LA-UR-12-20338
Approved for public release; distribution is unlimited.

Title: On-The-Fly Neutron Doppler Broadening for MCNP

Author(s): Brown, Forrest B.
Martin, William R.
Yesilyurt, Gokhan
Wilderman, Scott

Intended for: MCNP reference, seminar at U. Michigan
Web

2012-03-26

On-The-Fly Neutron Doppler Broadening for MCNP

Forrest Brown[1], William Martin[2], Gokhan Yesilyurt[3], Scott Wilderman[2]

[1]Monte Carlo Methods (XCP-3), LANL
[2]University of Michigan
[3]Argonne National Laboratory

Abstract

On-The-Fly Neutron Doppler Broadening for MCNP

Forrest Brown, William Martin, Gokhan Yesilyurt, Scott Wilderman

The University of Michigan, ANL, and LANL have been collaborating on a US-DOE-NE University Programs project “Implementation of On-the-Fly Doppler Broadening in MCNP5 for Multiphysics Simulation of Nuclear Reactors.” This talk describes the project and provides results from the initial implementation of On-The-Fly Doppler broadening (OTF) in MCNP and testing.

The OTF methodology involves high precision fitting of Doppler broadened cross-sections over a wide temperature range (the target for reactor calculations is 250-3200K). The temperature dependent fits are then used within MCNP during the neutron transport, for OTF broadening based on cell temperatures. It is straightforward to extend this capability to cover any temperature range of interest, allowing the Monte Carlo simulation to account for a continuous distribution of temperature ranges throughout the problem geometry.

- **Introduction**
  - Doppler Broadening - Obvious Stuff
  - Methods for Handling Temperature Variations
- **OTF Doppler Broadening in MCNP**
  - OTF Methodology
  - Union Energy Mesh
  - Temperature Fitting
  - OTF Doppler in MCNP
  - Testing
  - Work-in-Progress

Introduction

Doppler Broadening

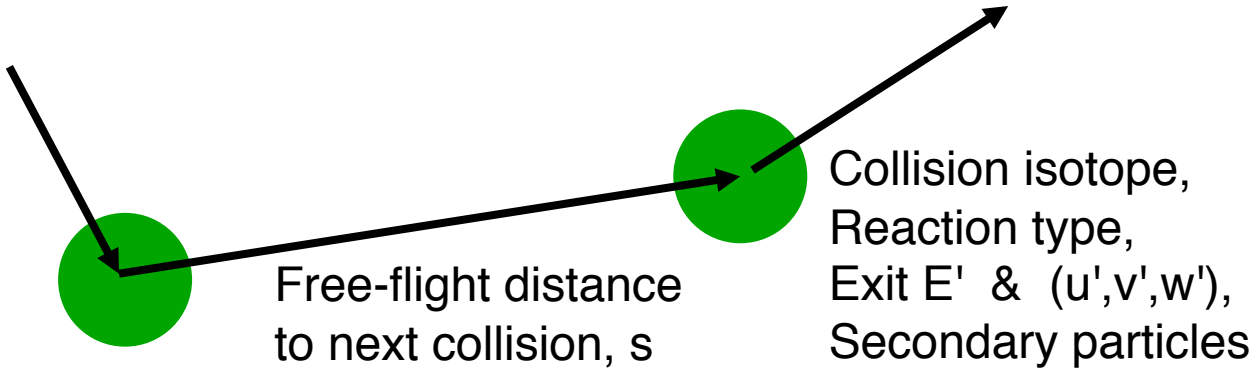
Temperature Variation in Monte Carlo Codes

- **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 scattering 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**

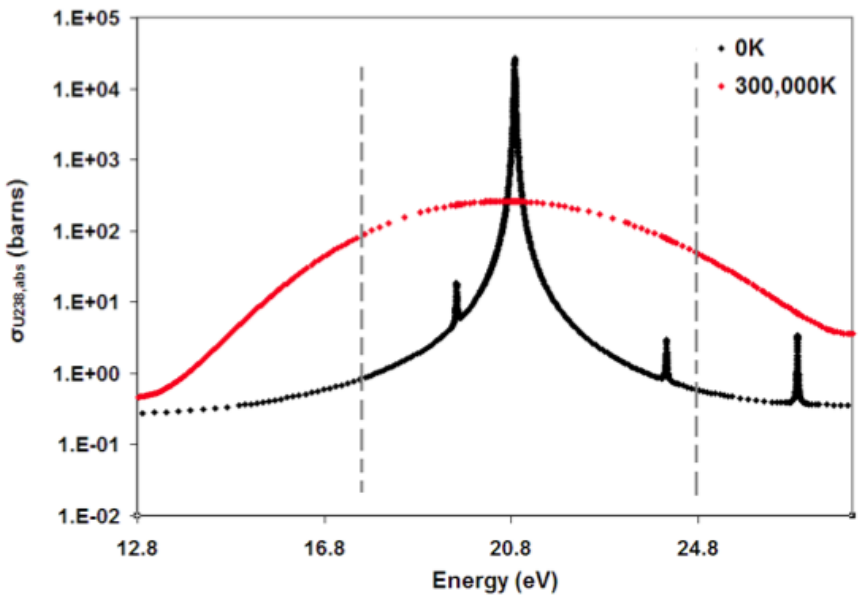
$$\sigma_{eff}(v) = \int \frac{|\vec{v} - \vec{V}|}{v} \sigma(|\vec{v} - \vec{V}|) P(\vec{V}) d\vec{V}, \qquad P(\vec{V}) = \left(\frac{M}{2\pi kT}\right)^{3/2} e^{-\left(M/2kT\right)V^2}$$

