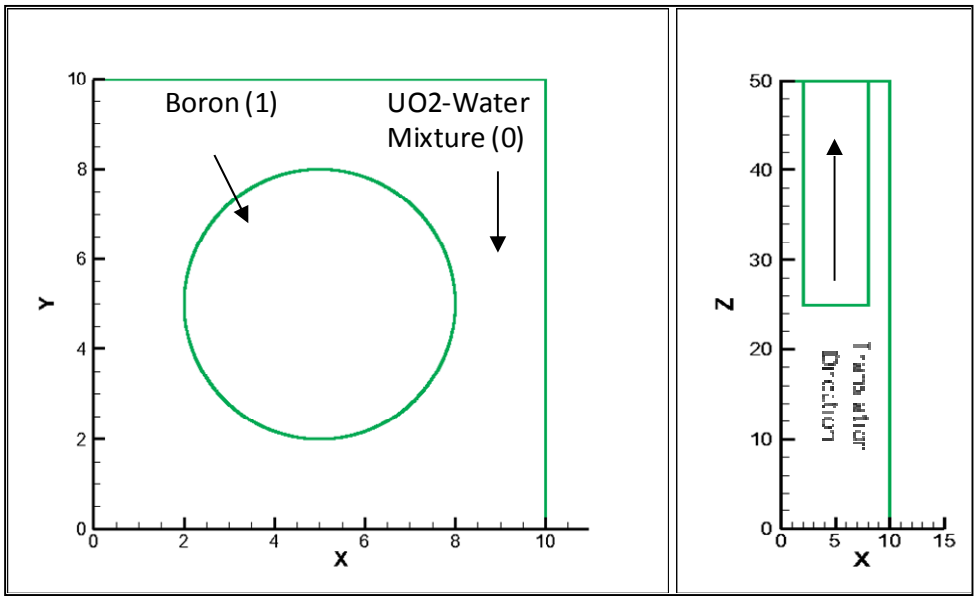


RE Morrow, TH Trumbull, TJ Donovan, TM Sutton, "A k_{eff} Search Capability in MC21," Proceedings of M&C 2007, Monterey, CA, April 15-19, 2007 (CD-ROM).

In-Line k_{eff} Search Capability

Example: Single Component Search

- Withdraw single rod until criticality



Default Search Procedure

```
<TIMESTEP> 1

movable_search  1 fully_inserted 0.0 50.0
{EXECUTE}       movable_search
```

With User Guess for Critical Position and Rod Worth

```
<TIMESTEP> 1

movable_search  1 fully_inserted 0 50.0 9.25 0.038
{EXECUTE}       movable_search
```

In-Line k_{eff} Search Capability

```
-------------------------------------------------------------------------------------------
Step 1, Iteration 1

  It      k-eff     pcm         CI              Loc      Histories     group ID  Ref Config

   1  0.5135646  -48644  4.839E-04      0.00000E+00        5500000            1   fully_inserted
   2  1.4389616   43896  6.809E-04      5.00000E+01        5500000            1   fully_inserted
   3  1.1834915   18349  8.227E-04      2.62825E+01        5500000            1   fully_inserted
   4  0.6244105  -37559  5.968E-04      9.24744E+00        5500000            1   fully_inserted
   5  1.0469380    4694  8.919E-04      2.06916E+01        5500000            1   fully_inserted
   6  1.0110453    1105  7.060E-04      1.94203E+01        5500000            1   fully_inserted
   7  0.9986132    -139  6.947E-04      1.90290E+01        5500000            1   fully_inserted


  Target Eigenvalue:                1.0000 +/- 0.0050
  Converged Eigenvalue:             0.9986 +/- 0.0007
  Total Histories:                  38500000
  Total Time:                         3.9390     mins
-------------------------------------------------------------------------------------------
```

