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Title: Progress with On-The-Fly Neutron Doppler Broadening in MCNP

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Progress with

On-The-Fly Neutron Doppler Broadening in MCNP

Forrest Brown (LANL), William Martin (Michigan),
Gokhan Yesilyurt (ANL), Scott Wilderman (Michigan)
US DOE NE-UP Project

Progress with
On-The-Fly Neutron Doppler Broadening in MCNP

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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

- Importance, Examples, Numerics
- Temperature Variation in Monte Carlo Codes

On-The-Fly Doppler Broadening in MCNP (OTF)

- Methodology
- Union Energy Mesh
- Temperature Fitting
- MCNP Implementation
- Testing

Work-in-Progress

Introduction – Doppler Broadening

^{238}U capture cross-section

Neutron Flux in Fuel per unit lethargy
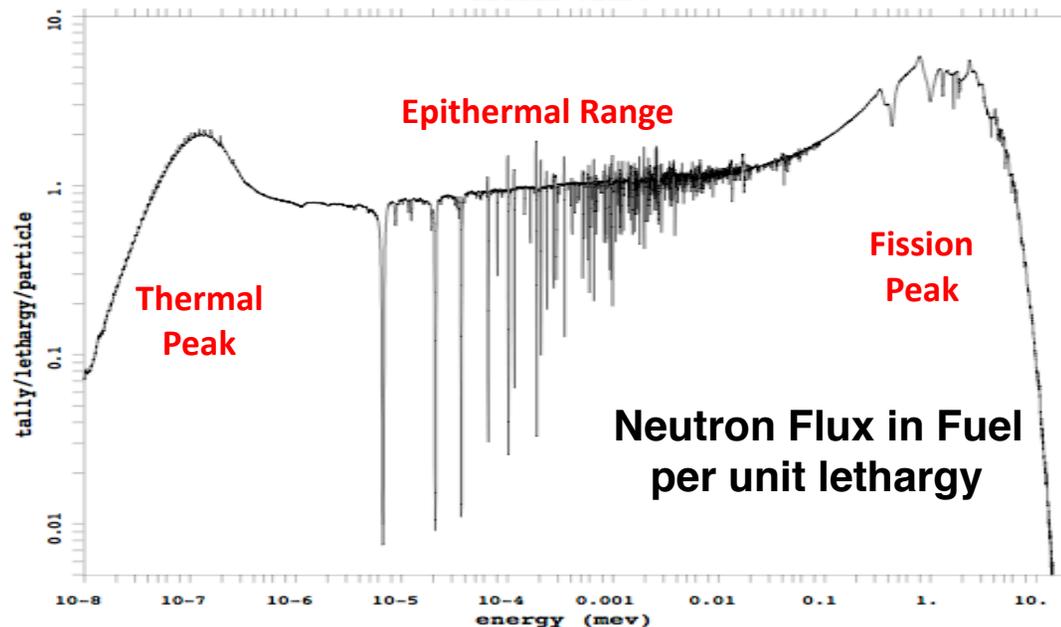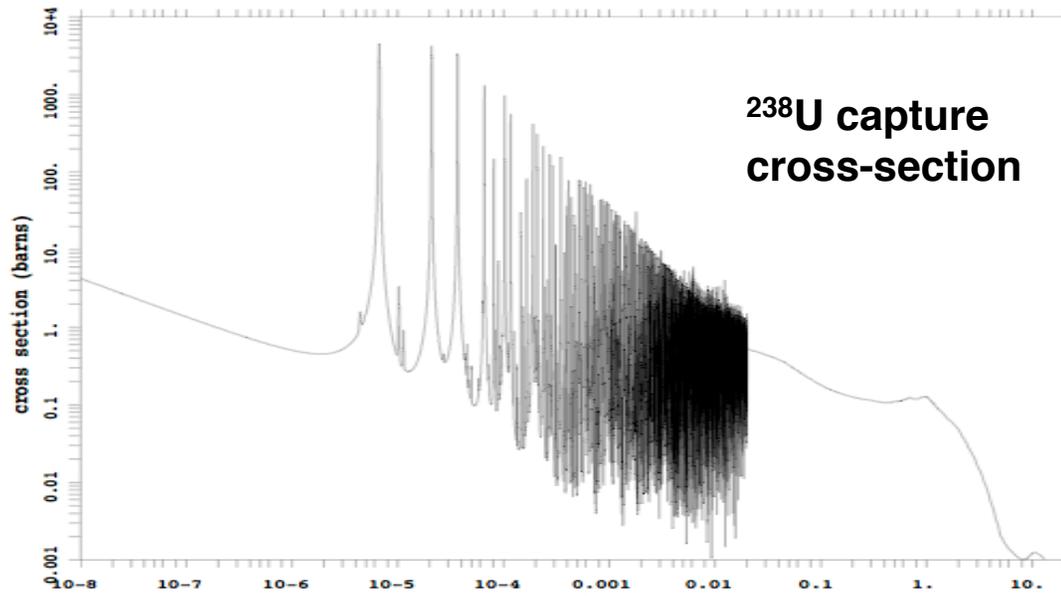
UO$_2$ Fuel Pin

