Nuclear data for high-fidelity, high performance reactor modelling and simulation

Benoit Forget

Massachusetts Institute of Technology
Department of Nuclear Science and Engineering
bforget@mit.edu

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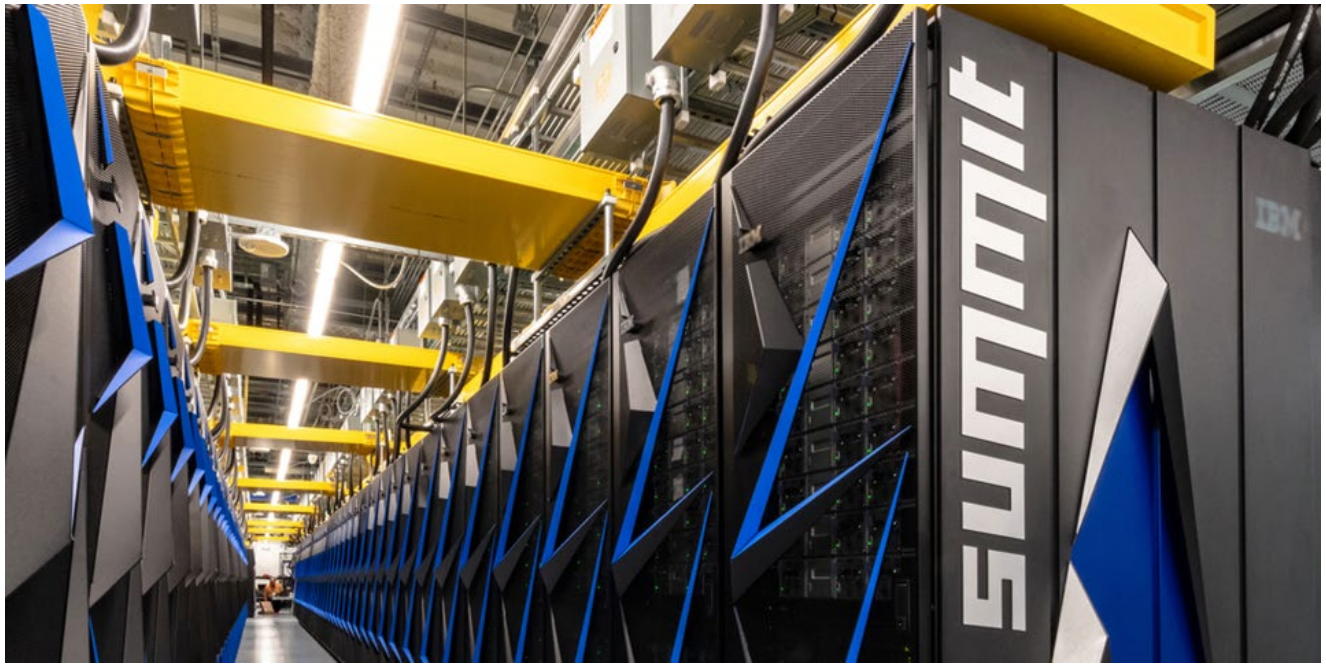
About Me

- Joined MIT in 2008
- Professor and Associate Department Head of Nuclear Science and Engineering
- Founded the Computational Reactor Physics Group
  - Major highlights:
    - OpenMC, an open source Monte Carlo code (lead developer Paul Romano)
    - OpenMOC, an open source Method of Characteristic transport code
    - BEAVRS benchmark, full core PWR with first 2 cycles of flux core mapping data

Our goal

- One of our primary goals has been the development of high-fidelity neutron transport methods for **full core nuclear reactor simulations**
  - Leverage high performance computing
  - Improve data representation
  - Reduce memory footprint
  - Develop novel algorithms for improved efficiency



Many of the roadblocks and bottlenecks identified for improving performance were tied to nuclear data

Outline

- Part I: Nuclear data for high-fidelity Monte Carlo simulations
  - Nuclear Data Requirements
  - Nuclear Data Options
  - Limitations and Opportunities

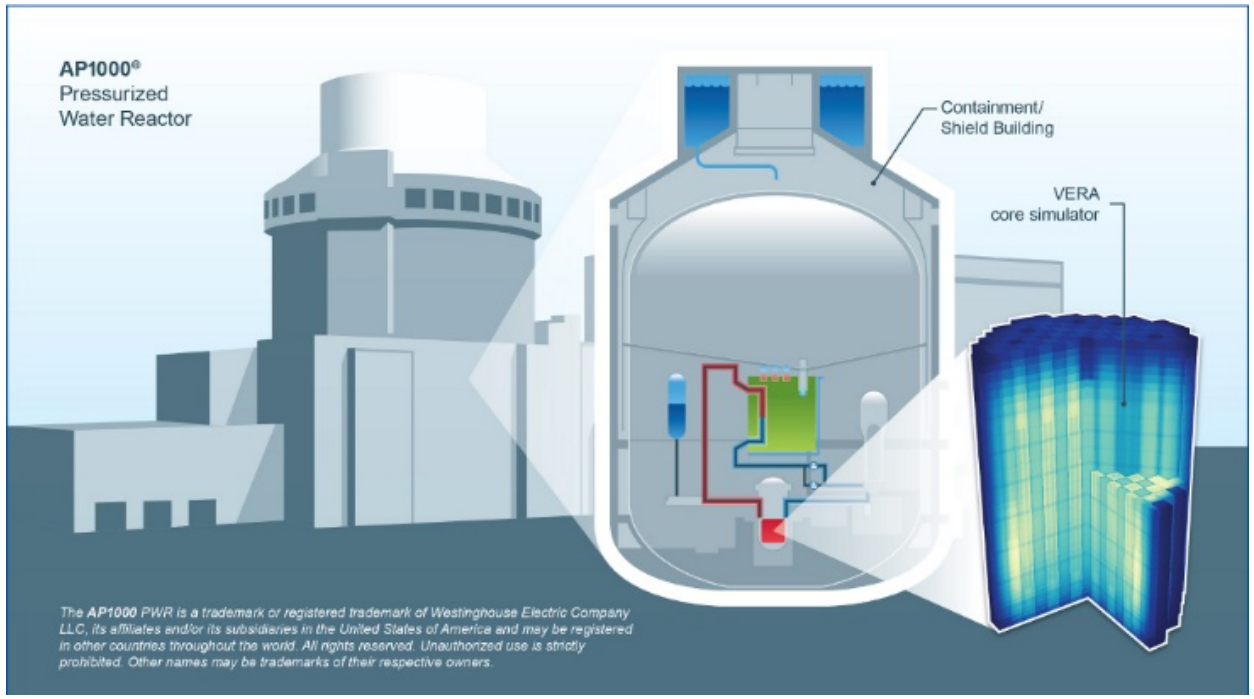
- Part II: Generating high-fidelity nuclear data for deterministic calculations
  - Transport cross-section
  - Equivalence Factors
  - Limitations and Opportunities

Assumptions

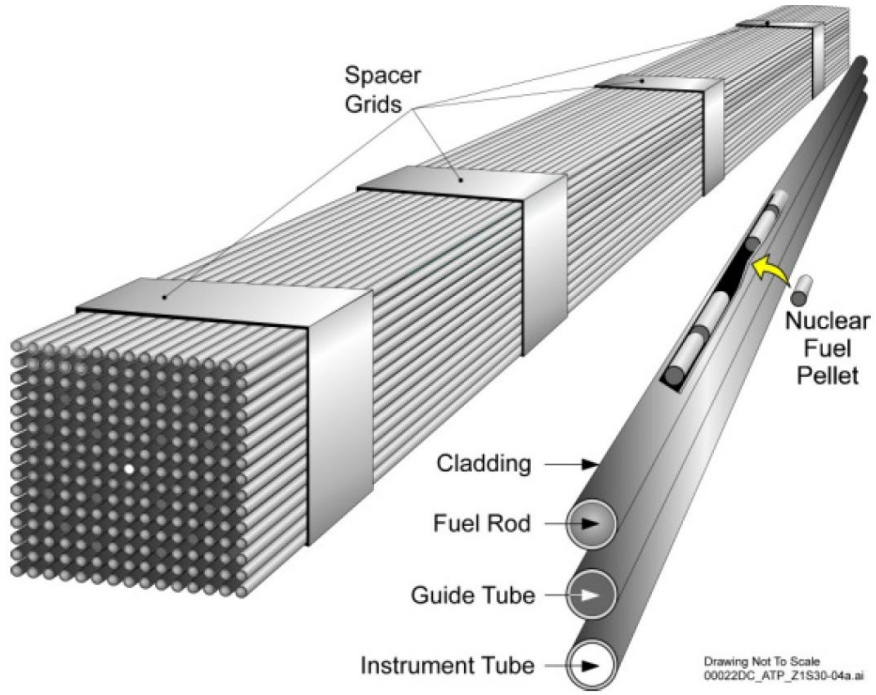
- When preparing this talk, I had to assume some level of knowledge, I thus assumed that most of you knew something about
  - Nuclear cross-sections
  - Neutron slowing down
  - Criticality
  - Multigroup cross-sections
  - Transport equation
  - Diffusion equation

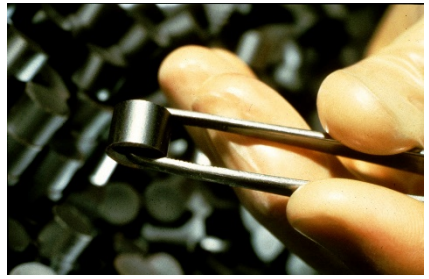
Part I: Nuclear data for high-fidelity Monte Carlo simulations

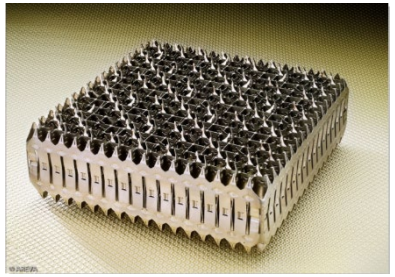
The Big Picture



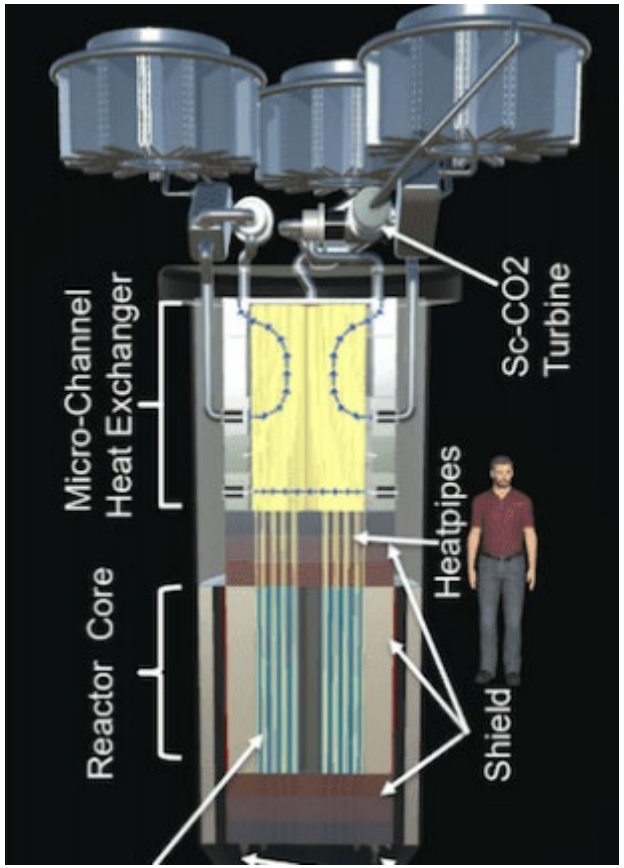
Oak Ridge National Laboratory, CASL News Release, 2014.