Default search procedure

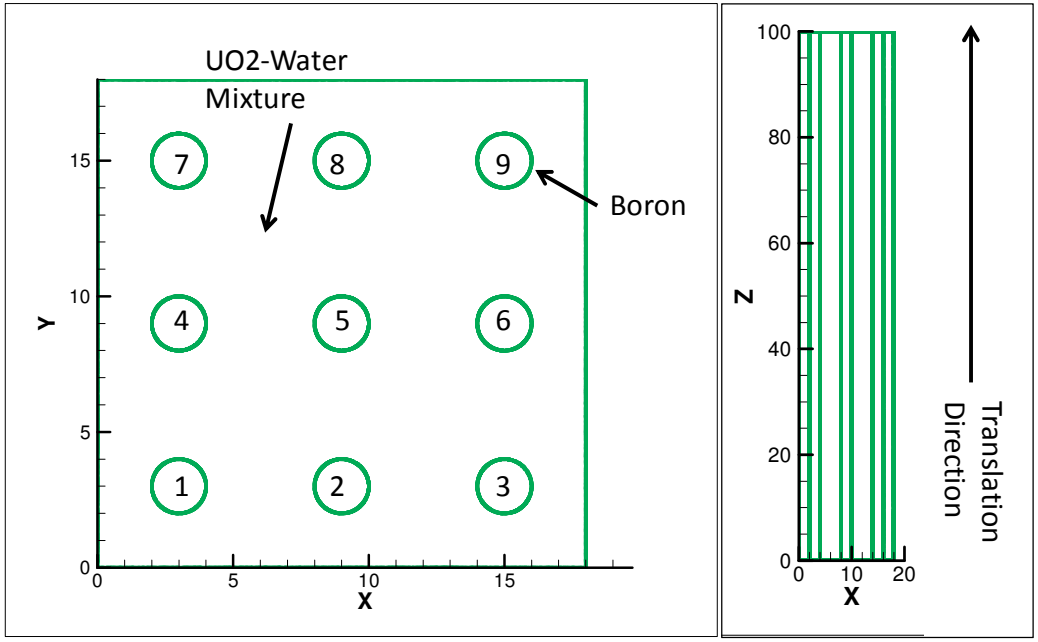
```
-------------------------------------------------------------------------------------------
Step 1, Iteration 1

  It      k-eff     pcm         CI              Loc      Histories     group ID  Ref Config

   1  0.6253822  -37462  5.732E-04      9.24744E+00        5500000            1   fully_inserted
   2  0.9993021     -70  8.077E-04      1.90398E+01        5500000            1   fully_inserted

  Target Eigenvalue:                1.0000 +/- 0.0050
  Converged Eigenvalue:             0.9993 +/- 0.0008
  Total Histories:                  11000000
  Total Time:                         1.0666     mins
-------------------------------------------------------------------------------------------
```

With initial guess and worth

In-Line k_{eff} Search Capability

Example: Search Sequence

- Withdraw individual rods until criticality



- Search sequences allow code to move components in a predetermined order until target eigenvalue is reached.

```
<SEQUENCE> 1
   move_group       all initial
   movable_search   1 all_rods_in   0.0 100.0
   movable_search   2 all_rods_in   0.0 100.0
   movable_search   3 all_rods_in   0.0 100.0
   movable_search   4 all_rods_in   0.0 100.0
   movable_search   5 all_rods_in   0.0 100.0
   movable_search   6 all_rods_in   0.0 100.0
   movable_search   7 all_rods_in   0.0 100.0
   movable_search   8 all_rods_in   0.0 100.0
   movable_search   9 all_rods_in   0.0 100.0
```