3.1% Enriched
293.6 ^{o}K

.01 eV – 20 MeV

- Neutrons born in MeV range from fission

- Most fissions caused by thermal neutrons

- **1/3 of neutron losses are due to ^{238}U capture in epithermal energy range during slowing down**

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Neutron Flux in Fuel per unit lethargy

^{238}U capture
6.67 eV resonance
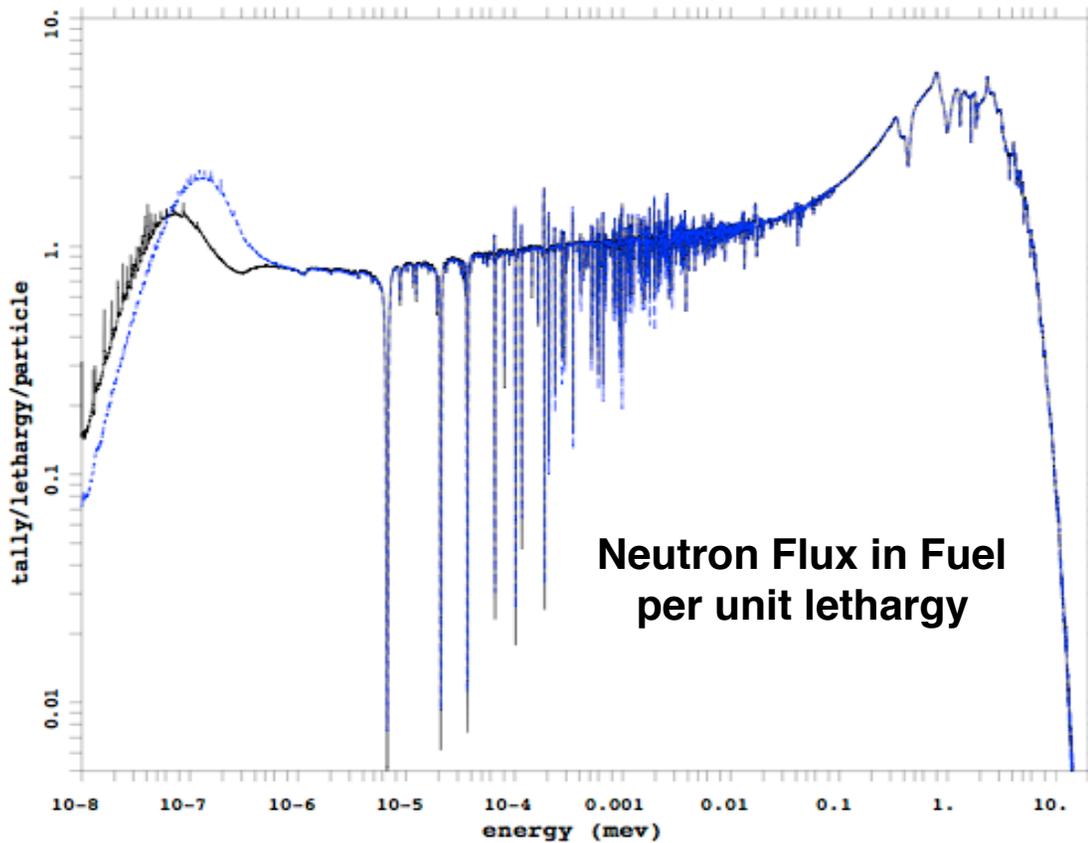
UO$_2$ Fuel Pin