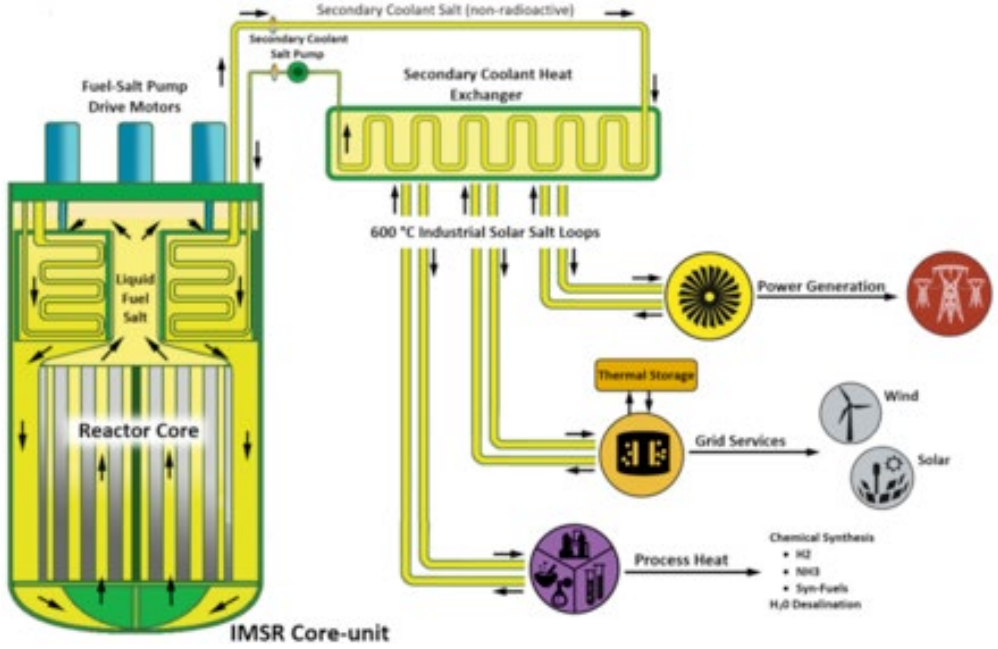




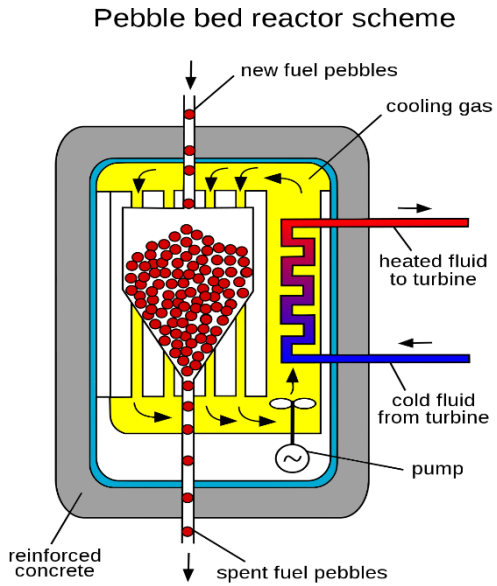
Beyond LWRs

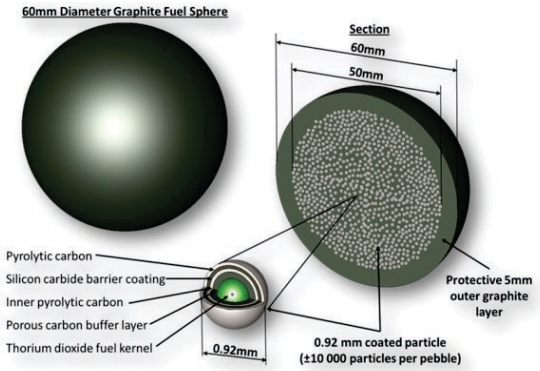


Microreactor



Molten Salt Reactor





Pebble Bed Reactor

Current state-of-the-art

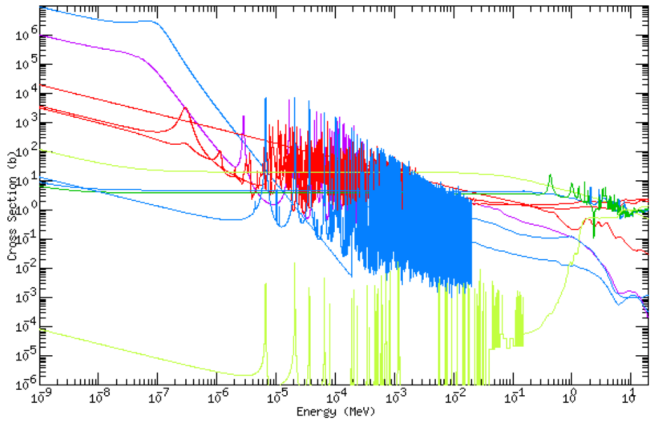
- Current methodologies rely on many-levels of approximation that have been extensively validated against experiments and operating nuclear fleet
  - Currently licensed methods are highly accurate for the current fleet of reactors
  - Most experiments were performed in the 60's and 70's

• New reactors promise much higher levels of heterogeneities.
• Experimental facilities in nuclear are increasingly costly and require very long lead times.

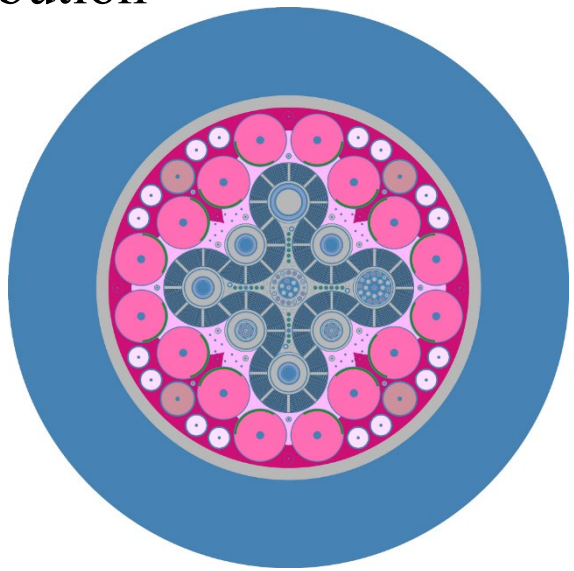
High-fidelity simulations are necessary to reduce the need for costly experiments for future nuclear reactor technologies

Why do we need high-fidelity Monte Carlo?

- Monte Carlo methods "faithfully" track neutrons through their lifetime
  - High-fidelity representation of the nuclear data
  - High-fidelity representation of the geometry
  - High-fidelity representation of the fission and scattering source distribution

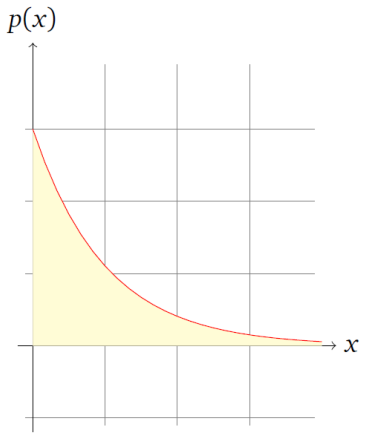


10 orders of magnitude in Energy

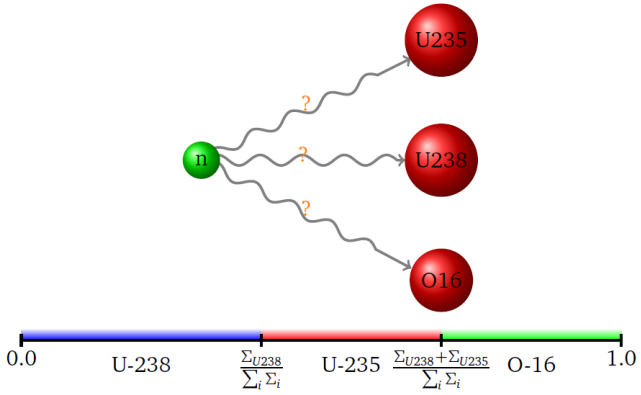


ATR Geometry in OpenMC

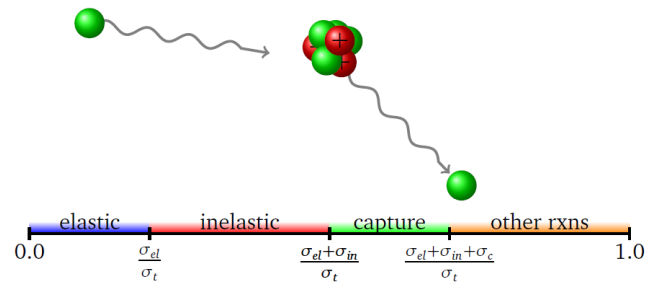
$$p(x)dx = \Sigma_t e^{-\Sigma_t x} dx$$



Path sampling



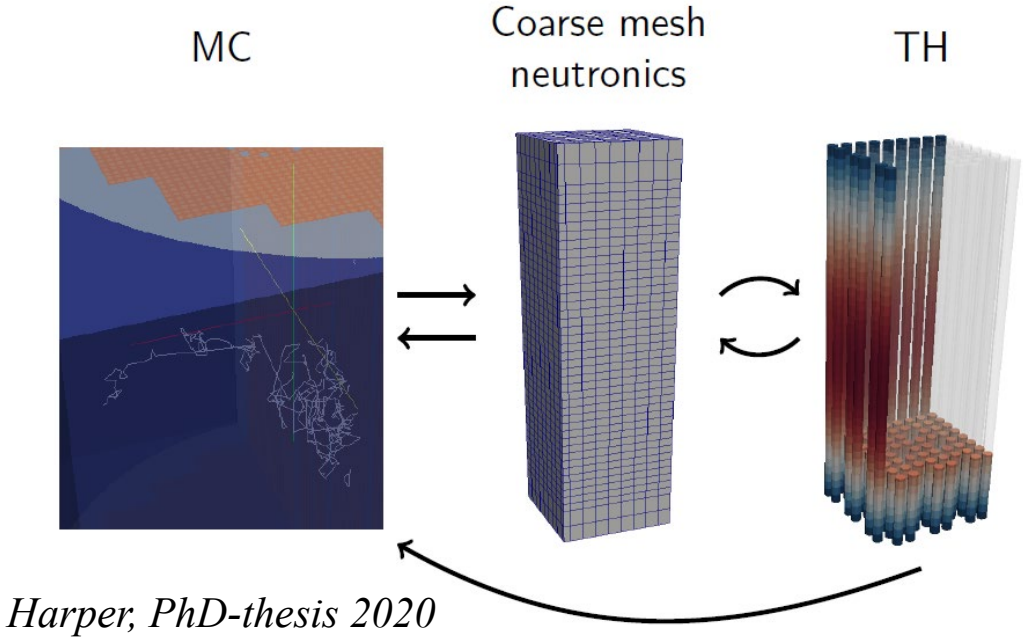
Nuclide sampling



Collision sampling

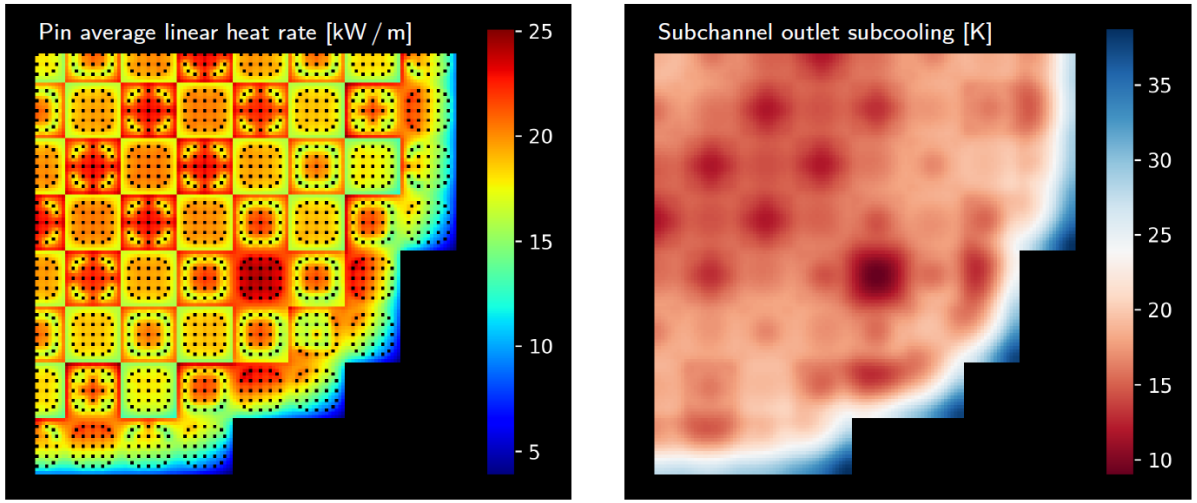
Multiphysics applications

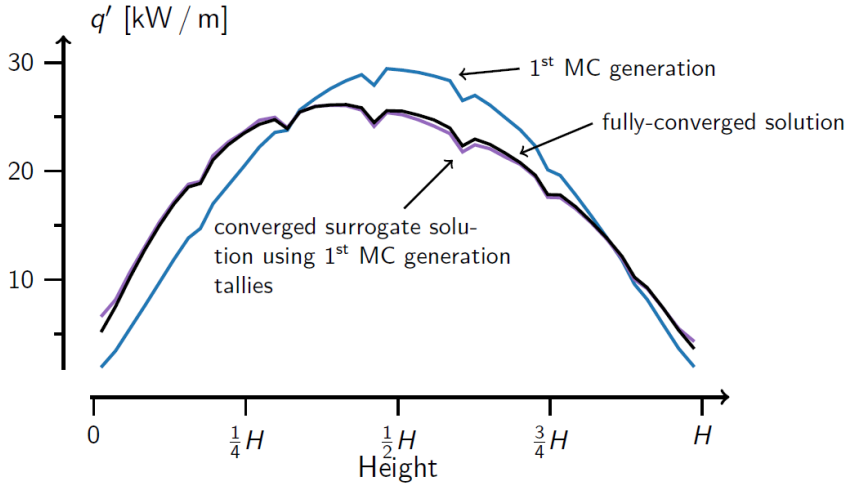
- High-fidelity simulations beyond benchmarking require at the very least thermohydraulic feedback
  - Example of 3D 1/4 PWR between OpenMC and subchannel
  - Power distribution shifts radially and axially based on temperature feedback



Harper, PhD-thesis 2020

$$\Sigma(T,\rho) \approx \Sigma(T_{\text{ref}},\rho_{\text{ref}}) + \frac{\partial \Sigma}{\partial T}(T - T_{\text{ref}}) + \frac{\partial \Sigma}{\partial \rho}(\rho - \rho_{\text{ref}})$$





Data Requirements (LWR Example)

- Our goal is to predict the power in every single fuel pellet as a function of time
  - PWR has ~20,000,000 fuel pellets
  - Every pellet has a **different average temperature**
  - Every pellet has a **unique temperature profile**
  - Fuel transmutes over its lifetime (each pellet resides ~5 years in the core)
    - We must track ~6 different reactions that can occur in the fuel.
    - We must follow ~300 nuclides being consumed and produced in the fuel.