In-Line k_{eff} Search Capability

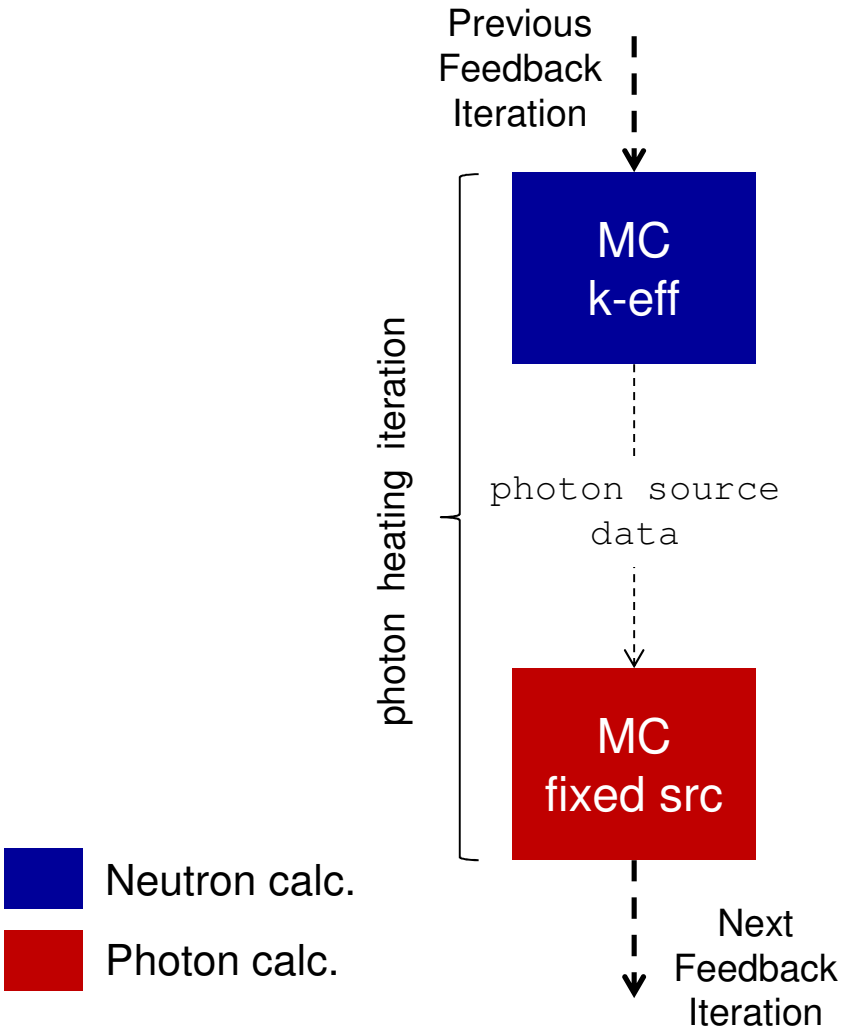
Search Iterations

Search Group ID

```
Timestep 1

  It    Step      k-eff      pcm         CI              Loc       Histories     group ID
   1       2  0.4393438  -56066  4.738E-04      0.00000E+00         7500000            1
   2       2  0.5295183  -47048  4.981E-04      1.00000E+02         7500000            1
   3       3  0.5293375  -47066  5.087E-04      0.00000E+00         7500000            2
   4       3  0.6258336  -37417  5.758E-04      1.00000E+02         7500000            2
   5       4  0.6270896  -37291  5.914E-04      0.00000E+00         7500000            3
   6       4  0.7277876  -27221  5.907E-04      1.00000E+02         7500000            3
   7       5  0.7281835  -27182  6.465E-04      0.00000E+00         7500000            4
   8       5  0.8121144  -18789  6.761E-04      1.00000E+02         7500000            4
   9       6  0.8124487  -18755  7.333E-04      0.00000E+00         7500000            5
  10       6  0.8991067  -10089  6.540E-04      1.00000E+02         7500000            5
  11       7  0.8994640  -10054  6.357E-04      0.00000E+00         7500000            6
  12       7  0.9885627   -1144  6.587E-04      1.00000E+02         7500000            6
  13       8  0.9886200   -1138  5.911E-04      0.00000E+00         7500000            7
  14       8  1.0661995    6620  6.888E-04      1.00000E+02         7500000            7
  15       8  0.9898617   -1014  6.899E-04      1.46689E+01         7500000            7
  16       8  0.9984339    -157  5.948E-04      2.60016E+01         7500000            7
  17       8  1.0001676      17  7.269E-04      2.80720E+01         7500000            7


  Target Eigenvalue:                  1.0000 +/- 0.0010
  Converged Eigenvalue:               1.0002 +/- 0.0007
  Total Histories:                    127500000
  Total Time:                           26.113     mins
```