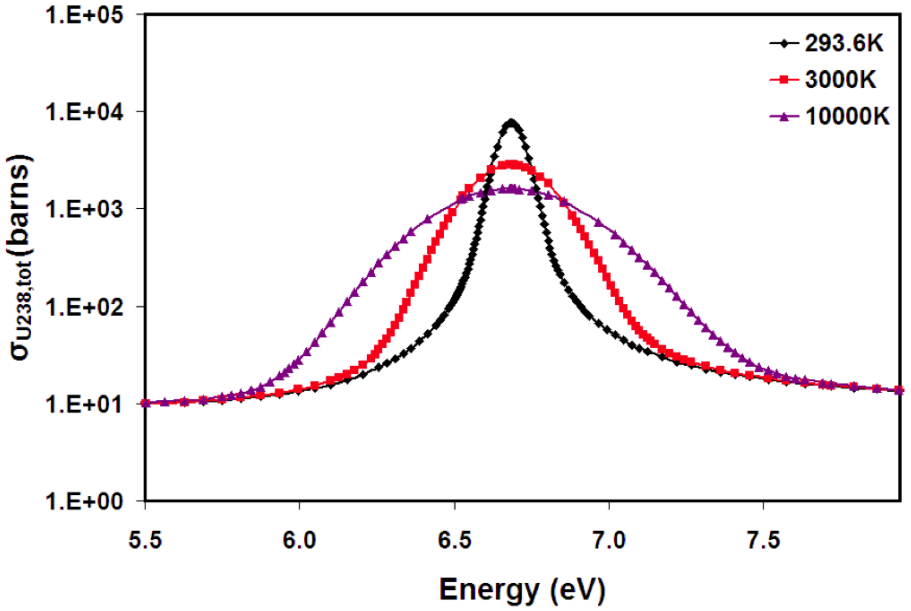
Doppler broadening equation v = neutron, V=nucleus

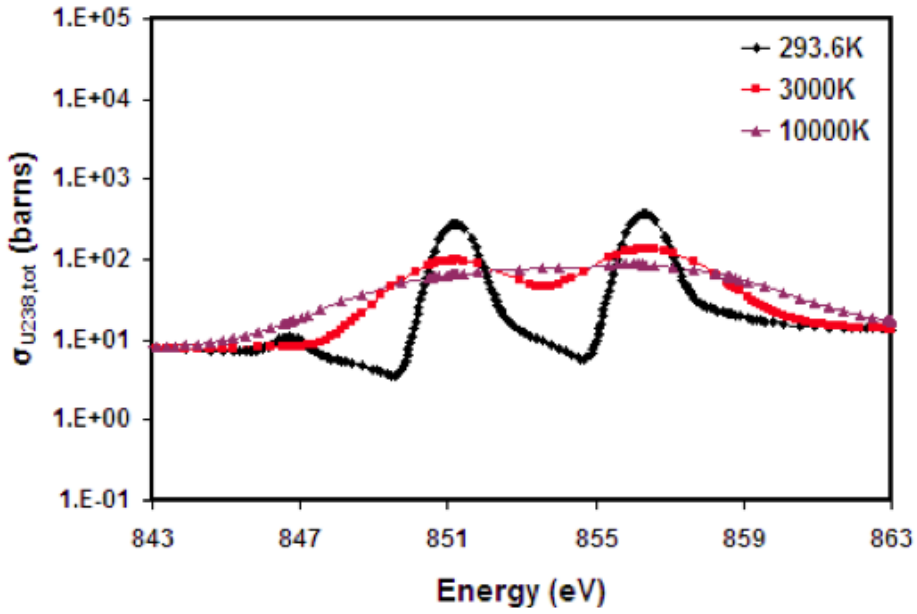
This is a convolution of the cross-section with the target energy or speed distribution.
Smears out & smoothes the cross-section, reduces peak values.