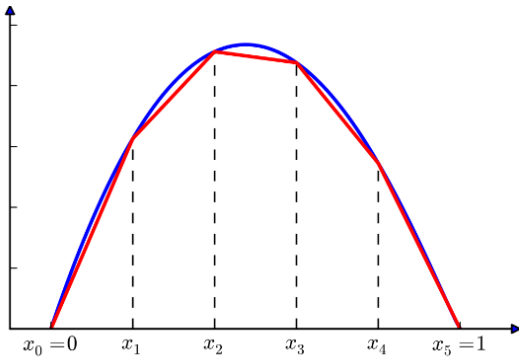
Each event requires accessing 100's of GBs of nuclear data!
Each time step requires ~3-5TB of data to be stored!

Detailed knowledge enables better fuel utilization, improves understanding of safety margins that can lead to a reduction of conservatism and improves predictability of the system.

Temperature dependence of data

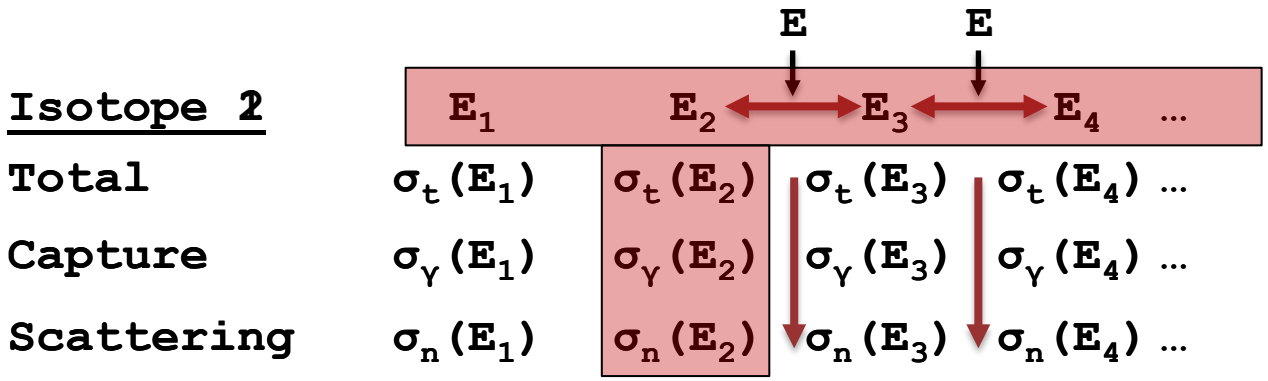
- Monte Carlo simulations are commonly used as reference calculations at fixed temperatures
- Cross sections are pre-generated at fixed temperatures using the BROADR (SIGMA1 algorithm) module of NJOY
- Nuclear data is commonly represented (in the resonance range) using models representative of the R-matrix theory (SLBW, MLBW, RM, …)
  - Requires only a few parameters per resonance (E_0,Γ, Γ_n, Γ_f …)
  - However, SIGMA1 requires a linearization of the data to perform the convolution integral

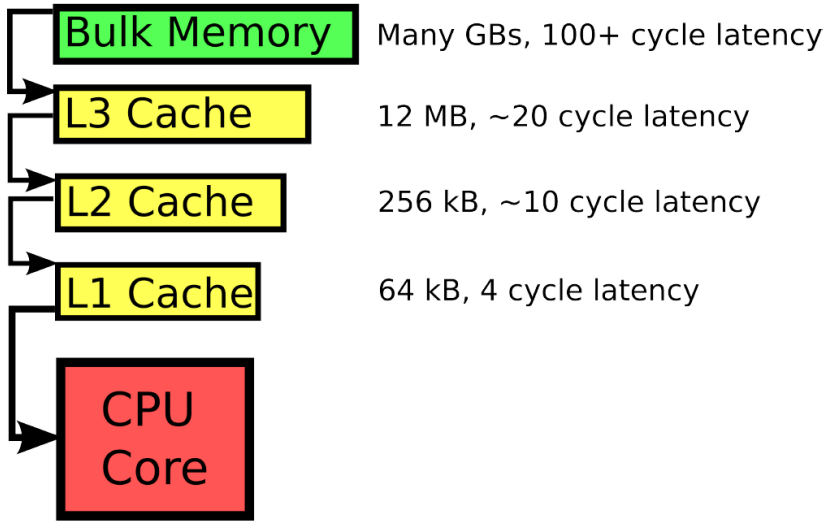
$$v\sigma(v,T) = \int d\mathbf{V}|\mathbf{v}-\mathbf{V}|\sigma_0(|\mathbf{v}-\mathbf{V}|)P(\mathbf{V},T)$$



Nuclear Data Reconstruction

- Every isotope has its own energy grid for each temperature
  - Requires a binary search over 1000's – 100,000's of points



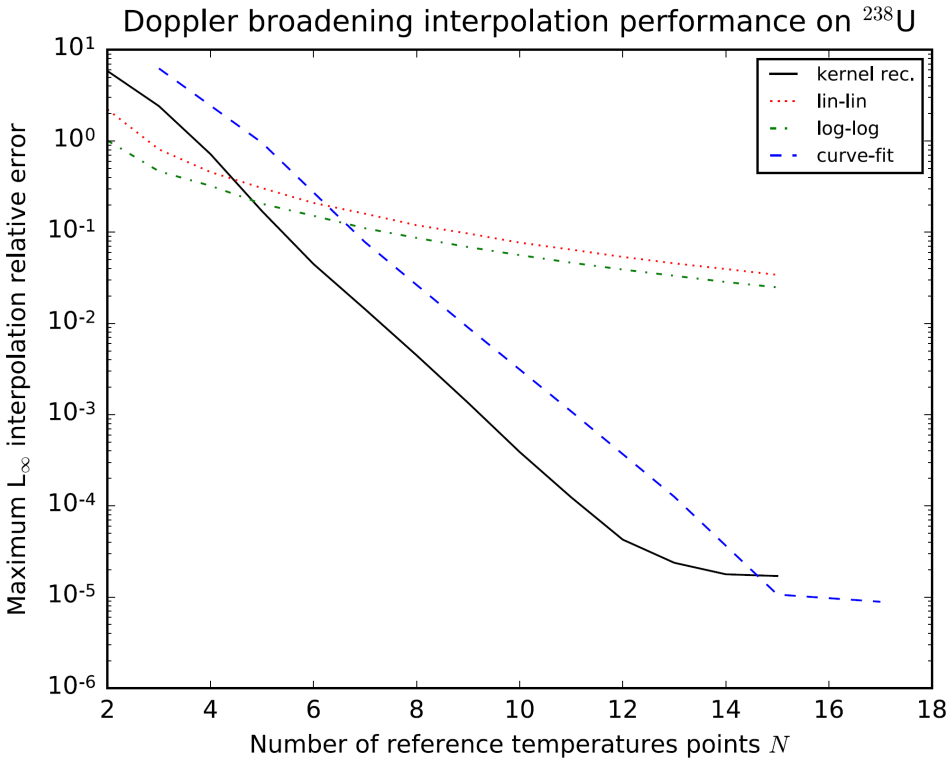


- Simple algorithmic fixes
  - Unionized grid over all temperatures and isotopes
    - Global or local (cell-based)
    - Serpent uses a global unionized grid
  - Hash table to accelerate search
    - MCNP6 and OpenMC use a hash table

The further you reach for data, the slower your code becomes!

Options in the Resolved Resonance Range

- SIGMA1
  - Linearize data and solve Solbrig kernel analytically over an energy band
  - Some are exploring off-loading this operation to GPU
- Stochastic Mixing
  - Randomly sample between bounding temperatures to mimic interpolation
  - Requires temperature spacings on the order of 10-50K for good accuracy
- Kernel Reconstruction
  - Reconstruct the Solbrig kernel effect using ~10 temperatures from which to randomly sample. Weights are determined analytically through an error minimization process.



Ducru et al, JCP, 2017

Options in the Resolved Resonance Range

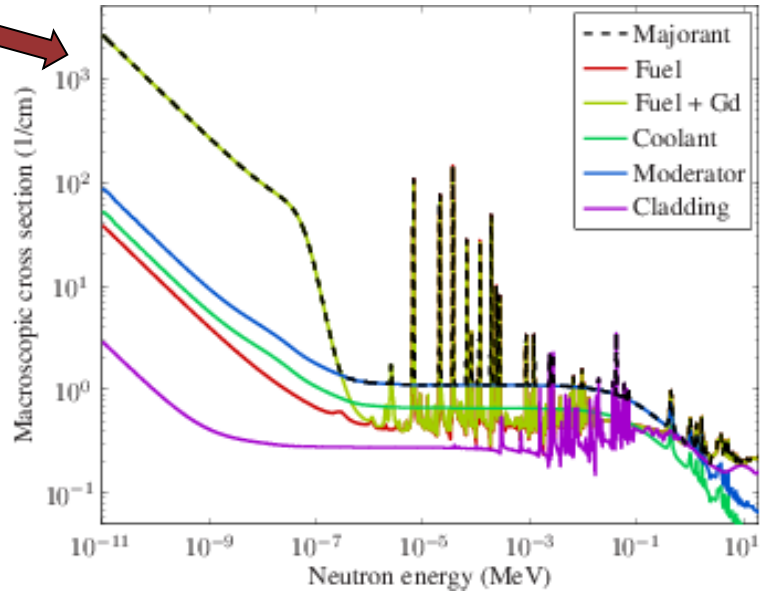
- Gauss-Hermite Quadrature
  - Replace convolution integral by a Gauss-Hermite quadrature

$$\int_{-\infty}^{\infty} dz e^{-z^2} f(z) \approx \sum_{k=1}^{N} w_k f(z_k)$$

- Polynomial fitting (e.g. MCNP)
  - High order fit across many temperatures

$$\sigma_\gamma(T, E_g) \approx \sum_{i=1}^{N} \frac{a_{g,i}}{T^{i/2}} + \sum_{i=1}^{N} b_{g,i} T^{i/2} + c_g$$

- Target Motion Sampling (e.g. SERPENT)
  - Sample target velocity at collision site and apply rejection sampling
- Windowed Multipole (e.g. OpenMC)
  - Transform the resonance parameters to an equivalent representation in complex space and perform convolution integral analytically
  - For performance benefits, broadening only performed over a surrounding energy window



Viitanen et al, NSE, 2012

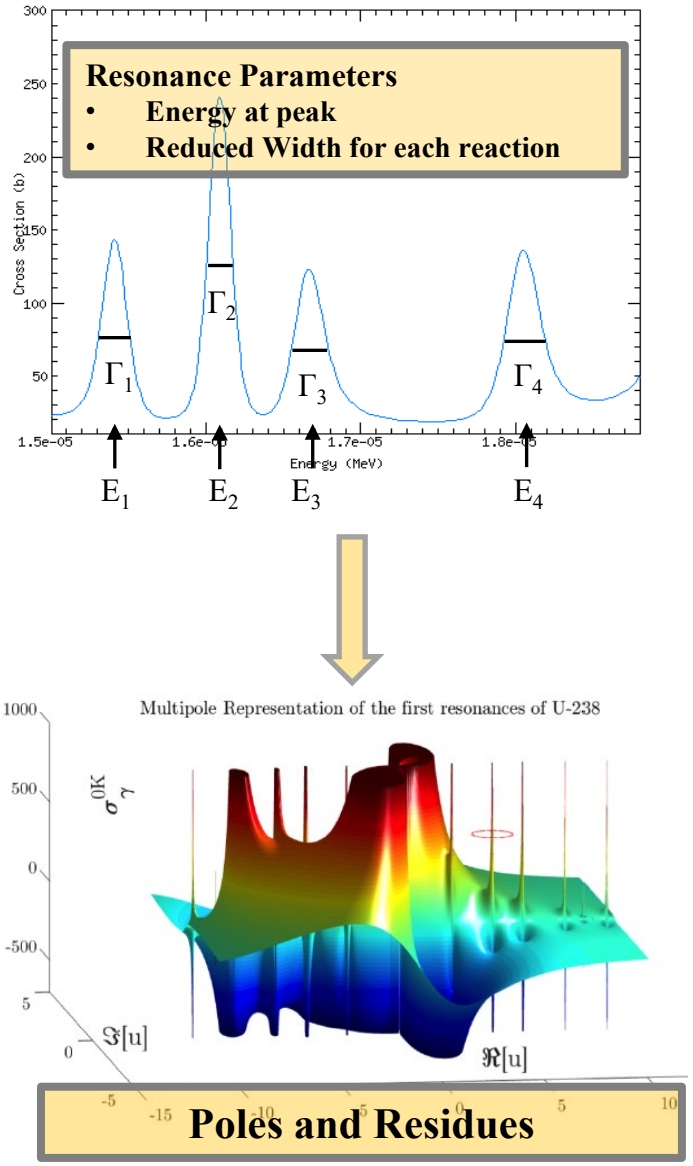
Multipole Formalism

- Developed by R.Hwang in 1987
  - Recognized that R-matrix formulation yielded a meromorphic function on which a partial fraction decomposition could be performed
  - *(E,Γ)* real parameters are transformed into *(p,r)* complex parameters

$$\sigma = \frac{1}{u^2}\sum_j \Re\left[\frac{r_j}{p_j - u}\right]$$

  - And the convolution integral yields

$$\sigma(u,T) = \mathfrak{D}\mathfrak{B}_{T_0}^{T}\left[\sigma(u,T_0)\right] = \frac{1}{2u^2\sqrt{\xi}}\sum_j \Re\left[ir_j\sqrt{\pi}W(z_j^0) - \frac{r_j}{\sqrt{\pi}}C\left(\frac{p_j}{\sqrt{\xi}}, \frac{u}{2\sqrt{\xi}}\right)\right]$$