3.1% Enriched
293.6 °K vs 900 °K

.01 eV – 20 MeV

Keeping same densities, but changing cross-sections:

k_{inf} (cold) = 1.34498 (8)

k_{inf} (hot)   = 1.31167 (8)
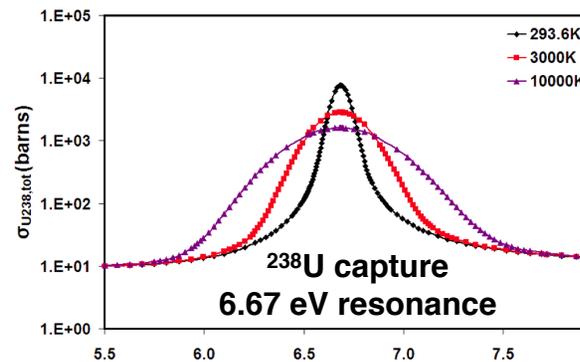
At higher temperatures, Doppler broadening of resonance cross-sections increases resonance capture

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Monte Carlo Simulation

Free-flight distance to next collision, s

Collision isotope,
Reaction type,
Exit E' & (u',v',w'),
Secondary particles
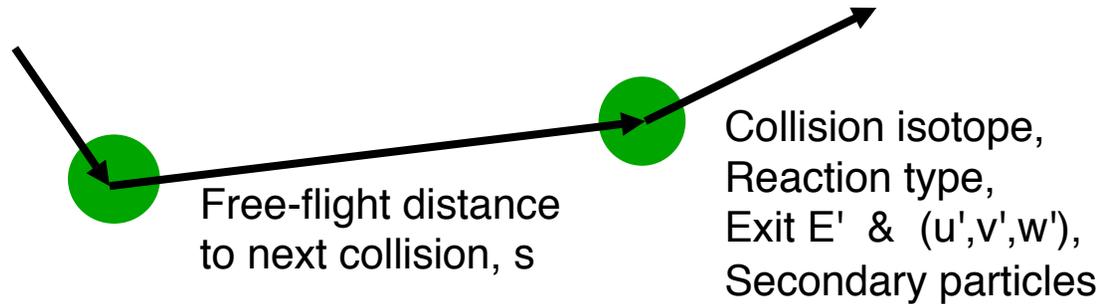
- **Target nucleus thermal motion important**
  - **Maxwell-Boltzmann energy distribution at temperature T, isotropic Ω**
  - **Detailed kinematics of collisions must include nucleus E & Ω**

- **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.