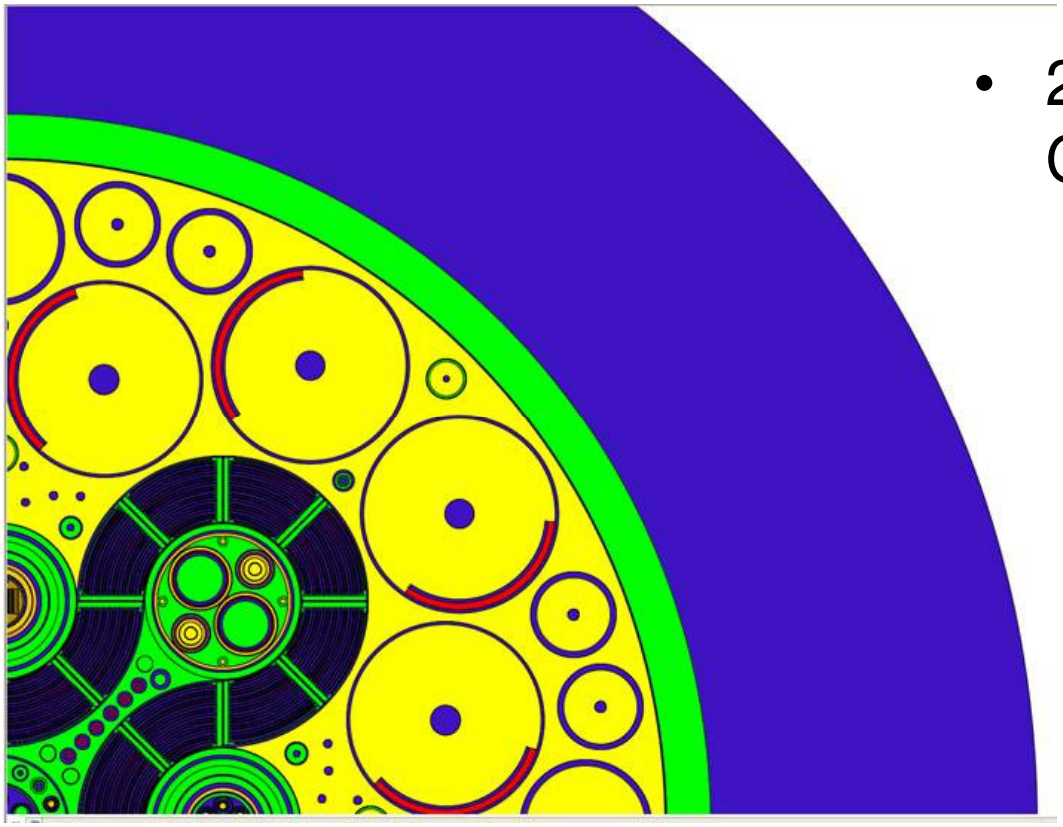
Convergence Information

In-Line Photon Heating Calculation



- Each photon heating calculation includes 2 transport simulations
- MC Neutron transport simulation
  - Samples fission and capture photons created during neutron transport and saves source information to a photon source data file
- MC Photon transport simulation
  - Photon source sites are read in from the photon source data file
  - MC code computes and saves
    - Global photon energy leakage
    - Photon energy deposited in every cell
  - All photon results are normalized to a per starting eV basis.

ATR Heating Model



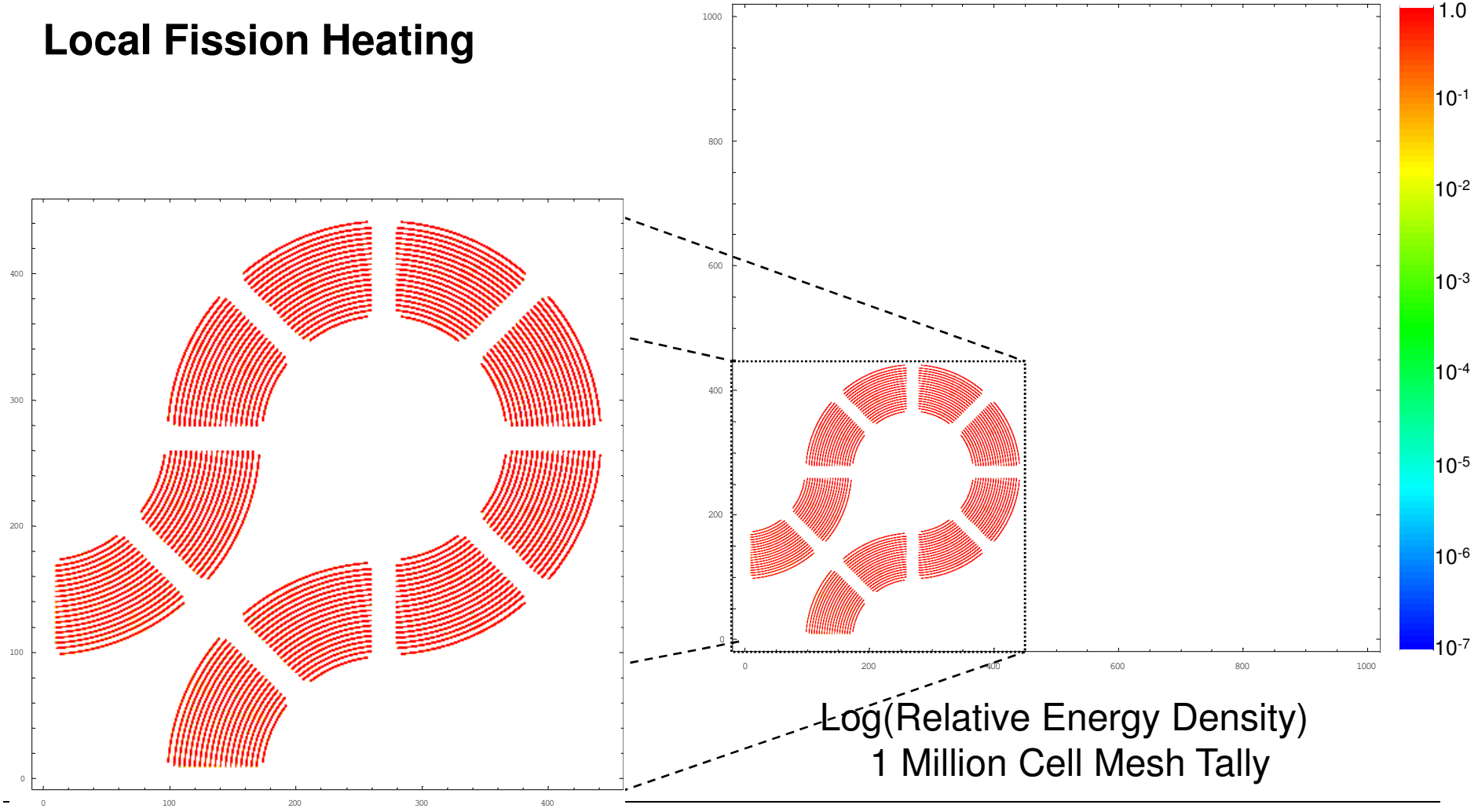
- 2D Slice of ATR Quarter Core (NE Quadrant)
  - z = 85.0 – 90.0 cm
  - 5,100 batches (100 discard)
  - 10,000 histories/batch
  - 50 million histories total
  - k_{eff} = 0.8367 ± 0.0002
  - In-line coupled neutron/photon heating