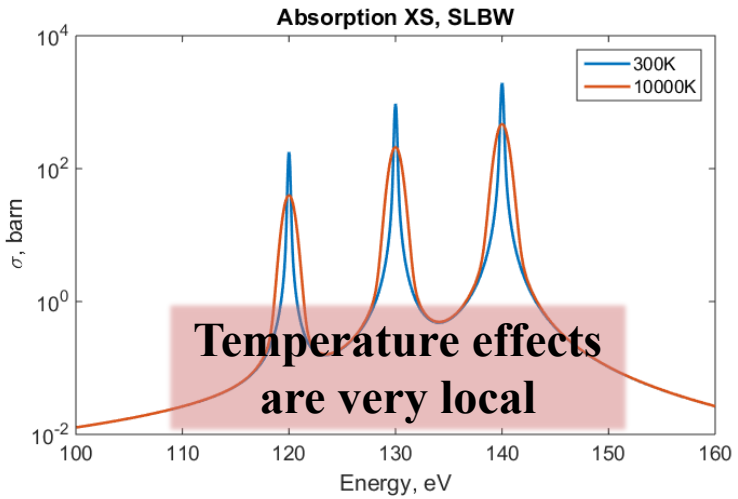


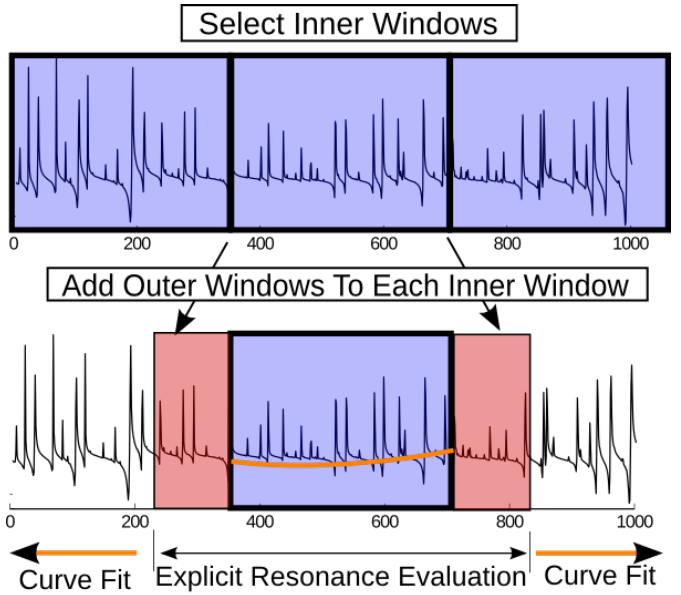
Josey and Ducru, JCP, 2016

Windowed multipole method

- Key observation was made that Doppler broadening effects are local
  - Far away resonances contribute to the local cross section but they exhibit little to no temperature dependence
- Windowed multipole method creates a system of inner windows and pointers to minimize the number of Faddeeva function evaluations
  - Far away resonances are fitted to a low order polynomial

$$\sigma(E) = \frac{1}{E} \sum_{j \in \mathcal{W}(E)} \mathrm{Re}\left[\frac{-ir_j}{p_j - \sqrt{E}}\right] + \sum_{n \geq -2}^{N} a_n (\sqrt{E})^n$$





For any point in the blue inner window

Josey and Ducru, JCP, 2016

Options in the Resolved Resonance Range

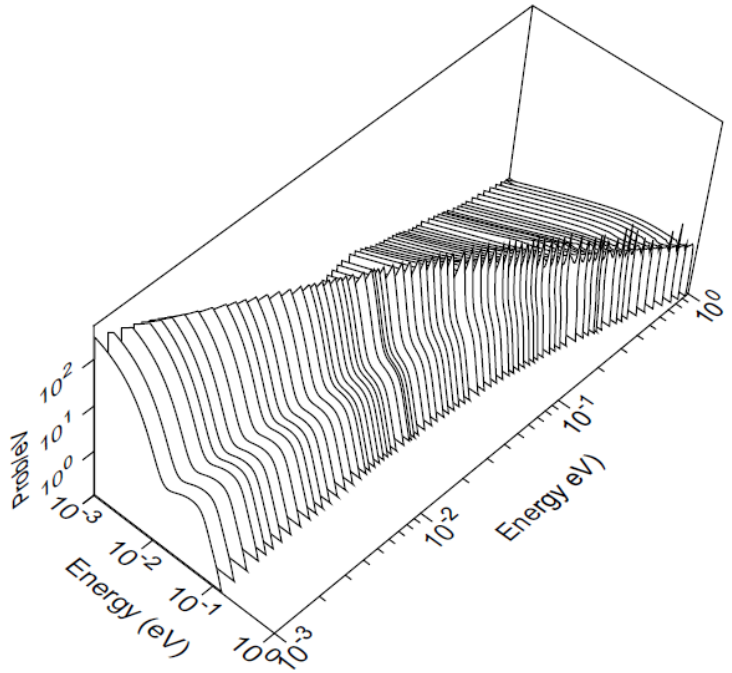
- SIGMA1
- Stochastic Mixing
- Kernel Reconstruction
- Gauss-Hermite Quadrature
- Polynomial fitting
- Target Motion Sampling
- Windowed Multipole

Method	Memory*	Efficiency*
Single T ACE	1	1
Stochastic Mixing / Interpolation	~100	~1.5-2
Kernel Reconstruction	**~10**	**~2**
Gauss-Hermite Quadrature	~1	~10-15
Polynomial Fitting	~20	~1.1-1.3
Target Motion Sampling	~2	~4-10
Windowed Multipole	**~0.5-0.7**	**~1.0-1.2**

* Estimated by the lecturer (lower is better)

Rest of the Energy Range

- Thermal scattering
  - Tables of (E, E', μ, T) with interpolation
  - PDF/CDF with temperature polynomial fitting
  - Rejection Sampling
- Unresolved Resonance Range
  - Equiprobable tables or surfaces
  - Multiple independent URR representations
- Threshold reactions, depletion tallies, …
  - (n,2n), (n,3n), (n,p), (n,α), …
- Secondary distributions
  - Multiple scattering laws, multiple formats, …



Outgoing Energy distribution Incoherent Inelastic Scattering for H in H2O at 293K (from NJOY)

Limitations

- Resonance upscattering is not always included by default
  - Observed in actinides with large low energy scattering resonances (<1000 eV)
  - Requires a rejection sampling algorithm or thermal scattering process that slows down computations
  - Impacts reactivity coefficients in LWRs by as much as 10%
- Nuclear data evaluations sometimes hinder the use and development of new formats
- More accurate data representation can significantly hinder performance but may have little impact on your problem of interest
  - Anisotropy of fission neutrons
  - Detailed outgoing angular distributions
- Coupled simulations and transients are still very costly

Resonance upscattering in U238 from energy just below 36.6 eV resonance

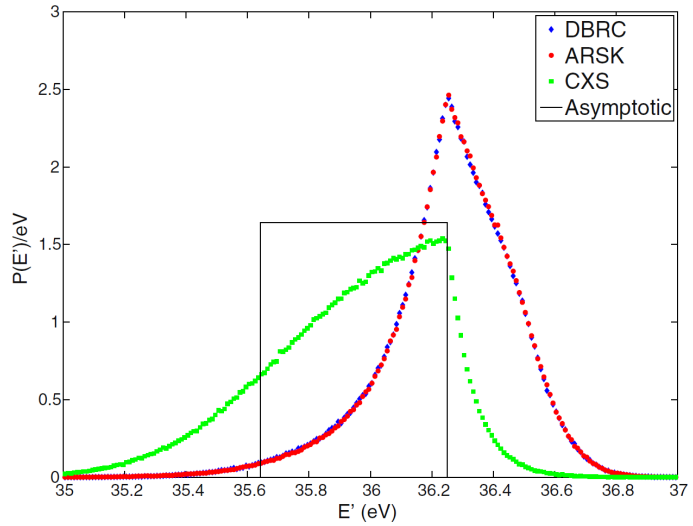
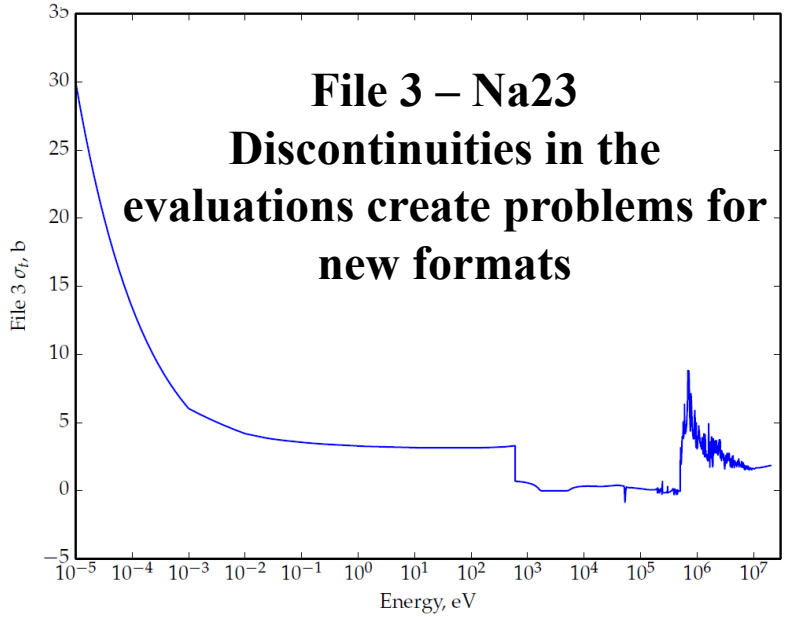


Fig. 2. 36.25 eV scattering kernel at 1000 K.



Opportunities

- Exposing the codes to more physics facilitates the integration of UQ methodologies with direct feedback on evaluations
  - Can we embed nuclear data uncertainty in a Monte Carlo simulations?
  - Can we provide valuable feedback to evaluators on where larger source of uncertainties are coming from?
- Neural network representations of complex data structures
  - Can advancements in data sciences provide a new path to data representation that can be both accurate and efficient?
- Modern computing architecture
  - Can we leverage power of GPU architectures to enable large skill steady-state and transient simulations?

Part II: Generating high-fidelity nuclear data for deterministic calculations

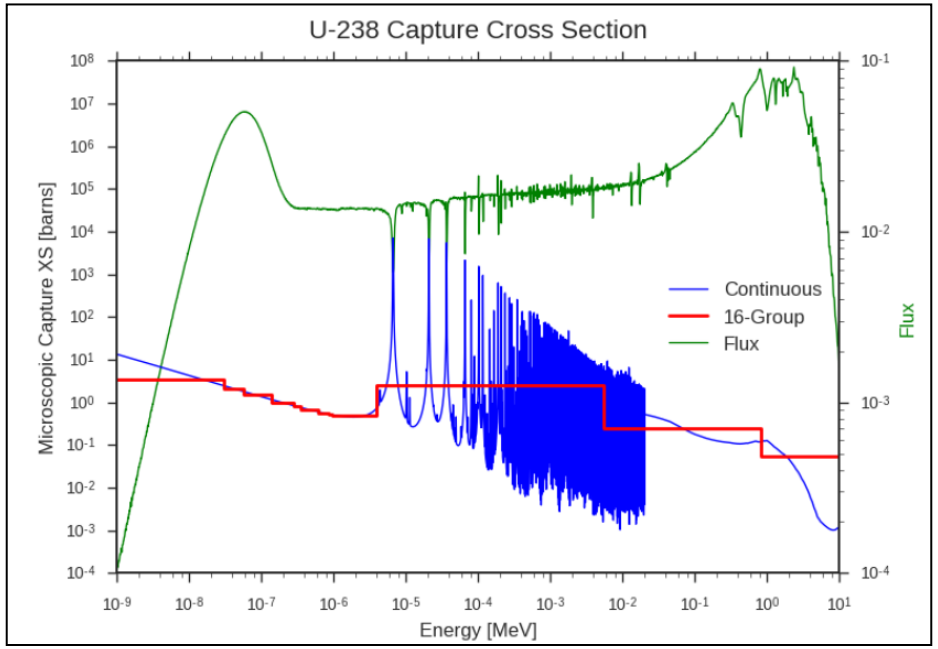
Why do we need high-fidelity deterministic codes?