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

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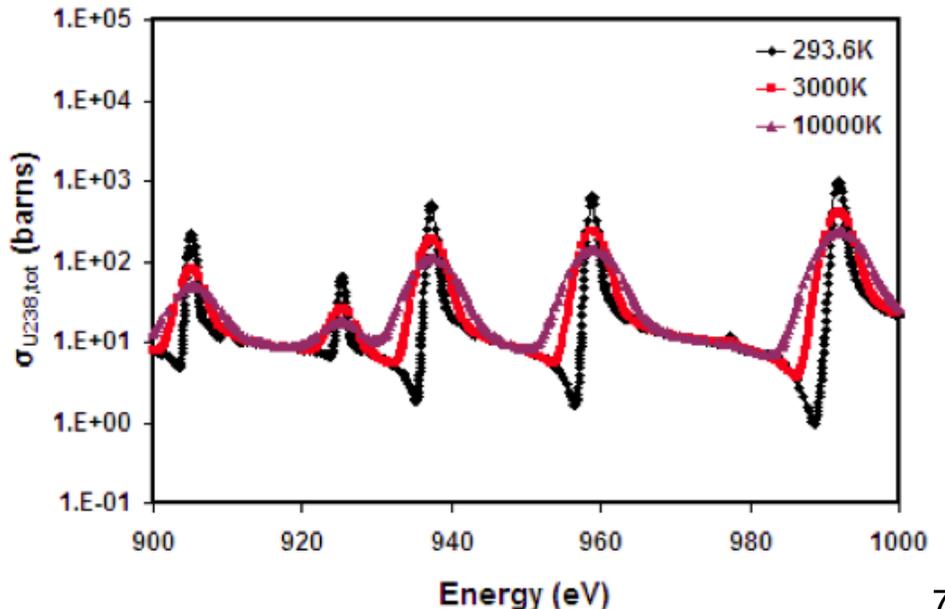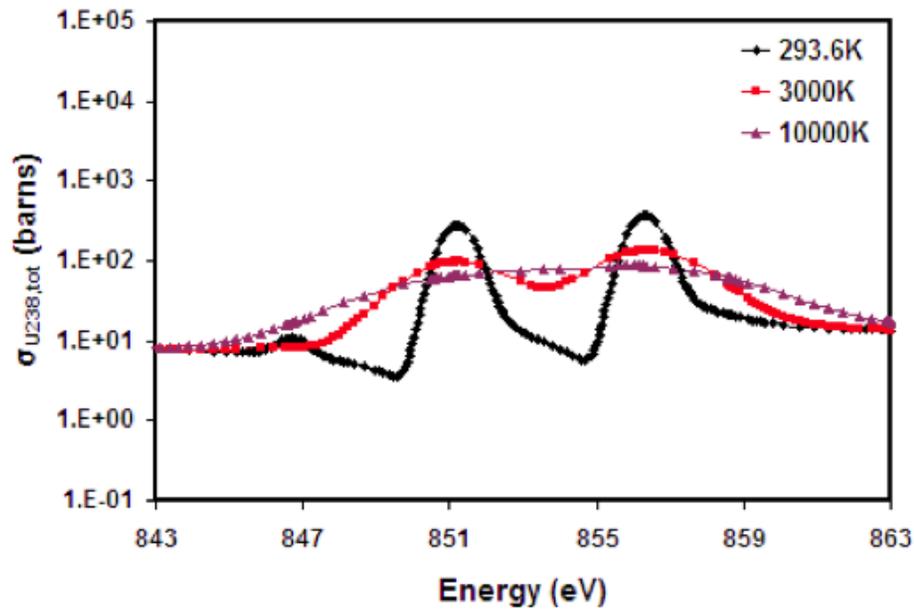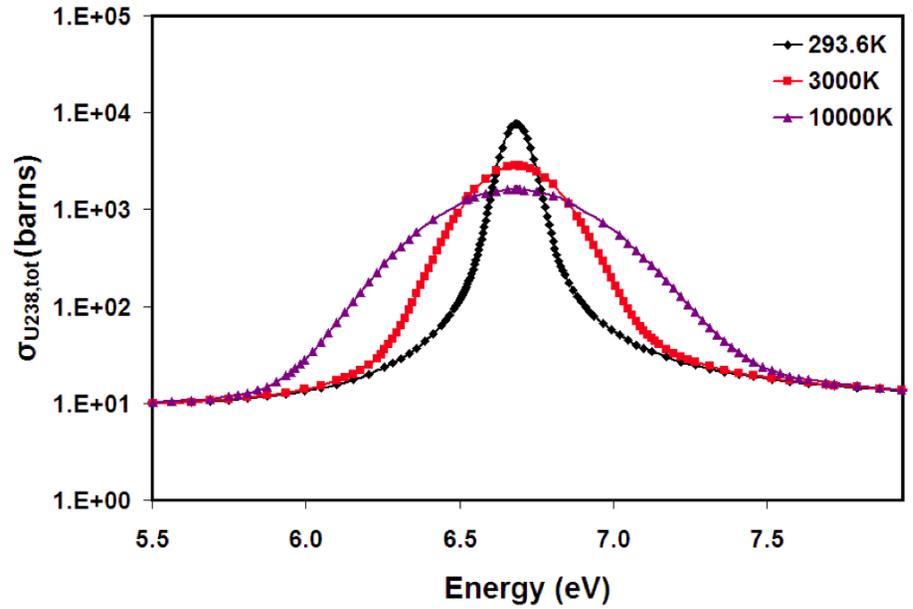
- **ENDF/B nuclear data is represented by piecewise-linear tabulation of σ(E)**
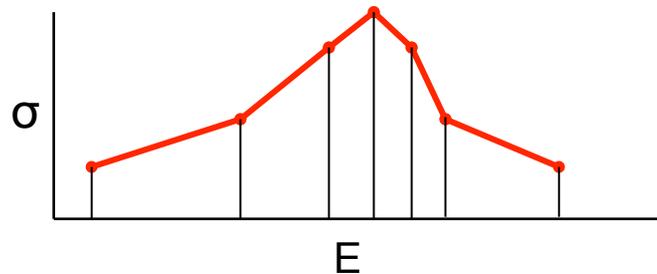
Typically, a linearization
tolerance of 0.1% is used

- **Doppler Broadened Neutron Cross-sections**

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

- 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

- $\sigma_{eff}(E)$ **has different E-mesh at different T's**

- **Very compute-intensive, typically performed prior to Monte Carlo in preparing nuclear data libraries**

Introduction – Temperature Variation in Monte Carlo

What if there are 1000s of T's ?