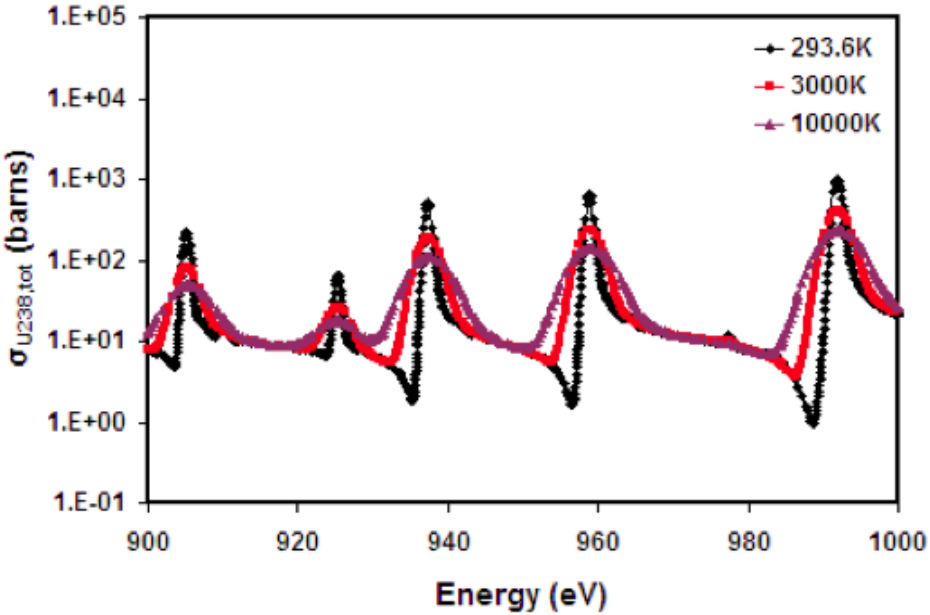
^{238}U Doppler Broadening Examples

Monte Carlo Codes
XCP-3, LANL



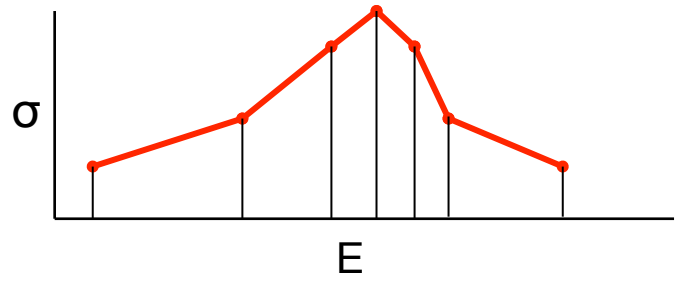






Doppler Broadening - Numerics

- **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**

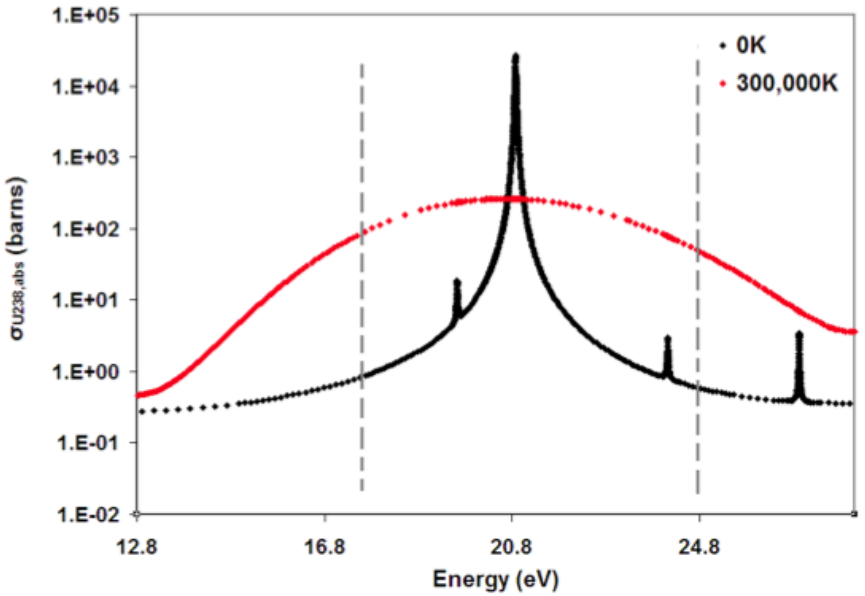
$$\sigma_{eff}(v) = \int_V \frac{|\vec{v}-\vec{V}|}{v}\,\sigma(|\vec{v}-\vec{V}|)\,P(\vec{V})\,d\vec{V}, \qquad P(\vec{V}) = \left(\frac{M}{2\pi kT}\right)^{3/2} e^{-\left(M/2kT\right)V^2}$$

  - 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

	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)

1. Prepare NJOY data at specific problem temperatures prior to MC
- Each region in MC calculation must use specific pre-broadened data
- **Exact, but very cumbersome, very large amount of xsec data**

2. Traditional NJOY+MC (approx.)

- Like (1), but round off temperatures to nearest 10-20 degrees
- **Aproximate, very cumbersome, very large amount of xsec data**

3. Stochastic Mixing (approx)

- Prepare NJOY data at a few bounding temperatures prior to MC
- Set up MC input with a mix of hot & cold data for a nuclide, such that average T for the mix matches problem 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)