Neutron Losses = **Neutron sources**

$$\underbrace{\boldsymbol{\Omega}\cdot\nabla\psi_g(\mathbf{r},\boldsymbol{\Omega})}_{\text{Net Leakage}}+\underbrace{\Sigma_t^g(\mathbf{r})\psi_g(\mathbf{r},\boldsymbol{\Omega})}_{\text{Neutron Interactions}}=\frac{1}{4\pi}\left(\underbrace{\frac{\chi_g(\mathbf{r})}{k}\sum_{g'=1}^{G}\nu_{g'}(\mathbf{r})\Sigma_f^{g'}(\mathbf{r})\phi_{g'}(\mathbf{r})}_{\text{Fission}}+\underbrace{\sum_{g'=1}^{G}\Sigma_s^{g'\to g}(\mathbf{r})\phi_{g'}(\mathbf{r})}_{\text{In-scattering}}\right)$$

- Deterministic methods represent the bulk behavior of neutrons and can thus typically converge faster
  - Transients!
- Energy condensation reduces the data size

$$\Sigma_f^g(\mathbf{r})=\frac{\int_{E_{g'-1}}^{E_{g'}}dE\,\Sigma_f(\mathbf{r},E)\phi(\mathbf{r},E)}{\int_{E_{g'-1}}^{E_{g'}}dE\,\phi(\mathbf{r},E)}$$



Full core performance of 3D OpenMOC vs OpenMC

	Machine	CPU-hours	Method
Gunow – PhD – 2017	Mira[4]	800,000[1]	3D MOC extruded geometry
Tramm – PhD – 2018	Theta[4]	220,000[2]	3D MOC Random Ray
Gaston – PhD – 2019	Lemhi[4]	200,000[3]	3D MOC Unstructured mesh
Giudicelli – PhD - 2020	Lemhi[4]	6,000	3D MOC extruded geometry

1: Estimated at 200,000 CPU hrs on Lemhi
2: Simplified geometry
3: Estimated
4: Theta is a Xeon Phi system, Lemhi is a Xeon Skylake system, Mira is POWERPC8 system

- Monte Carlo (OpenMC) Full core PWR with pin powers
  - 1% statistical accuracy in each pellet
  - ~100,000 CPU-hours on Lemhi-like system
  - Very difficult for transients due to time scales
    - Prompt neutrons of ~10^{-5} s and delayed neutrons ~1 s

Multigroup data generation is a solution and a problem

- Starting from a simplified continuous energy form of the transport equation

$$\vec{\Omega} \cdot \nabla \psi(\vec{r}, \vec{\Omega}, E) + \Sigma_t(\vec{r}, E)\psi(\vec{r}, \vec{\Omega}, E) = Q(\vec{r}, \vec{\Omega}, E)$$

- Energy condensation is used to preserve reaction rates

$$\Sigma_{t,g}(\vec{r}, \vec{\Omega}) = \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(\vec{r}, E)\psi(\vec{r}, \vec{\Omega}, E)dE}{\int_{E_g}^{E_{g-1}} \psi(\vec{r}, \vec{\Omega}, E)dE} = \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(\vec{r}, E)\psi(\vec{r}, \vec{\Omega}, E)dE}{\psi_g(\vec{r}, \vec{\Omega})}$$

Approximation 1

- Energy condensation introduces angular dependence to the multigroup cross-section, so we apply the following approximation

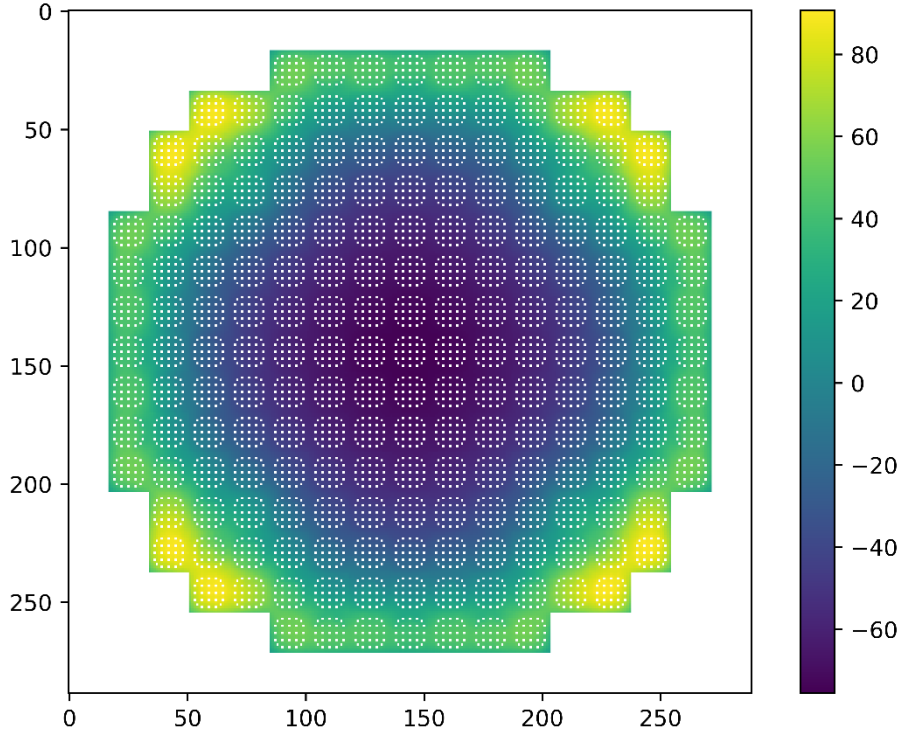
$$\Sigma_{t,g}(\vec{r}, \vec{\Omega}) \approx \Sigma_{t,g}(\vec{r}) = \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(\vec{r}, E)\phi(\vec{r}, E)dE}{\int_{E_g}^{E_{g-1}} \phi(\vec{r}, E)dE} = \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(\vec{r}, E)\phi(\vec{r}, E)dE}{\phi_g(\vec{r})}$$

Approximation 2

What if I only preserved reaction rates?

Approximation 3

$$\vec{\Omega} \cdot \nabla \psi(\vec{r}, \vec{\Omega}, E) + \Sigma_t(\vec{r}, E)\psi(\vec{r}, \vec{\Omega}, E) = \frac{Q(\vec{r}, E)}{4\pi}$$



- OpenMC vs. OpenMOC for the 2D BEAVRS core
  - 70-group **isotropic-in-lab scattering**
  - 64 azimuthal and 3 polar angles in OpenMOC
  - Ray spacing is 0.05 cm
  - Fine spatial discretization

	k_{eff}	Error (pcm)	Pin power relative error	
			RMS	Max
OpenMC	**1.00490**	(ref)	(ref)	(ref)
OpenMOC	1.02358	+ 1868	46.3%	90.2%

Liu, PhD thesis, 2020

Neutron migration

- If we start again from the simplified transport equation

$$\vec{\Omega} \cdot \nabla \psi(\vec{r}, \vec{\Omega}, E) + \Sigma_t(\vec{r}, E)\psi(\vec{r}, \vec{\Omega}, E) = Q(\vec{r}, \vec{\Omega}, E)$$

- We now apply the method of characteristic where we solve follow the neutron along its direction of travel (path s)

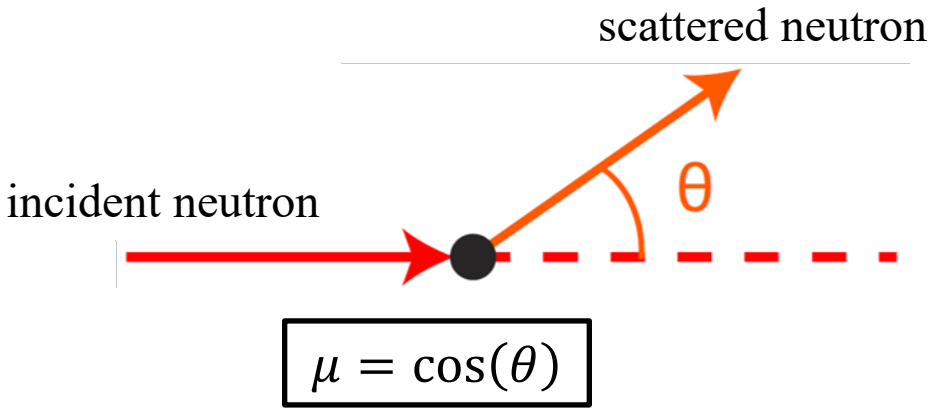
$$\frac{d\psi(\vec{r} - \vec{\Omega}s, \vec{\Omega}, E)}{ds} + \Sigma_t(\vec{r} - \vec{\Omega}s, E)\psi(\vec{r} - \vec{\Omega}s, \vec{\Omega}, E) = Q(\vec{r} - \vec{\Omega}s, \vec{\Omega}, E)$$

- Introducing an integrating factor (for a homogeneous system)

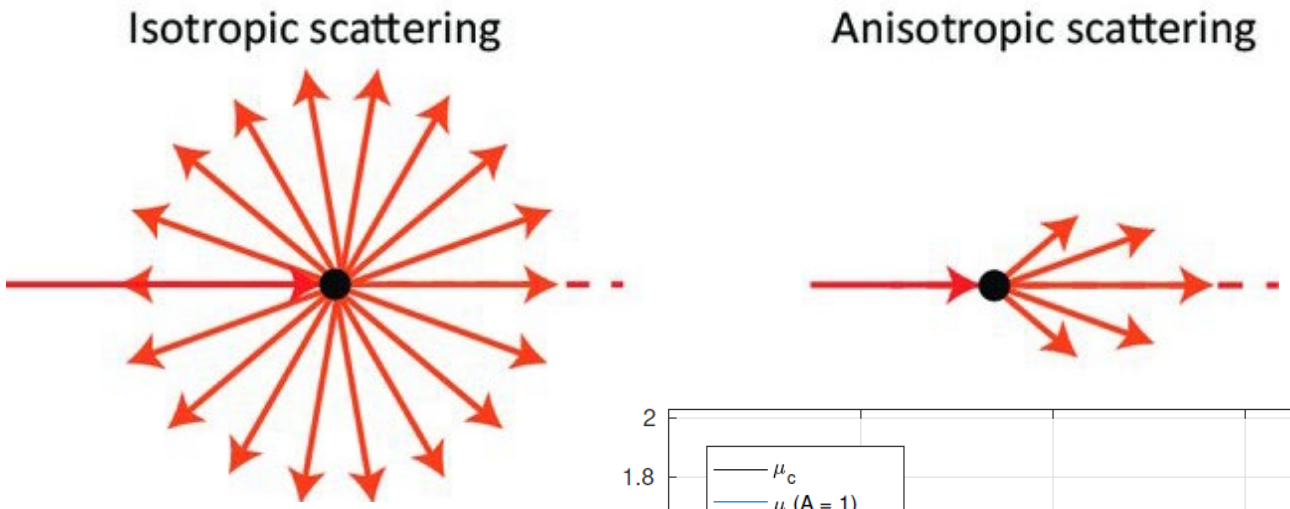
$$\psi(\vec{r}, \vec{\Omega}, E) = \psi_{BC}(\vec{r} - \vec{\Omega}s_{BC}, \vec{\Omega}, E)\, e^{-\Sigma_t(E)s_{BC}} + \int_0^{s_{BC}} Q(\vec{r} - \vec{\Omega}s, \vec{\Omega}, E)\, e^{-\Sigma_t(E)s}\, ds$$

Preserving the reaction rate will not preserve the attenuation! – This invalidates approximation 1.

Anisotropy must also be accounted for properly

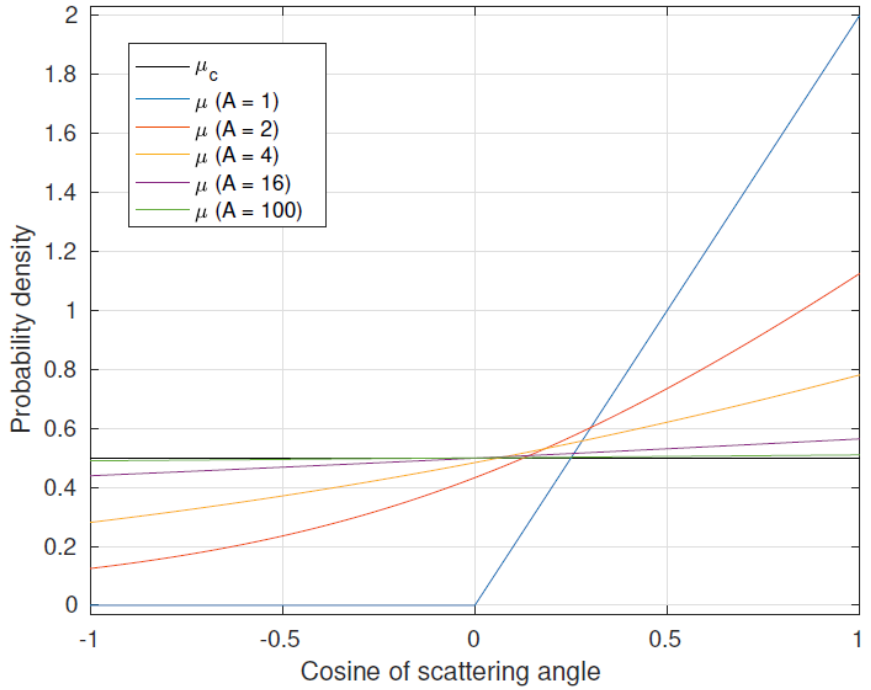


(Figure source:, Baptiste Jayet, 2015)



- Light nuclei have a large forward scattering component.
- Typically, scattering cosine angle is represented using Legendre polynomials (orthogonal between -1 and 1)
- H-1 requires high order scattering for accurate representation of neutron movement

This invalidates approximation 3.