Six approaches:

(OTF = On-The-Fly)

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**

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**

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- **OTF Methodology (for each nuclide)**

  – **Create union energy grid for a range of temperatures**

  – **Create fits for σ_{eff}(T,E), for range of temperatures, on union E-grid**

  – **MCNP – evaluate σ_{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

mcnp
LA-UR-12-xxxxx

- ^{238}U energy grid, 35-36 eV, various temperatures   (ENDF/B-VII.0)
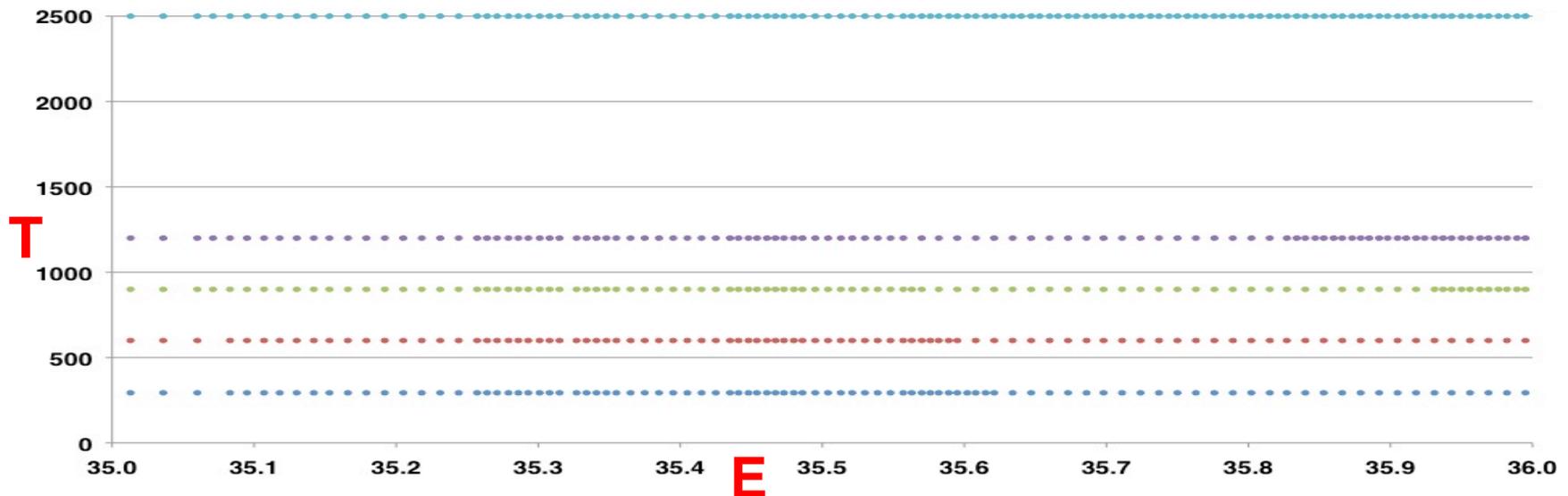
NJOY adapts the energy grid (for each nuclide, at given T)
to preserve linearization tolerance

Temperature (K)	Number of E pts
293.6	157754
600	133964
900	122581
1200	115361
2500	99631

Union E-grid:

Need to determine 1 energy grid
(for each nuclide) that preserves
linear interpolation tolerance in E
over the entire T range

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OTF Methodology – Union Energy Grid   (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

  - **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 (E,T) ranges**
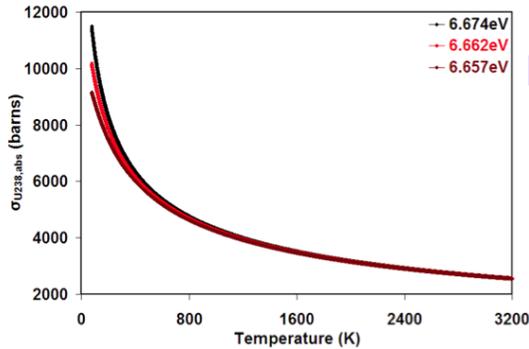
Near resonance peaks:

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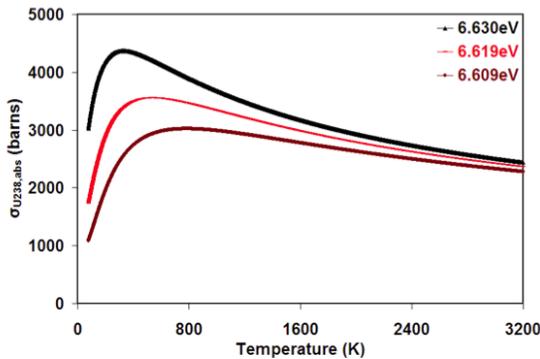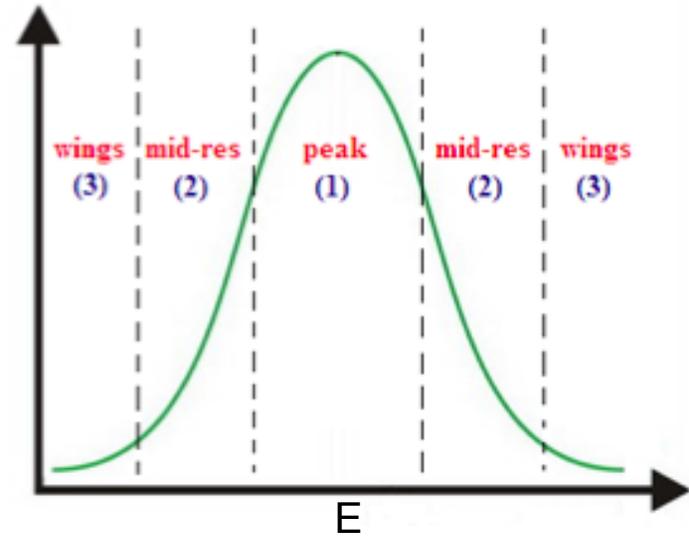
Mid resonance:

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

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

- **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**

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- **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 <u>once</u>, & 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

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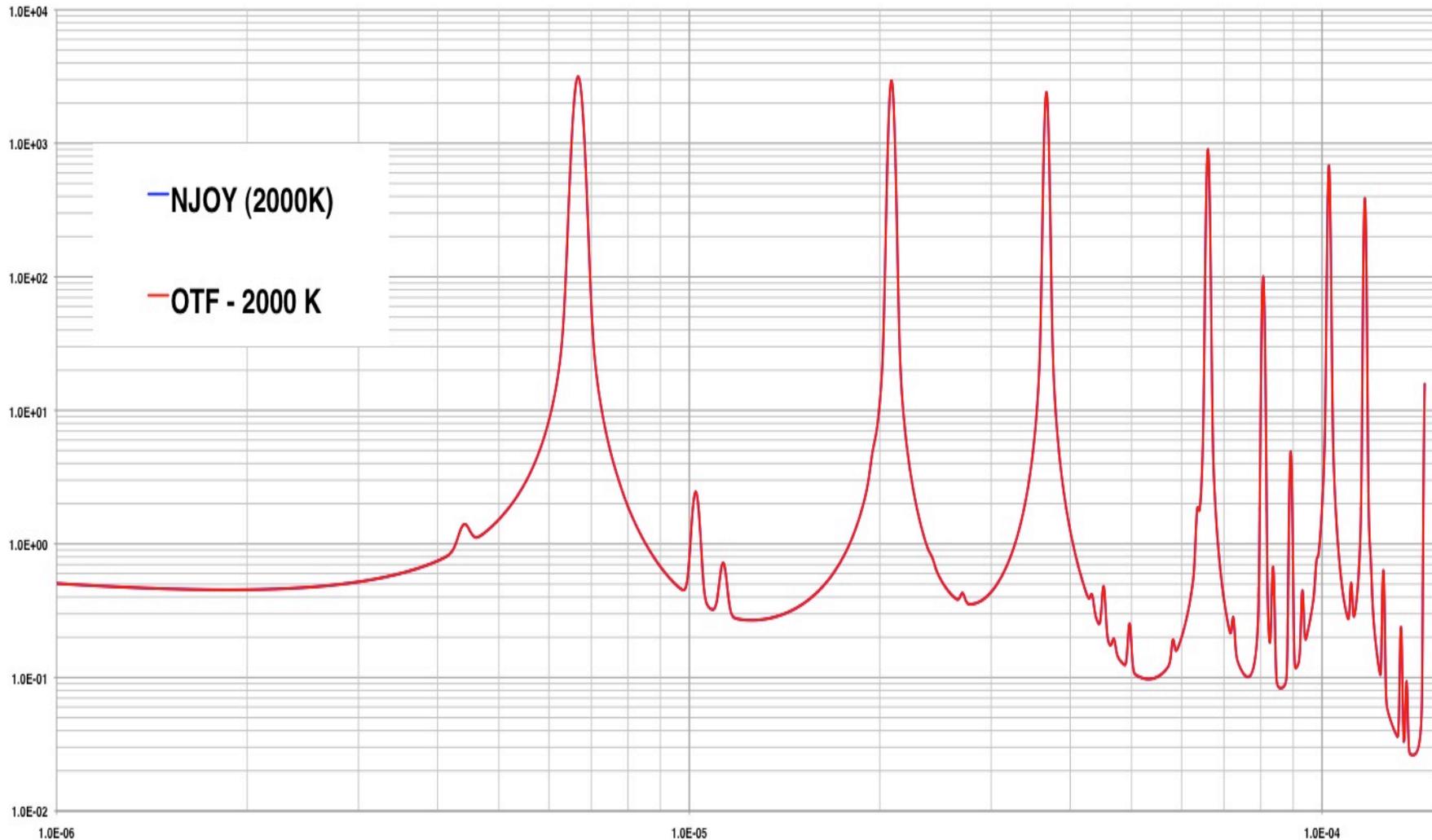
Cross-sections from NJOY & OTF match within linearization tolerance 0.1% at all energies