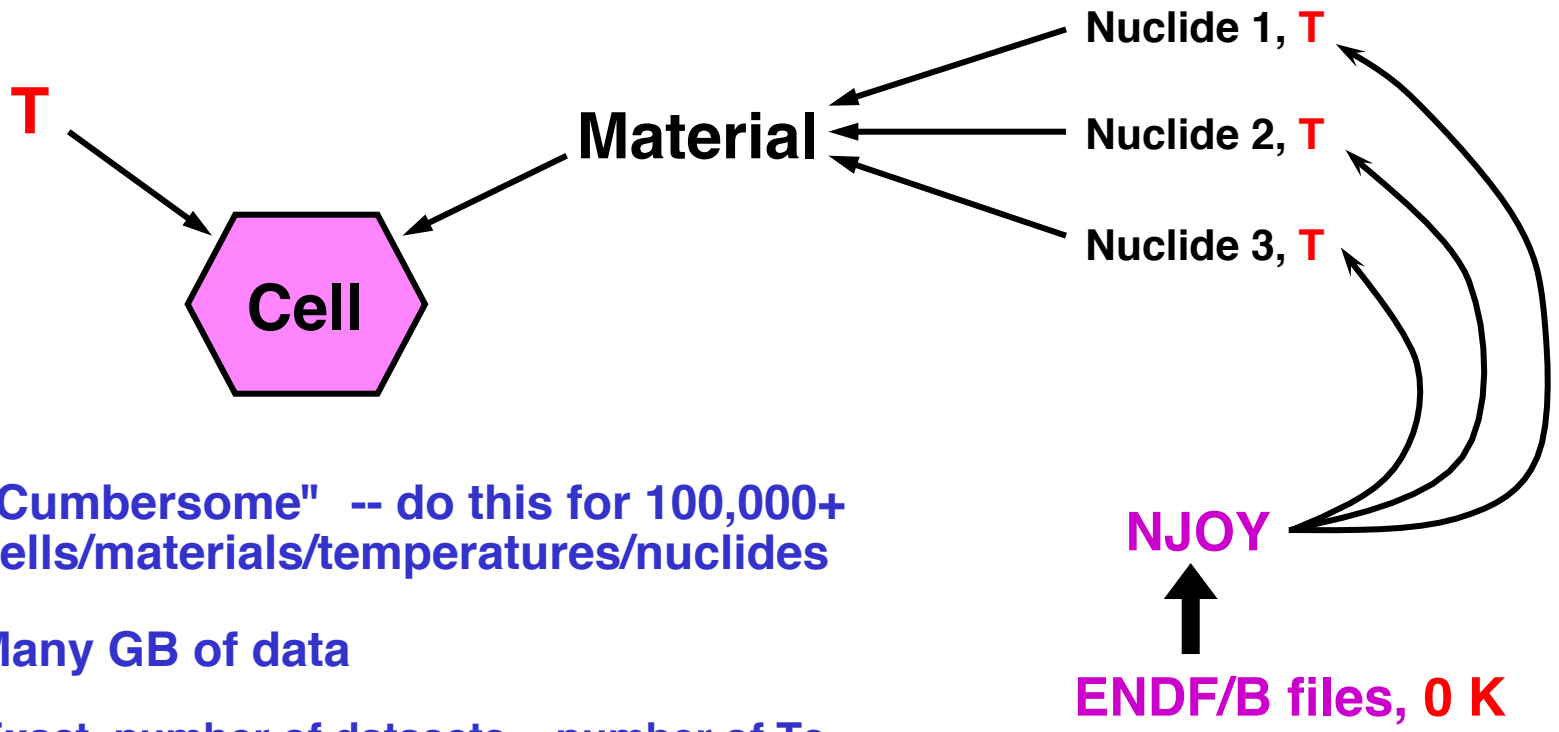
- Use only 1 set of NJOY datafiles
- During MC, use delta-tracking rejection method to broaden data as needed
- **Exact, but complex & expensive, ~4x increase in computer time**
- **Cannot do pathlength MC estimators or point-detector estimators**

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" -- do this for 100,000+ cells/materials/temperatures/nuclides
  - Many GB of data

(1) Exact, number of datasets = number of Ts

(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" -- do this for 100,000+ cells/materials/temperatures/nuclides (could be scripted…..)
- Many GB of 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
  - 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

-

U. Michigan + ANL + LANL

DOE NE-UP Project

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

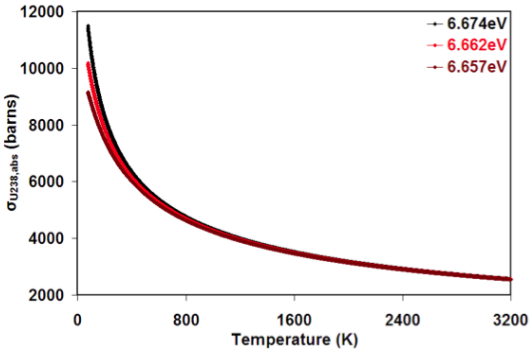
OTF Methodology – Union Energy Grid

- **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**

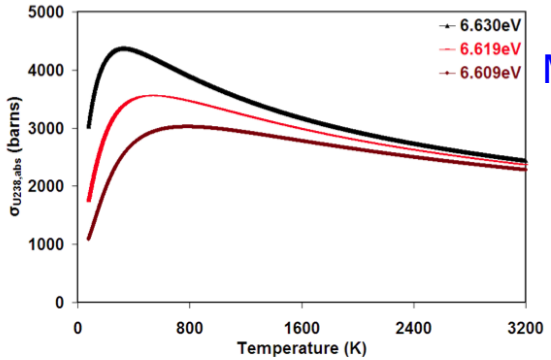
OTF Methodology – Doppler Broadening vs Temperature

Monte Carlo Codes
XCP-3, LANL



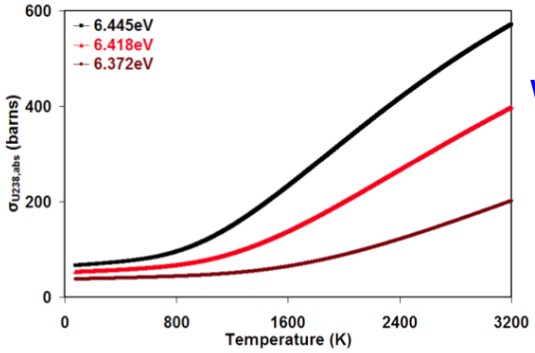
Near resonance peaks:

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



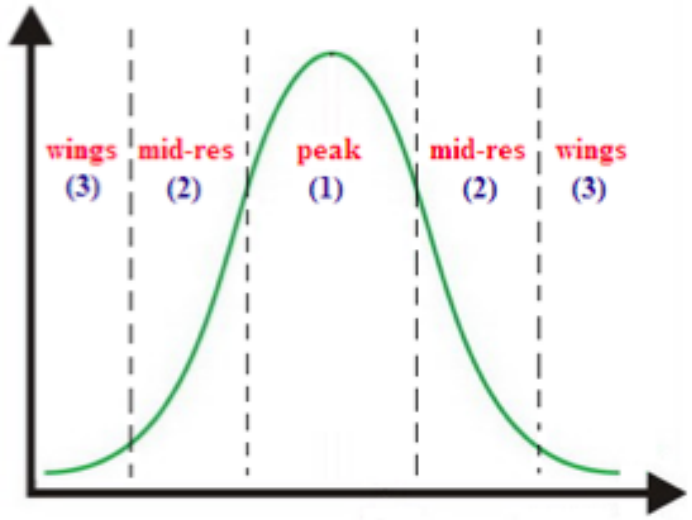
Mid resonance:

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



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

- **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 $1/T^{1/2}$

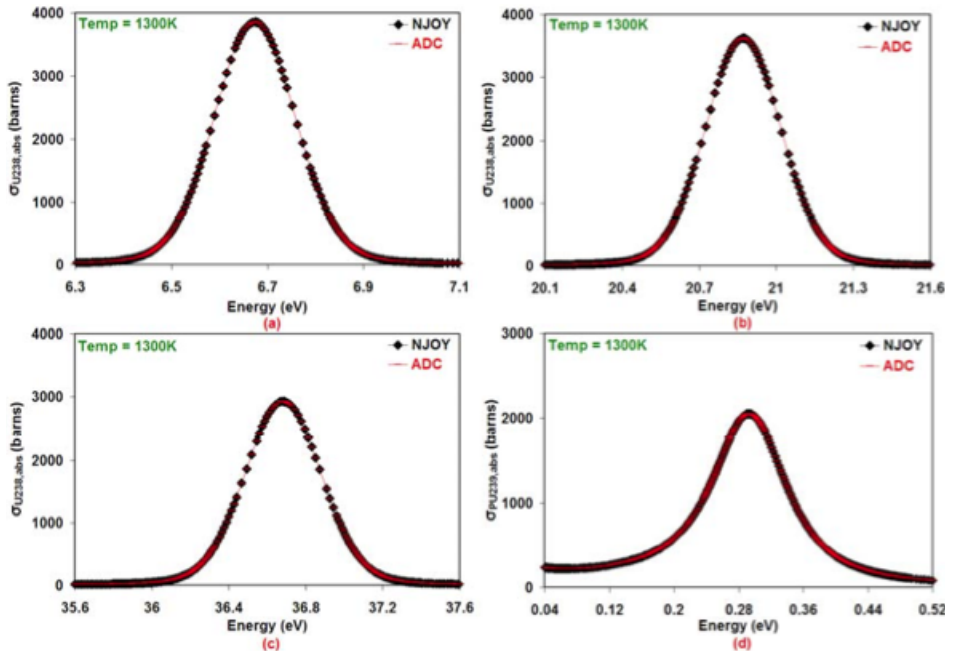
- **For 1 nuclide, at each point in the union E grid:**
  - **Exact Doppler broadening from T_{base} to all T's in range**, using sigma1 method
  - **Least-squares fitting over T**
    - Singular value decomposition, least squares for temperature dependence
    - **Fitting order chosen adaptively for 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**