Blue = Water; Red = Hafnium; Green = Aluminum; Yellow = Beryllium

Model and illustration courtesy of C.M. Rodenbush

ATR Heating Model

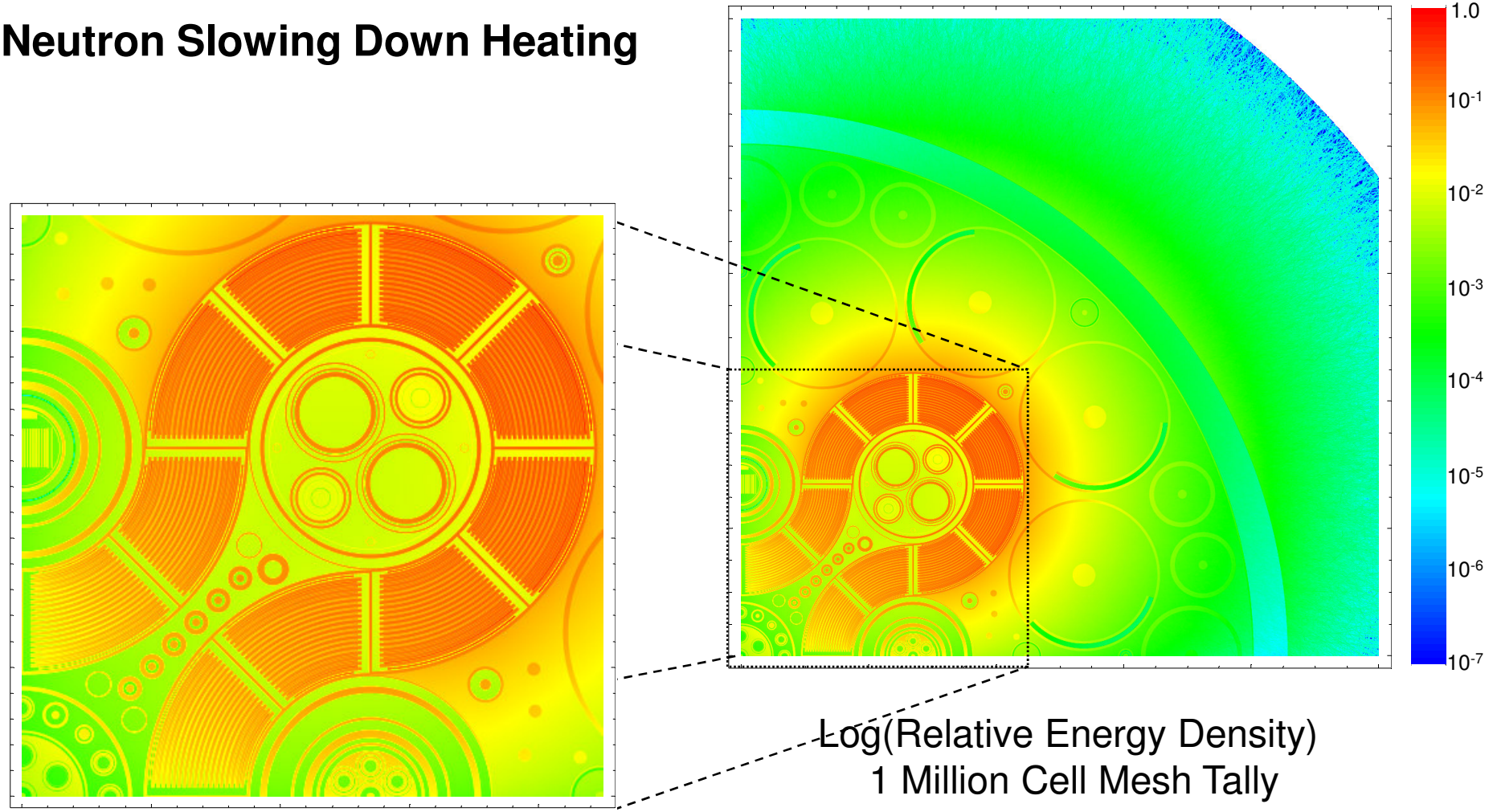
Local Fission Heating



Log(Relative Energy Density)
1 Million Cell Mesh Tally

ATR Heating Model

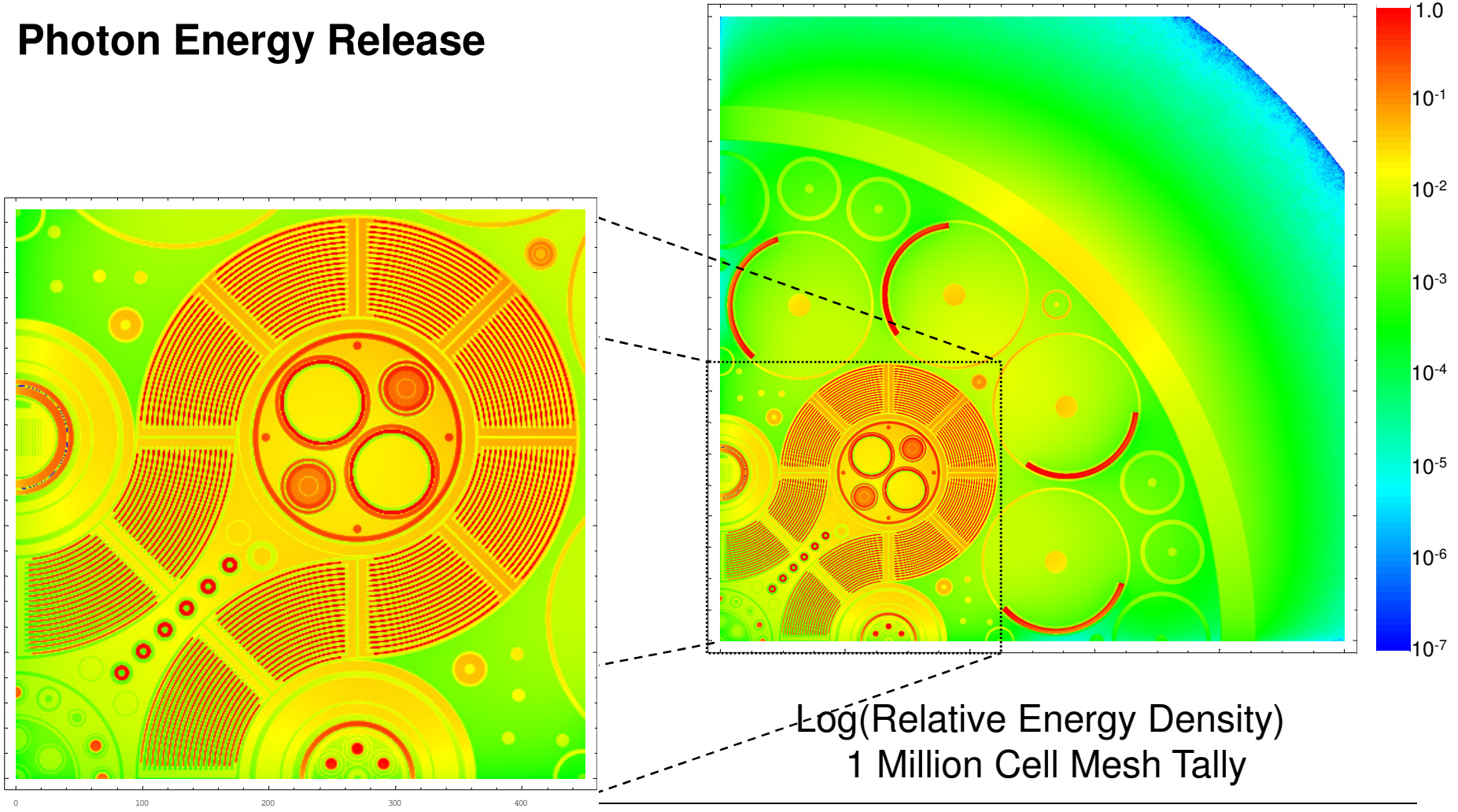
Neutron Slowing Down Heating



Log(Relative Energy Density)