NJOY vs OTF ²³⁸U Capture Cross-Section

- **NJOY vs OTF at 1000 K**
  (curves with higher peak)

- **NJOY vs OTF at 2000 K**
  (curves with lower peak)

Cross-sections from NJOY & OTF match within linearization tolerance 0.1% at all energies
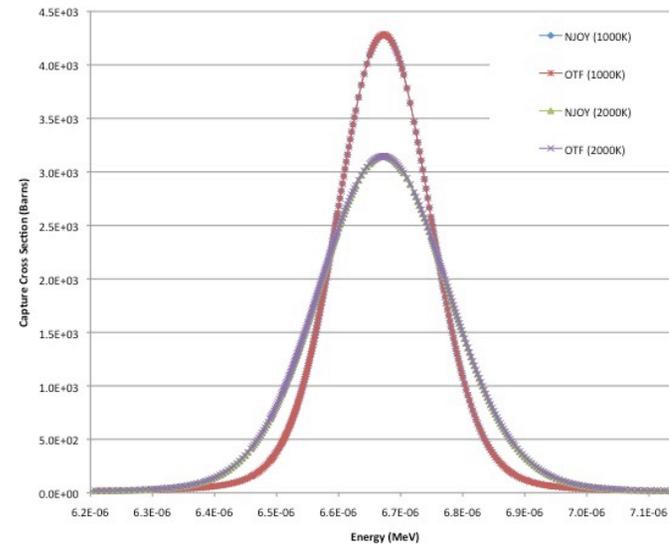
6.67 eV resonance
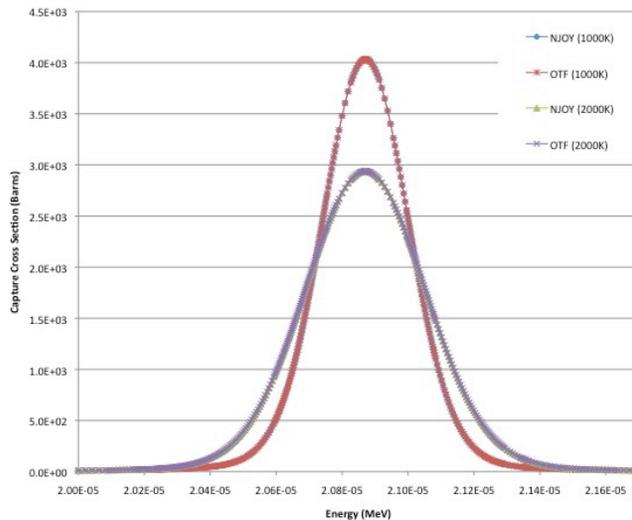
20.9 eV resonance