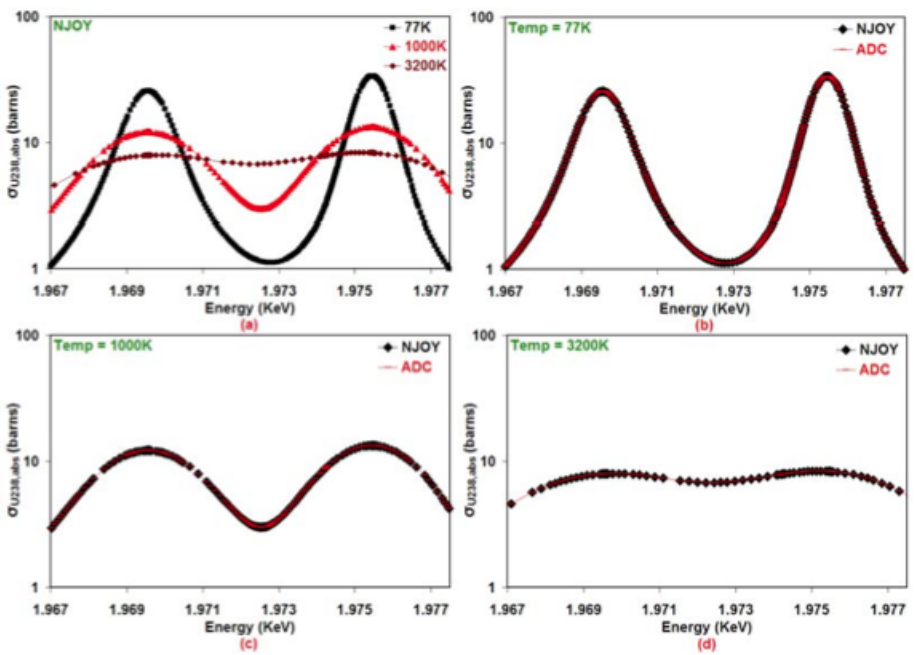
OTF Methodology – MCNP OTF

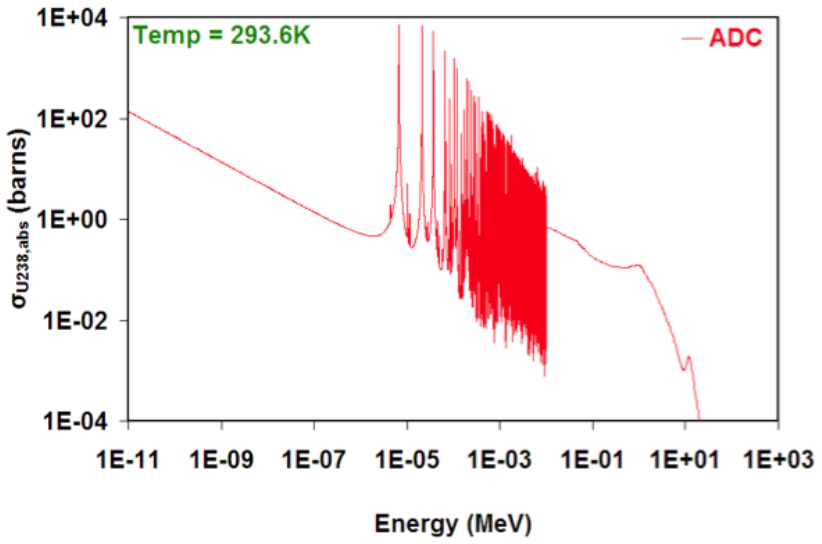
- **At problem setup, read in OTF data for various nuclides**
  - Each OTF nuclide set can have different fit orders & union E-grid & reactions
- **During simulation, if neutron in E-T range of fits**
  - Use OTF data for each nuclide to create on-the-fly Doppler broadened cross-sections at current cell 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

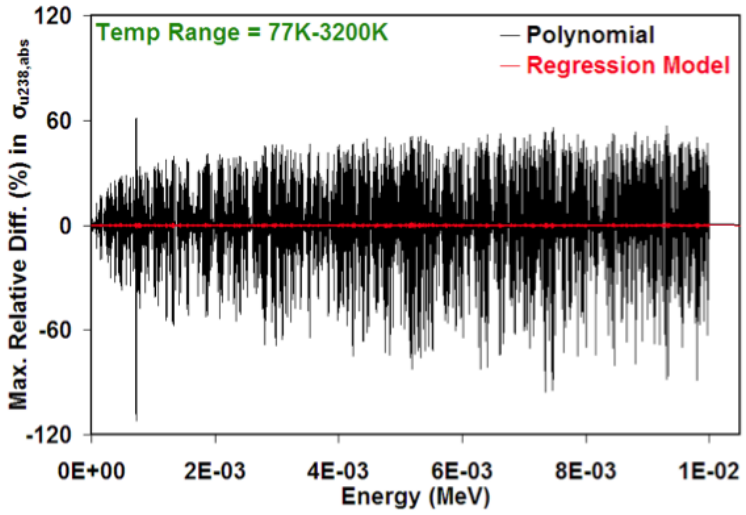
OTF Testing - Yesilyurt

Monte Carlo Codes
XCP-3, LANL

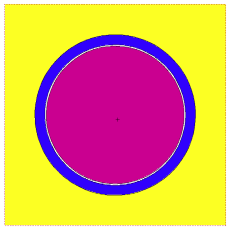








- **Doppler Reactivity Benchmark**
  - Compare k-effective for **HZP** (hot, zero power) and **HFP** (hot, full power) conditions for a unit fuel cell typical of a PWR
  - **Basic model:**