High order scattering is needed

- Scattering source

$$Q_g^{scat}(\vec{r},\vec{\Omega}) = \frac{1}{2\pi}\sum_{g'=1}^{G}\int_{4\pi} d^2\Omega' \Sigma_{s,g'\to g}(\vec{r},\vec{\Omega}\cdot\vec{\Omega}')\psi_{g'}(\vec{r},\vec{\Omega}')$$

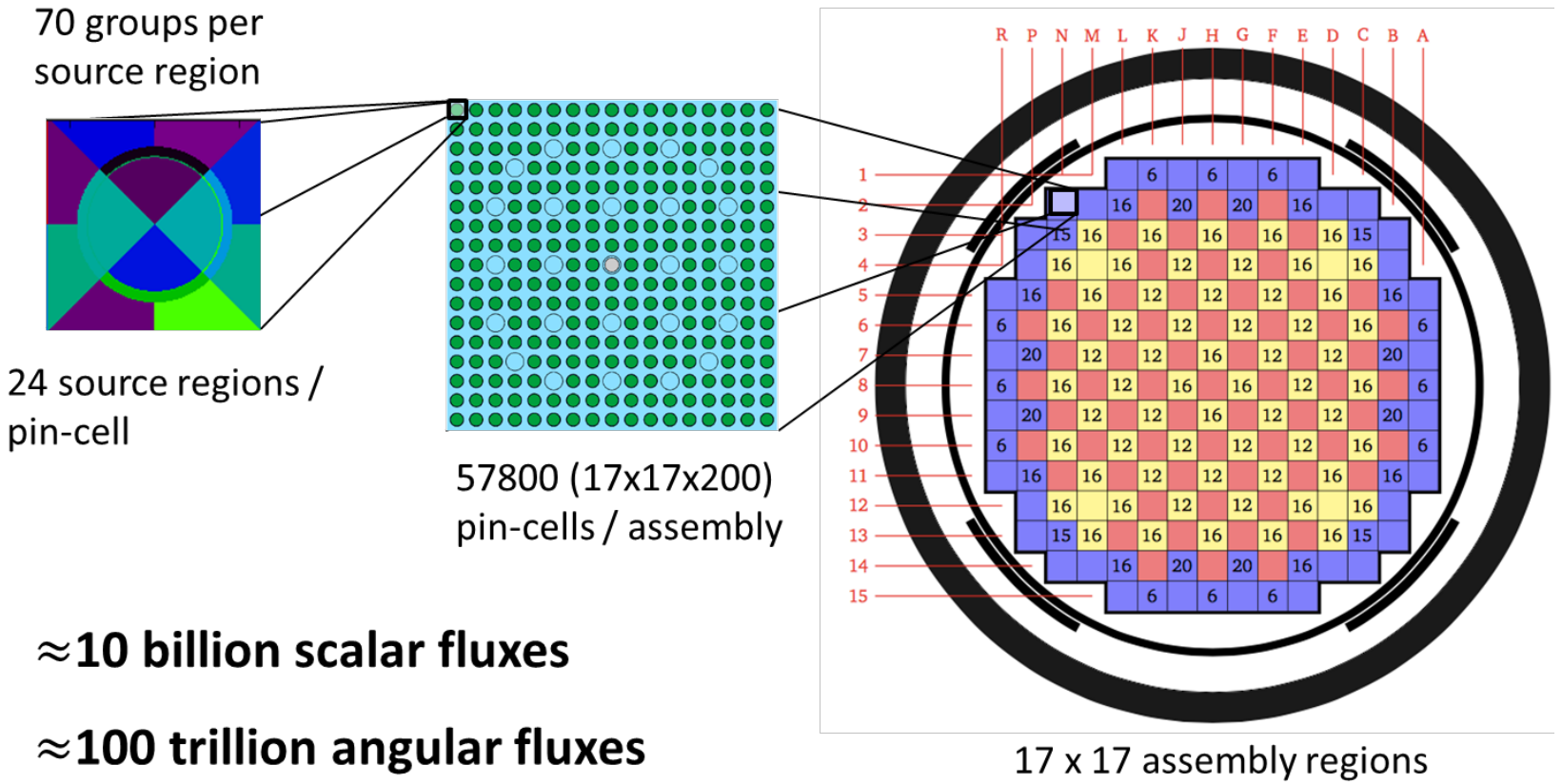
where the scattering cross-section is expanded using Legendre polynomials

$$\Sigma_{s,g'\to g}(\vec{r},\vec{\Omega}\cdot\vec{\Omega}') = \sum_{l=0}^{L}\frac{2l+1}{2}\Sigma_{sl,g'\to g}(\vec{r})P_l(\vec{r},\vec{\Omega}\cdot\vec{\Omega}')$$

- An anisotropic source complicates the solution of the neutron transport equation over a segment immensely!
  - Angular fluxes or flux moments are needed (x10-100 in memory)
  - Number of operations increases substantially (x10-100 in operations)

Scale of full core PWR problem

- Storing angular fluxes is not possible or desirable
  - Methods are developed that only store scalar flux or low order angular flux moments
- High order scattering can become quite costly
  - P_3 scattering requires storing 16 spherical harmonics flux moments



≈10 billion scalar fluxes

≈100 trillion angular fluxes

10 billion unknowns in double precision is ~75GB

Transport cross-section

- To capture the high order scattering effects while keeping memory costs comparable to the isotropic-in-lab case, we introduce the transport correction

$$\Sigma_{tr}(E) = \Sigma_t(E) - \Delta_{tr}(E)$$

- This correction will allow us to capture the anisotropic scattering and preserve the migration area during the condensation process

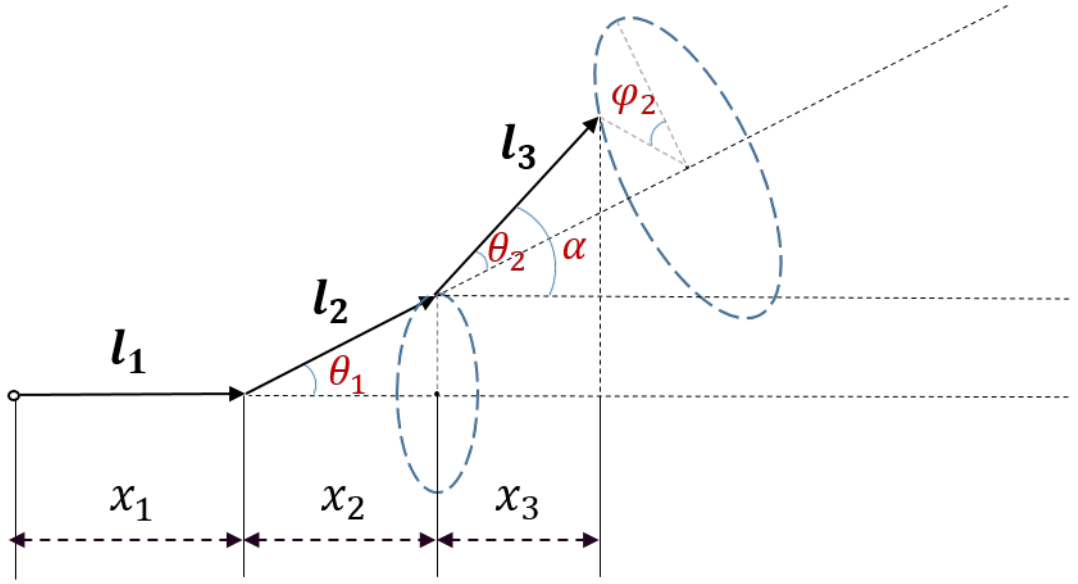
$$\vec{\Omega} \cdot \nabla \psi(\vec{r}, \vec{\Omega}, E) + \Sigma_{tr}(\vec{r}, E)\psi(\vec{r}, \vec{\Omega}, E) = \frac{Q^*(\vec{r}, E)}{4\pi}$$

- How do we calculate the transport cross-section?

If done correctly, this could allow for approximations 1 and 3 to work.

One group model

- Textbook definition from Lamarsh (1961)
  - Measures the true distance travelled after an infinite number of collisions
  - μ-bar is the average cosine angle after a collision, equal to 2/3A for elastic scattering isotropic in the COM



- There is however a strong energy dependence!

$$\lambda_{tr} = \lambda_t + \lambda_t\bar{\mu} + \lambda_t\bar{\mu}^2 + \cdots$$

$$= \frac{\lambda_t}{1-\bar{\mu}}$$

For H-1, $\Sigma_{tr} = (1-\bar{\mu})\Sigma_t = \frac{1}{3}\Sigma_t$

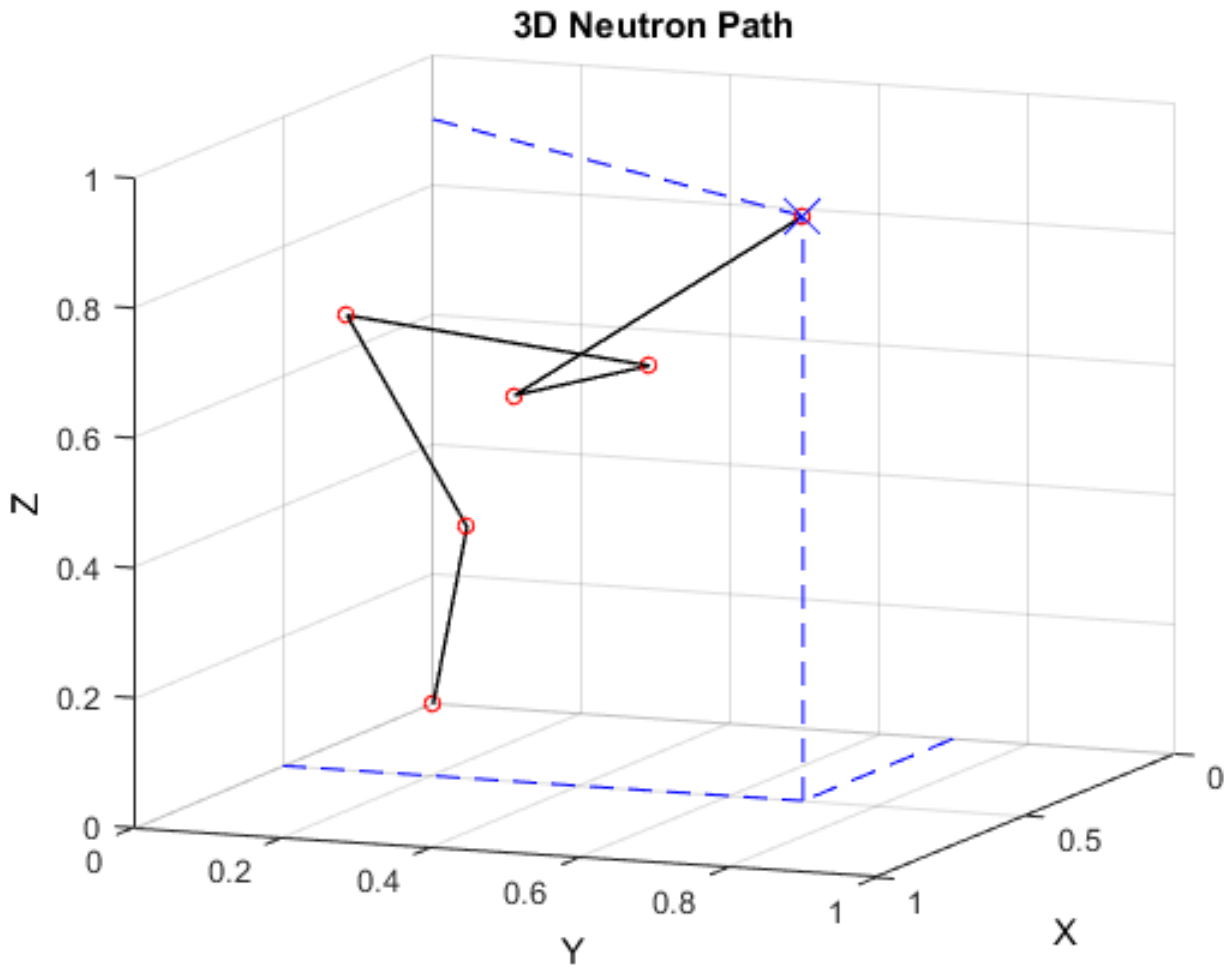
Migration area

- Migration area is a relation between the square of the distance travelled by a neutron and the probability of getting absorbed by the medium along the way
- In one group diffusion theory, we can show that

$$M^2 \equiv \frac{D}{\Sigma_a}$$

which can also be related to the square distance from birth to absorption

$$M^2 = \frac{1}{6}\langle r^2 \rangle$$



From the P_1 equations (in 1D), we can relate Σ_{tr} to D

- Expand the angular flux using a first order Legendre polynomial expansion

$$\nabla \cdot \vec{J}(\vec{r},E) + \Sigma_t(\vec{r},E)\,\phi(\vec{r},E) = \int_0^\infty \Sigma_{s0}(\vec{r},E' \to E)\,\phi(\vec{r},E')\,dE' + \frac{\chi(\vec{r},E)}{k_{eff}} \int_0^\infty \Sigma_f(\vec{r},E')\,\phi(\vec{r},E')\,dE'$$

$$\nabla\phi(\vec{r},E) + 3\Sigma_t(\vec{r},E)\,\vec{J}(\vec{r},E) = 3\int_0^\infty \Sigma_{s1}(\vec{r},E' \to E)\,\vec{J}(\vec{r},E')\,dE'$$