36.6 eV resonance

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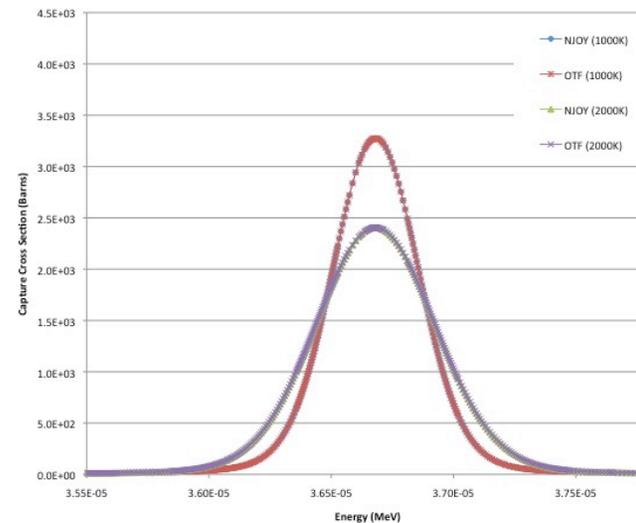
- **Doppler Reactivity Benchmark**
  - Compare k-effective for **HZP** (hot, zero power) and **HFP** (hot, full power) conditions for a unit fuel cell typical of a PWR
  - **Basic model:**
    - **PWR fuel pin cell** with reflecting BCs,   various enrichments
    - **HZP** cases**:   fuel at 600K**,   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
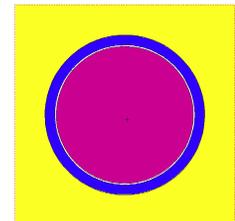
  - **NJOY+MCNP**:   NJOY-broadened data at exact temperatures
  - **OTF+MCNP**:   OTF data for ^{16}O, ^{234}U, ^{235}U, ^{238}U in fuel

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

Doppler Defect Benchmark Results

MCNP

		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)

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

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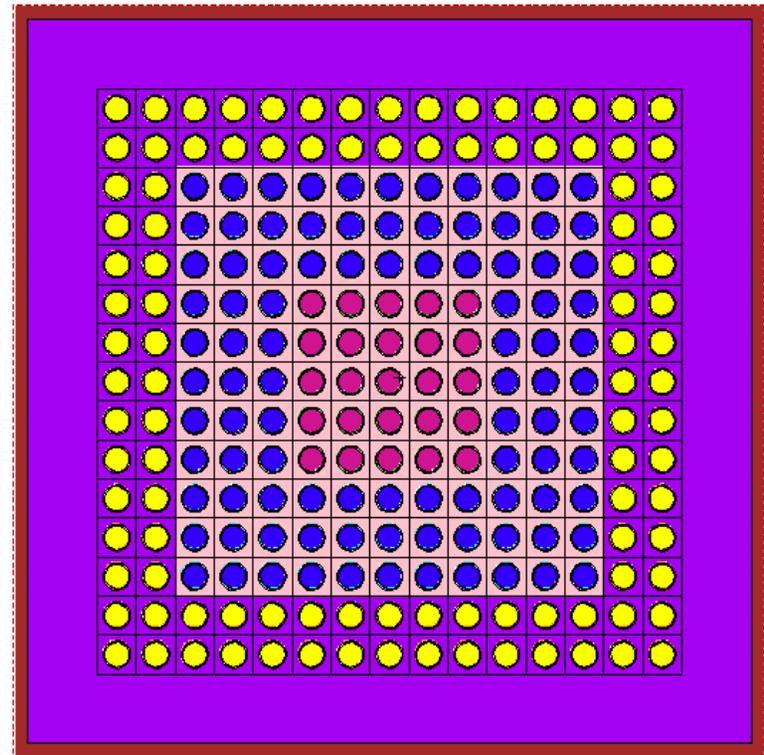
Fuel=900K, clad=900K, mod=600K
Fuel=600K, clad=600K, mod=600K
Fuel=300K, clad=300K, mod=300K

k-effective:

STD	1.11599	(15)
OTF	1.11592	(15)
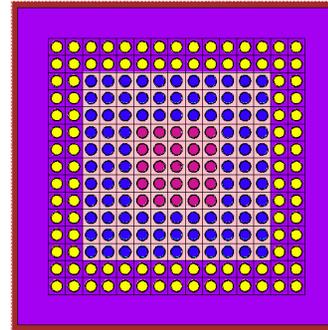
Fuel=900K, clad=900K, mod=600K
Fuel=600K, clad=600K, mod=600K
Fuel=300K, clad=300K, mod=300K

	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%)

- **Better integration & optimization in MCNP**

- **FIT_OTF fitting program**
    - Investigate scaling & Chebychev, for better numerical stability **[done]**
    - Investigate regression, to vary fit order by energy & reaction **[done]**

- **U. Michigan work**
    - Create OTF libraries for all nuclides in ENDF/B-VII.0 **[in progress]**
    - 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

- **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", *Nuclear Science & Engineering* **171**, 239-257 (2012).

- **F.B. Brown, B.C. Kiedrowski, D. Brown, W.R. Martin, D. Griesheimer**, "Advanced Monte Carlo for Reactor Core Analysis", technical workshop for PHYSOR-2012, Knoxville, TN, April 15 [also LA-UR-12-20397] (2012).

- **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)