1 Million Cell Mesh Tally

ATR Heating Model

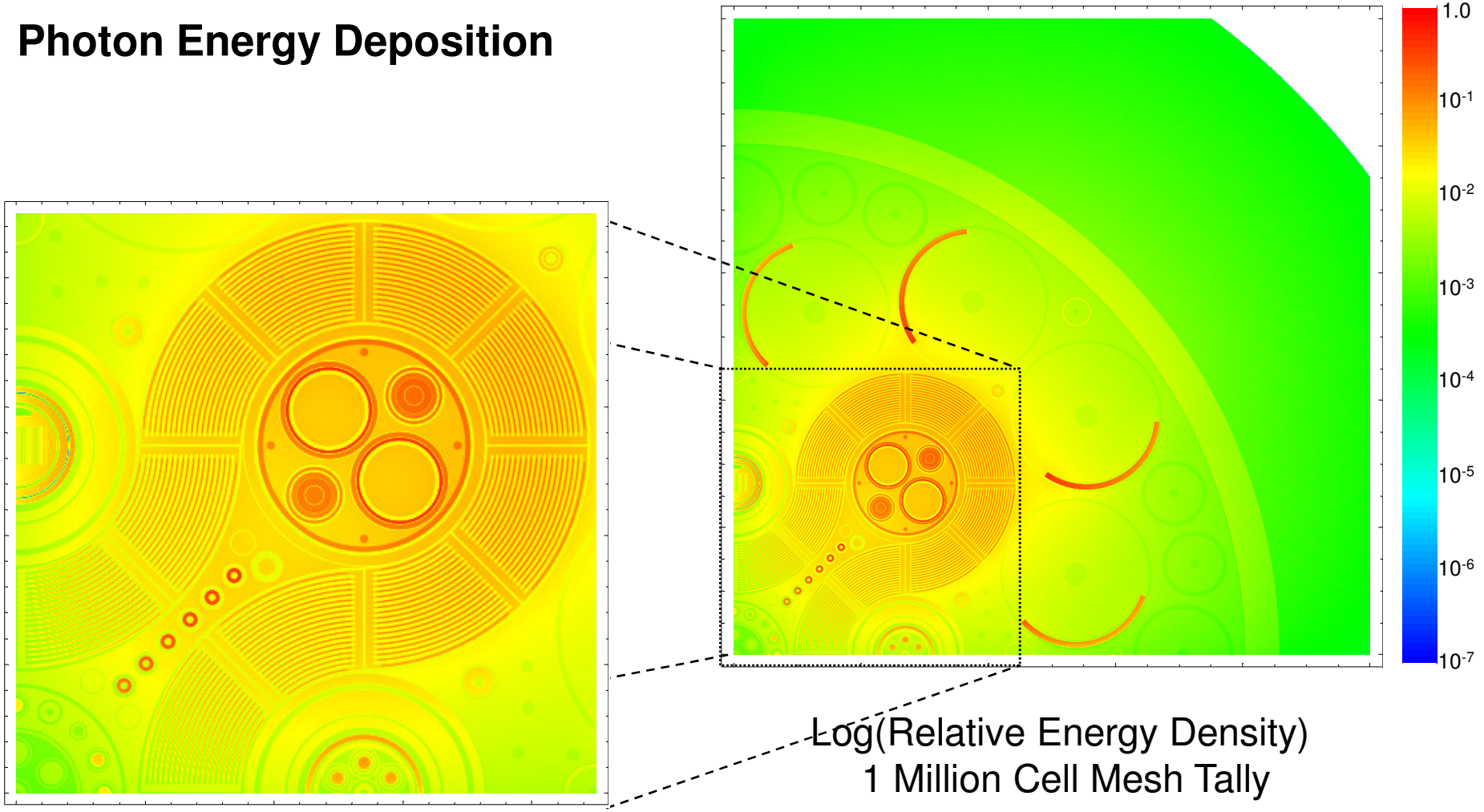
Photon Energy Release



Log(Relative Energy Density)
1 Million Cell Mesh Tally

ATR Heating Model

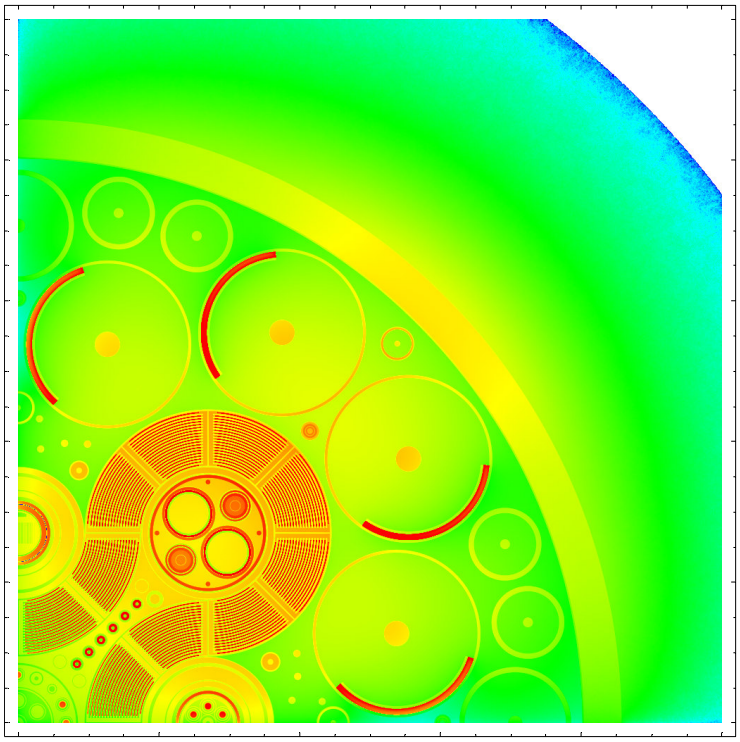
Photon Energy Deposition



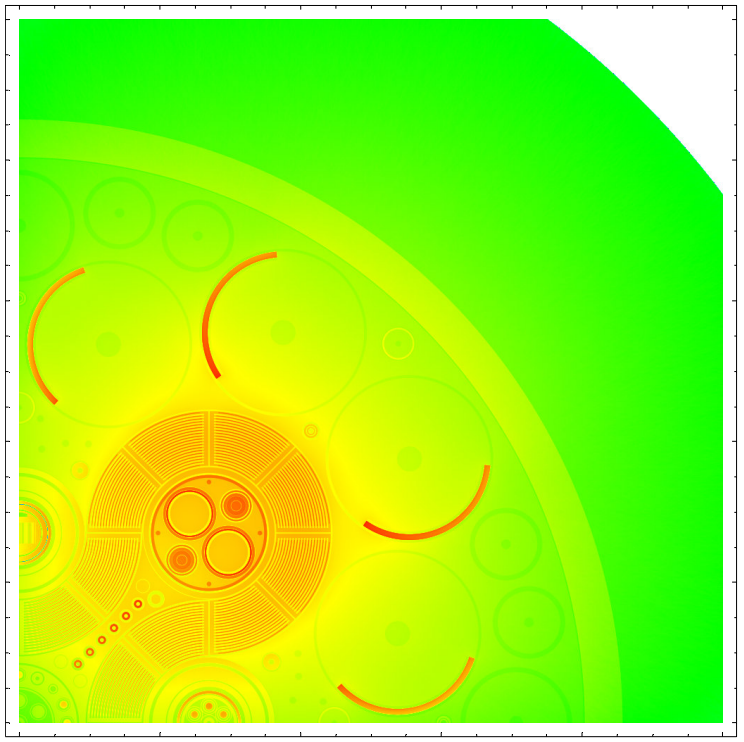
Log(Relative Energy Density)
1 Million Cell Mesh Tally

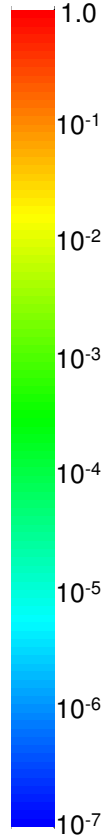
ATR Photon Redistribution

Emission



Deposition





Log(Relative Energy Density)
1 Million Cell Mesh Tally

Conclusions

- In order to achieve full potential as a tool for reactor design and analysis, MC methods must match the capabilities of existing deterministic design tools

- In addition to overcoming the traditional challenges of computational speed and management of statistical uncertainty, MC methods must incorporate in-line support for important feedback effects

- Many in-line feedback methods have been prototyped, typically for one effect at a time. However additional research and development is still needed, especially on feedback sequences, the propagation of error, convergence criteria, and convergence in the presence of statistical uncertainty is still needed.