- From the second equation, we can write

$$\vec{J}(\vec{r},E) = -\frac{1}{3\left[\Sigma_t(\vec{r},E) - \frac{1}{J(\vec{r},E)}\int_0^\infty \Sigma_{s1}(\vec{r},E' \to E)\,J(\vec{r},E')\,dE'\right]}\nabla\phi(\vec{r},E)$$

$$\downarrow$$

$$\Sigma_{tr}$$

Common approximations

$$\Sigma_{tr}(E) = \Sigma_t(E) - \frac{1}{J(E)}\int_0^{\infty} \Sigma_{s1}(E' \rightarrow E)\, J(E')\, dE'$$

- Many approximations have been introduced throughout the years, the most accurate being the in-scatter method which requires an approximate current spectrum
  - Out-scatter (and asymptotic) approximation are common in most textbook, but perform very poorly for most thermal systems
  - In-scatter is often difficult to implement since current can often be 0 in symmetric problems

- In-scatter

  from solving P_1 Equations with small buckling

$$\Sigma_{tr,g}^{in} = \Sigma_{t,g} - \sum_{g'=1}^{G} \frac{\Sigma_{s1,g'\rightarrow g} J_{g'}}{J_g}$$

- Commonly-used approximations
  - out-scatter approximation

$$\Sigma_{tr,g}^{os} = \Sigma_{t,g} - \bar{\mu}_g \Sigma_{s0,g}$$

  - ***asymptotic*** result of out-scatter approximation

$$\Sigma_{tr,g}^{as} = \Sigma_{t,g} - \frac{2}{3}\Sigma_{s0,g} \approx \frac{1}{3}\Sigma_{t,g}$$

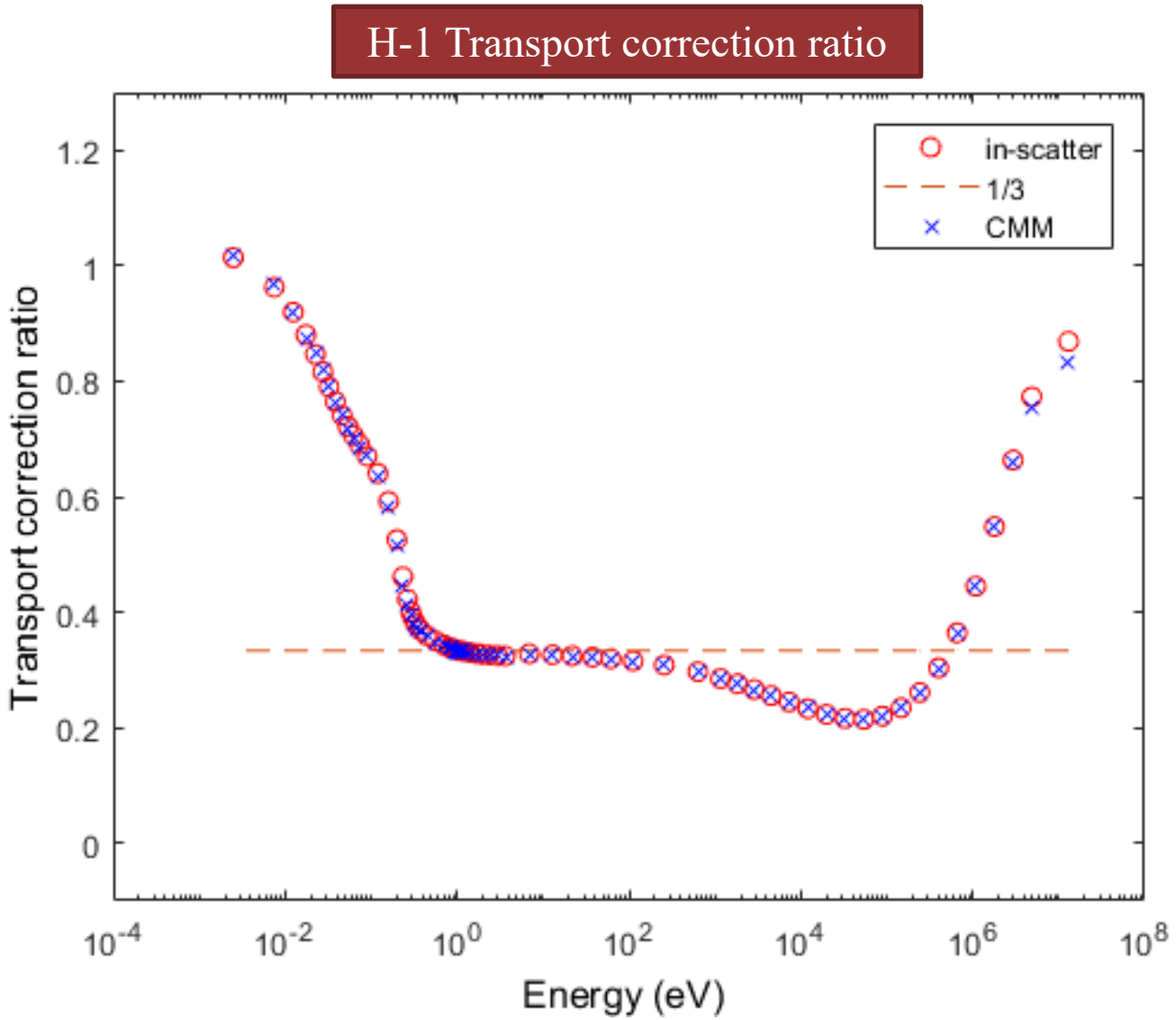
  - flux-limited approximation

$$\Sigma_{tr,g}^{fl} = \Sigma_{t,g} - \sum_{g'=1}^{G} \frac{\Sigma_{s1,g'\rightarrow g} \phi_{g'}}{\phi_g}$$

Keep in mind the strong energy dependence!

- Figure shows the transport correction ratio (Σ_{tr} / Σ_t) as a function of energy for H-1

- Many collisions are needed to reach the asymptotic value
  - In H-1 this comes with a large change in energy
  - Poor energy resolution can lead to large errors in the fast leakage



Always perform energy condensation on $1/\Sigma_{tr}$

- The transport correction is introduced to preserve migration of neutrons, thus when condensing in energy, it should preserve the migration area.

$$\psi(\vec{r},\vec{\Omega},E)=\psi_{BC}(\vec{r}-\vec{\Omega}s_{BC},\vec{\Omega},E)\,e^{-\Sigma_{tr}s_{BC}}+\int_0^{s_{BC}}Q^*(\vec{r}-\vec{\Omega}s,\vec{\Omega},E)\,e^{-\Sigma_{tr}s}ds$$

- Two ways to think of this
  - From Diffusion theory

$$D_g=\frac{1}{3\Sigma_{tr,g}}\approx\frac{\int_{E_g}^{E_{g-1}}D(E)\phi(E)dE}{\int_{E_g}^{E_{g-1}}\phi(E)dE}=\frac{\int_{E_g}^{E_{g-1}}\frac{1}{3\Sigma_{tr}(E)}\phi(E)dE}{\phi_g}=\frac{1}{3}\frac{\int_{E_g}^{E_{g-1}}\lambda_{tr}(E)\phi(E)dE}{\phi_g}$$

  - Or from Transport theory

$$\Sigma_{tr,g}=\frac{\int\int\int\Sigma_{tr}(E)\psi(\vec{r},\vec{\Omega},E)dEdVd\Omega}{\int\int\int\psi(\vec{r},\vec{\Omega},E)dEdVd\Omega}=\frac{\int\int\int\Sigma_{tr}(E)\psi(\Omega,E)e^{-\Sigma_{tr}s}dEdVd\Omega}{\int\int\int\psi(\Omega,E)e^{-\Sigma_{tr}s}dEdVd\Omega}=\frac{\int\lambda_{tr}(E)\phi(E)dE}{\frac{1}{\Sigma_{tr,g}^2}\phi_g}$$

Never energy collapse Σ_{tr}, always $1/\Sigma_{tr}$!

$$\frac{1}{\Sigma_{tr,g}} = \frac{\int_{E_g}^{E_{g-1}} \lambda_{tr}(E)\phi(E)dE}{\phi_g}$$

	Fast Group Diffusion Coefficient			
Energy Collapse Weighting	P1 with Inscatter	P1 with Outscatter	B1 with Inscatter	Monte Carlo Cumulative Migration*
Diffusion Coefficient	1.435	1.544	1.393	1.426
Difference From MC	0.6%	8.3%	-2.3%	
Sigma Transport	1.169	1.149	1.397**	
Difference From MC	-18.0%	-19.4%	-2.0%	

*See Companion Paper by Liu, Smith, and Forget

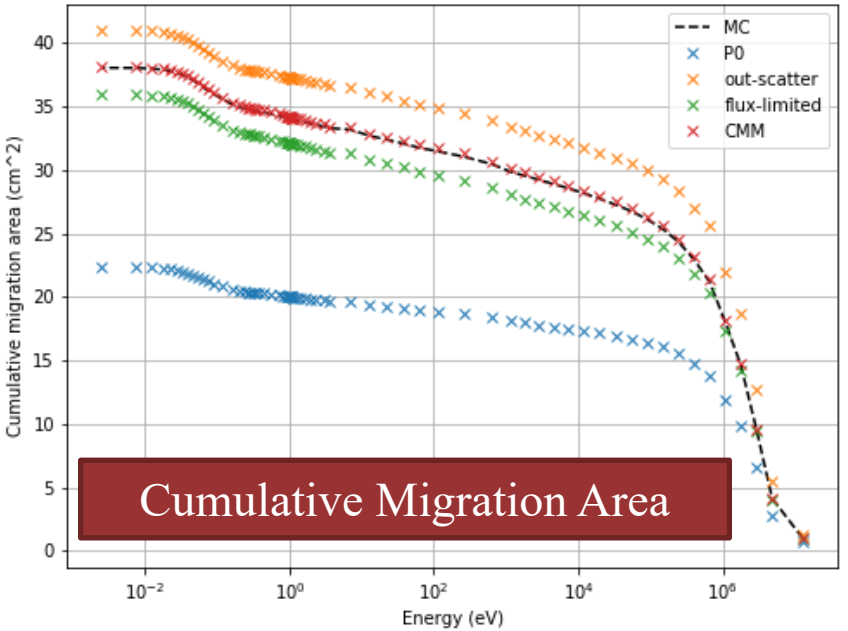
** Lepannen for 2.4% lattice wth 12 Pyrex BP

In diffusion theory, it can lead to a 20% error in the fast group diffusion coefficient.

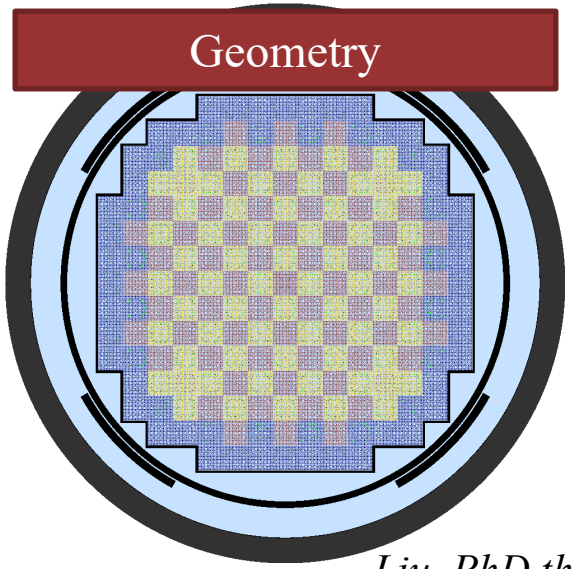
Liu, PhD thesis, 2020

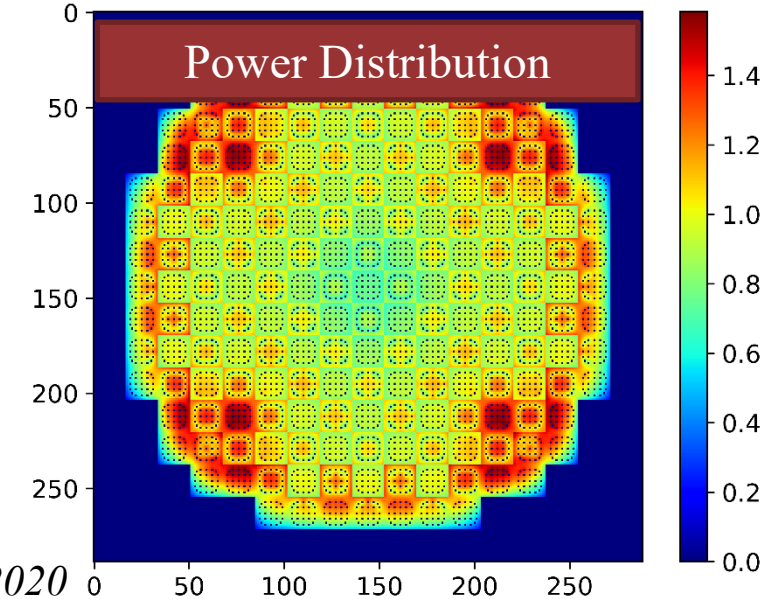
Transport cross-section

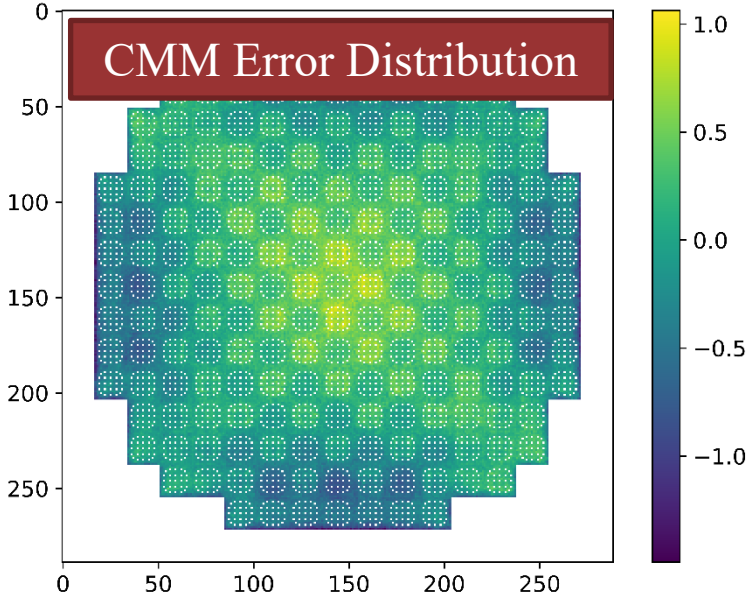
	k_{eff}	Error (pcm)	M^2 (cm^2)	Relative error
OpenMC	**1.00490**	(ref)	**55.56**	(ref)
Consistent-*P*	1.02358	1868	33.30	-40.06%
Out-scatter	1.00129	-361	58.79	5.82%
Flux-limited	1.00411	-79	52.83	-4.90%
CMM (hom)	1.00213	-277	55.65	0.16%