    - **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

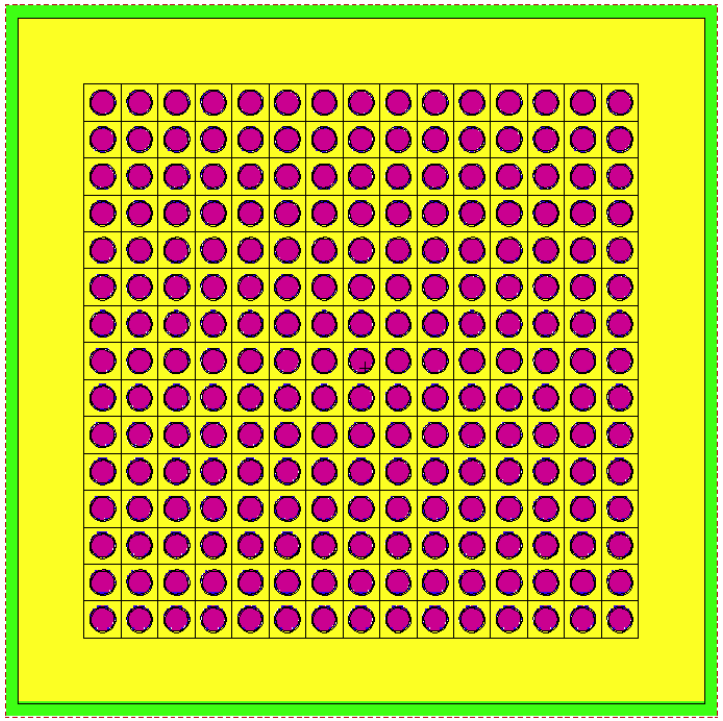
Monte Carlo Codes
XCP-3, LANL

		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 I

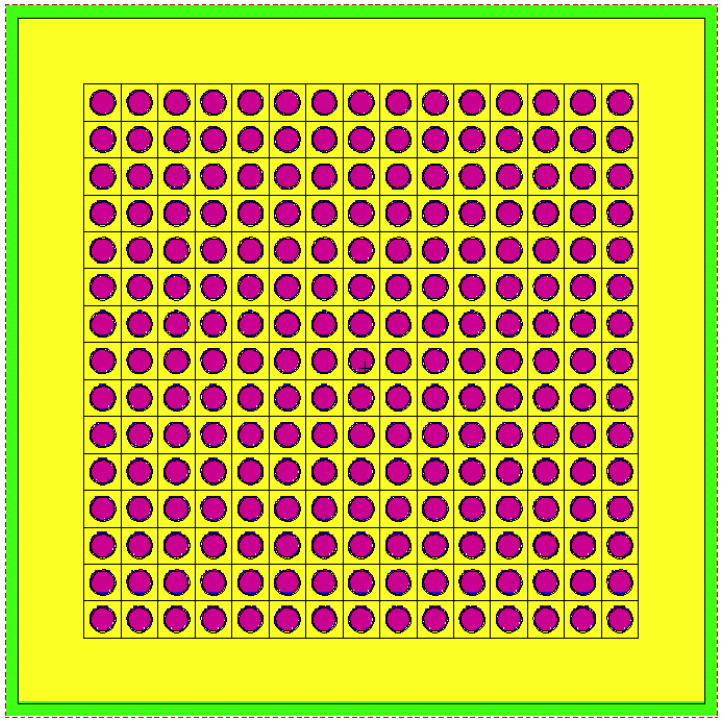
- **Simplified PWR 15 x 15 fuel assembly**
  - **From OECD/NEA fuel storage vault benchmark**
    - Fuel = 900 K
    - Clad & water = 600 K
    - Outer iron rack = 293.6K
  - **Standard NJOY+MCNP5:**
    - 900K ACE data for fuel,
    - 600K ACE data for clad & mod
    - 293.6K ACE data for iron
  - **OTF+MCNP5**
    - 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



Results - Fuel Assembly I

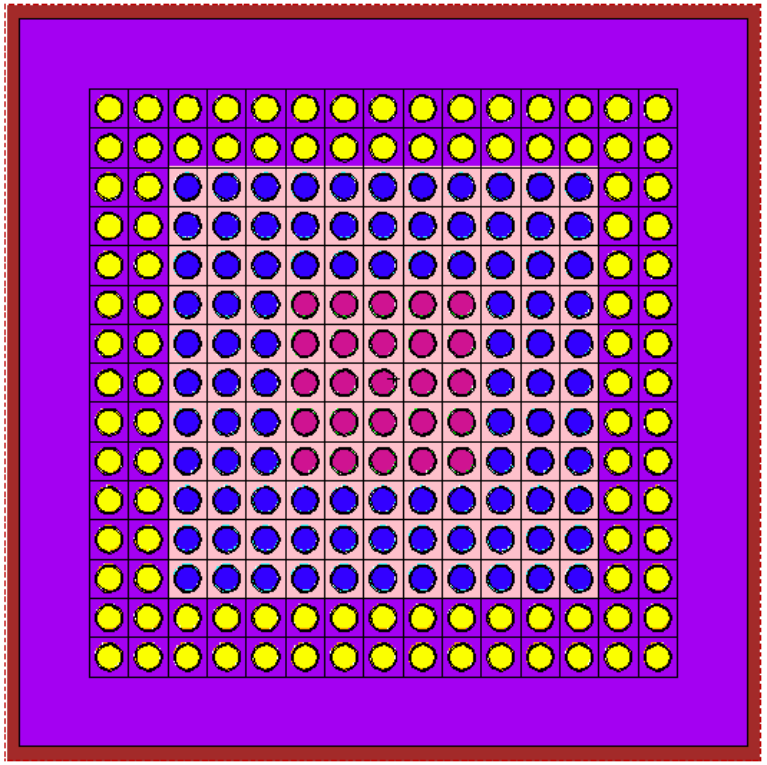
Monte Carlo Codes
XCP-3, LANL

- **K-effective**
  - NJOY+MCNP5: 1.13891 (15)
  - OTF+MCNP5: 1.13892 (15)
- **Total Fission**
  - NJOY+MCNP5: 0.464506 (.02%)
  - OTF+MCNP5: 0.464499 (.02%)
- **Total Capture in fuel**
  - NJOY+MCNP5: 0.250912 (.02%)
  - OTF+MCNP5: 0.250918 (.02%)
- **U235 capture in fuel**
  - NJOY+MCNP5: 0.089478 (.02%)
  - OTF+MCNP5: 0.089475 (.02%)
- **U238 capture in fuel**
  - NJOY+MCNP5: 0.160302 (.03%)
  - OTF+MCNP5: 0.160311 (.03%)
- **O16 capture in fuel**
  - NJOY+MCNP5: 9.73621e-4 (.11%)
  - OTF+MCNP5: 9.73248e-4 (.11%)



Results – Fuel Assembly II

- **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



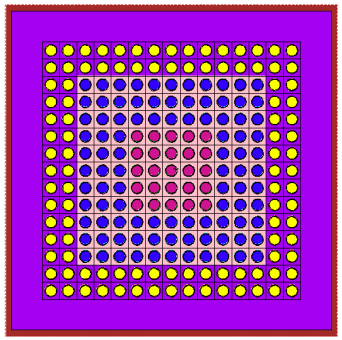
Fuel=900K, clad=900K, mod=600K
Fuel=600K, clad=600K, mod=600K
Fuel=300K, clad=300K, mod=300K

Results – Fuel Assembly II

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).

Fit_OTF Example (1)


```
=================================================================
 =  Fit_OTF:  Command-line options:
 =
 =       perform_fitting  =  T
 =
 =       zaid             = 92238.70c
 =       ace_file         =
 =       ugrid_file       = ugrid_92238.70c.txt
 =       otf_file         = otf_file.txt
 =       fit order min    =            1
 =       fit order max    =            8
 =       fit   min temp   =    293.600000000000       (if > ACE temp)
 =       fit   max temp   =    1000.00000000000
 =       fit   inc temp   =    10.0000000000000
 =
 =       print n-th lines =           20
 =
 =       create ugrid     =  F
 =
 =       testing?         =  T
 =       test_emin        =   5.500000000000000E-006
 =       test_emax        =   7.500000000000000E-006
 =================================================================
```

Fit_OTF Example (2)


```
.....read ACE file =
    92238.70c
        xsdir = /Volumes/fbb/fbrown/LANL/MCNP_DATA/xsdir
        file  = /Volumes/fbb/fbrown/LANL/MCNP_DATA/endf70j
   ..............................................................................
   Info from ACE data file for ZAID = 92238.70c

        Number of energies  =   157754
        Atomic weight ratio = 236.005800 amu
        Temperature         =  2.530100E-08 MeV,     293.6 K
        Date                = 08/25/07
        Info                = 92-U -238 at 293.6K from endf/b-vii.0 njoy99.248
        endf MAT            = mat9237

        MT reactions (std+gpd+mtlist), n= 52
                 1  101    2  301  202   16   17   18   37   51
                52   53   54   55   56   57   58   59   60   61
                62   63   64   65   66   67   68   69   70   71
                72   73   74   75   76   77   78   79   80   81
                82   83   84   85   86   87   88   89   90   91
               102  444
        MT reactions for fission, n=  1
                18

        URR-probability tables are present
             energy range:  2.000001E-02 MeV -  1.490287E-01 MeV

        Doppler broadening info:
             energy range:  1.000000E-11 MeV -  2.000001E-02 MeV
             MT reactions for Doppler broadening, n=  8
                      1  101    2  301  202   18  102  444
   ..............................................................................
```

Fit_OTF Example (3)

Monte Carlo Codes
XCP-3, LANL

```
 .....read ugrid

 .....  ugrid e pts =       168626
 .....  ugrid min e =   9.999999999999999E-012
 .....  ugrid max e =   2.074926000000000E-002


Broadening & fitting info:
     number of ugrid pts =   168603
     min energy          =  1.000000E-11 MeV
     max energy          =  2.000001E-02 MeV
     number of temps     =       71
     min temp            =    293.6 K
     max temp            =    993.6 K
     temp increment      =     10.0 K
     number of reactions =   8
     MT numbers          =     1  101    2  301  202   18  102  444
     MT for tot fission  =  18

     fitting order is variable, to meet tolerance
       min order         =   1
       max order         =   8
       max number coefs  =  17
```

Fit_OTF Example (4)


```
                                        MT-order for kprt lines. Errors given if >tolerance.

   k=   460, e=  5.60999     ev:     1-1  101-2    2-3  301-1  202-4   18-1  102-5  444-1
   k=   480, e=  6.03017     ev:     1-2  101-3    2-4  301-1  202-5   18-1  102-6  444-1
   k=   500, e=  6.28893     ev:     1-2  101-3    2-4  301-1  202-5   18-1  102-6  444-1
   k=   520, e=  6.41344     ev:     1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-1
   k=   540, e=  6.47134     ev:     1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-1
   k=   560, e=  6.50794     ev:     1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-8
   k=   580, e=  6.53025     ev:     1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-8
   k=   600, e=  6.55195     ev:     1-3  101-4    2-5  301-1  202-6   18-1  102-7  444-8
   k=   620, e=  6.57375     ev:     1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-8
   k=   640, e=  6.59798     ev:     1-3  101-4    2-5  301-1  202-6   18-7  102-8  444-8
   k=   660, e=  6.65659     ev:     1-3  101-4    2-5  301-1  202-6   18-7  102-8  444-8
   k=   680, e=  6.70483     ev:     1-3  101-4    2-5  301-1  202-6   18-7  102-8  444-8
   k=   700, e=  6.76322     ev:     1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-8
   k=   720, e=  6.79844     ev:     1-3  101-4    2-5  301-1  202-6   18-1  102-7  444-8
   k=   740, e=  6.85025     ev:     1-4  101-5    2-6  301-1  202-7   18-1  102-8  444-8
   k=   760, e=  6.89968     ev:     1-3  101-4    2-5  301-1  202-6   18-1  102-7  444-1
   k=   780, e=  6.98755     ev:     1-3  101-4    2-5  301-1  202-6   18-1  102-7  444-1
   k=   800, e=  7.18240     ev:     1-2  101-3    2-4  301-1  202-5   18-1  102-6  444-1
>>>>> e-points/minute =     3624.46836348410
```

Fit_OTF Example (5)


```
Overall error checks:
     mt=  1  max-err= 0.100%     for   e=  2883.54     eV,  t=  303.6 K
     mt=101  max-err= 0.100%     for   e=  5967.96     eV,  t=  313.6 K
     mt=  2  max-err= 0.097%     for   e=  20.2401     eV,  t=  313.6 K
     mt=301  max-err= 0.079%     for   e=  7089.62     eV,  t=  313.6 K
     mt=202  max-err= 0.026%     for   e=  2664.37     eV,  t=  313.6 K
     mt= 18  max-err= 0.002%     for   e=  723.161     eV,  t=  333.6 K
     mt=102  max-err= 0.005%     for   e=  4264.86     eV,  t=  333.6 K
     mt=444  max-err= 0.000%     for   e=  20.6344     eV,  t=  333.6 K

     Overall maximum error                =  0.100%

     Number of energies with err > 0.10% =      0

  nctot_max =     22930008
  nctot     =     11074134
```