Geometry





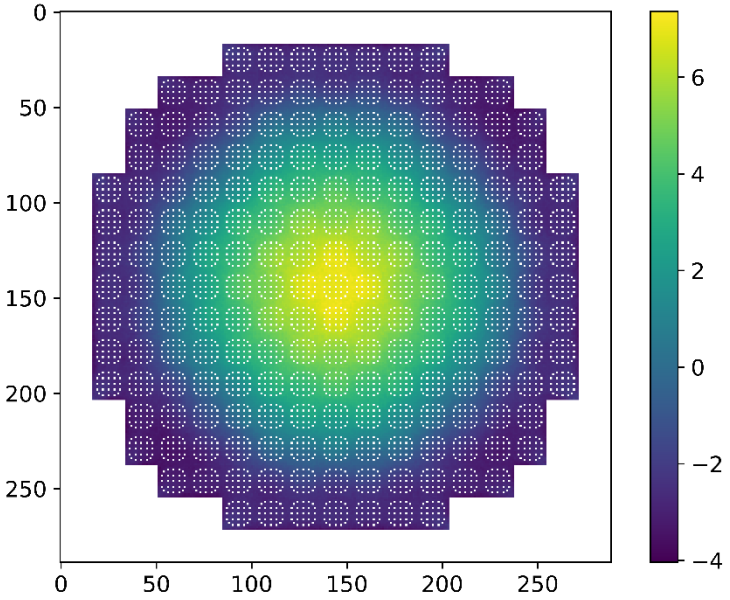


Liu, PhD thesis, 2020

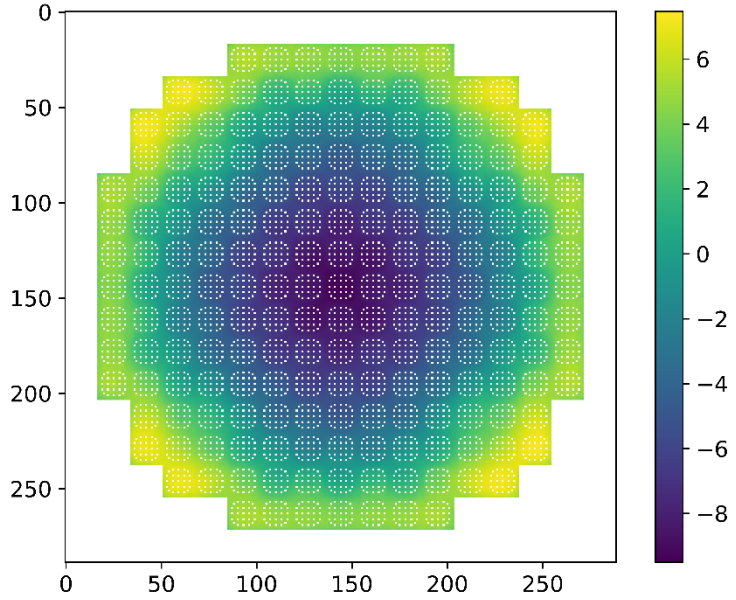
Migration area is key!

Liu, PhD thesis, 2020

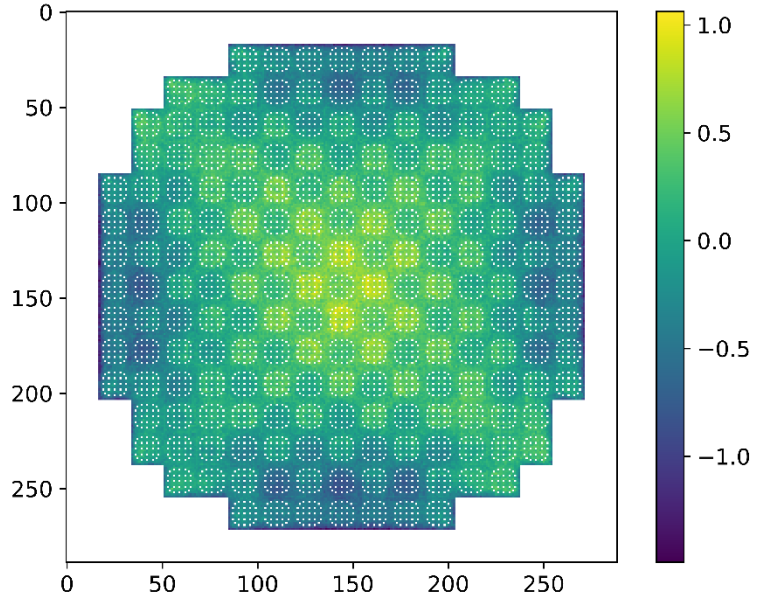
Out-scatter Error Distribution



Flux Limited Error Distribution



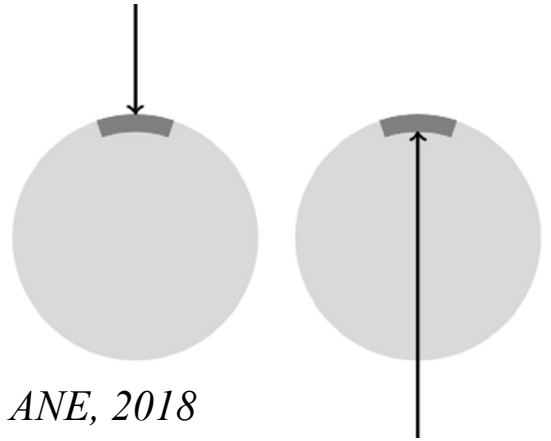
CMM and In-scatter Error Distribution



	Migration area error (%)	Pin Power RMS Error (%)	Pin Power Max Error (%)
Out-scatter	**5.8**	**3.0**	**7.4**
Flux Limited	**-4.9**	**4.6**	**9.5**
In-scatter / CMM	**0.2**	**0.4**	**1.5**

Angular dependence of the cross-sections

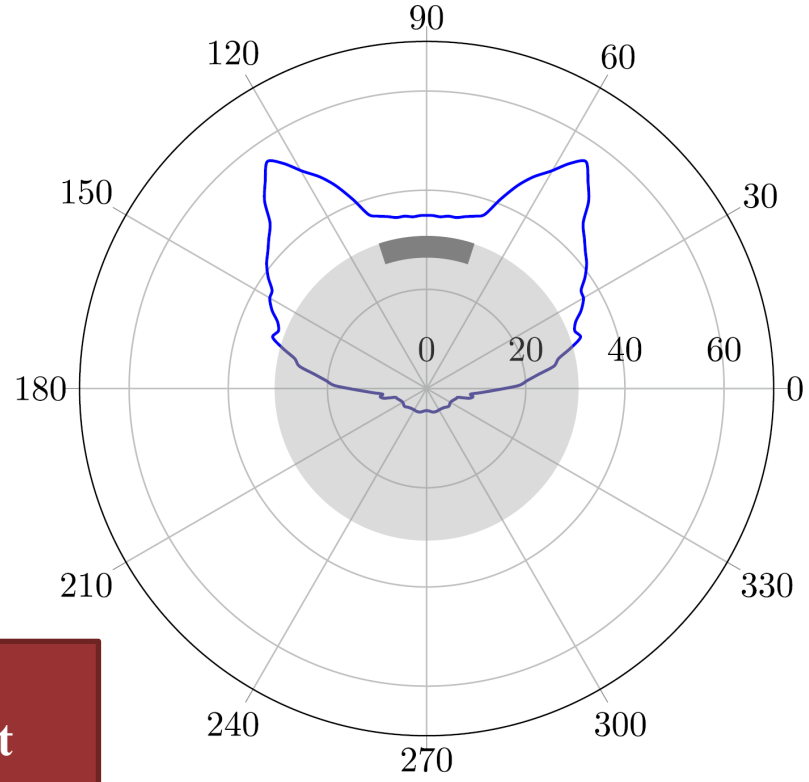
- Ignoring the angular dependence of the cross-section is problematic for heterogeneous geometries
  - In LWRs, leads to errors on the order of 200-300 pcm. Mostly on the over estimation of absorption in U-238 resonances.



Boyd et al, ANE, 2018

The eigenvalue bias in pcm with isotropic-in-lab scattering. The number of radial rings is varied, holding the number of azimuthal sectors constant.

	FSR Discretization		
# Groups	1×	4×	16×
1	80	55	66
2	141	29	34
4	27	−43	−57
8	26	−85	−102
16	35	−91	−111
25	−31	−158	−182
40	−38	−174	−202
70	−39	−182	−211



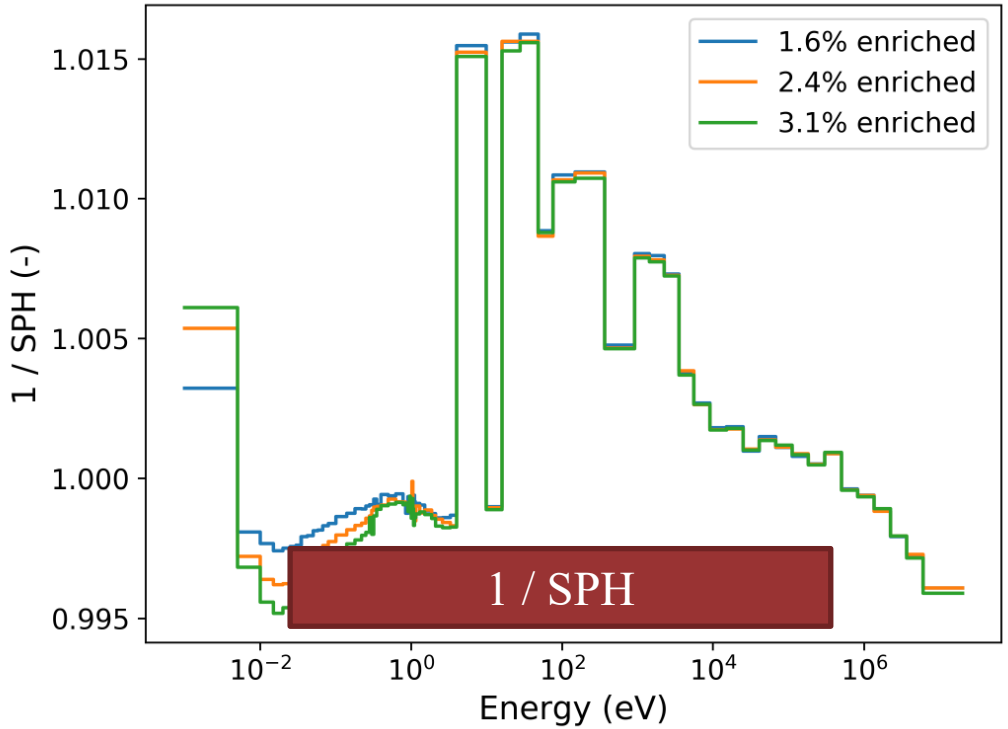
Approximation 2 will always lead to a minus 200-300 pcm error in coarse group structures (for LWRs), regardless of the scattering order or transport cross-section. Adding more groups >5000's will eventually eliminate this error.

Equivalence factors

- Most common approach is called SPH factors

$$(f_{ig}\Sigma_{ig})\Phi_{SPH} = \Sigma_{ig}\Phi_{ig}$$

  - Iterative approach
    - Solve OpenMC to get Σ and Φ_{MC} in each region
    - Set SPH factors (f) to 1
    - Iterate
      - $\Sigma^* = \Sigma$ x f
      - Solve OpenMOC to get Σ^* and Φ_{MOC}
      - Calculate SPH factor (f)
  - Typically done on small scale problem (e.g. pin cell) and used on larger problem



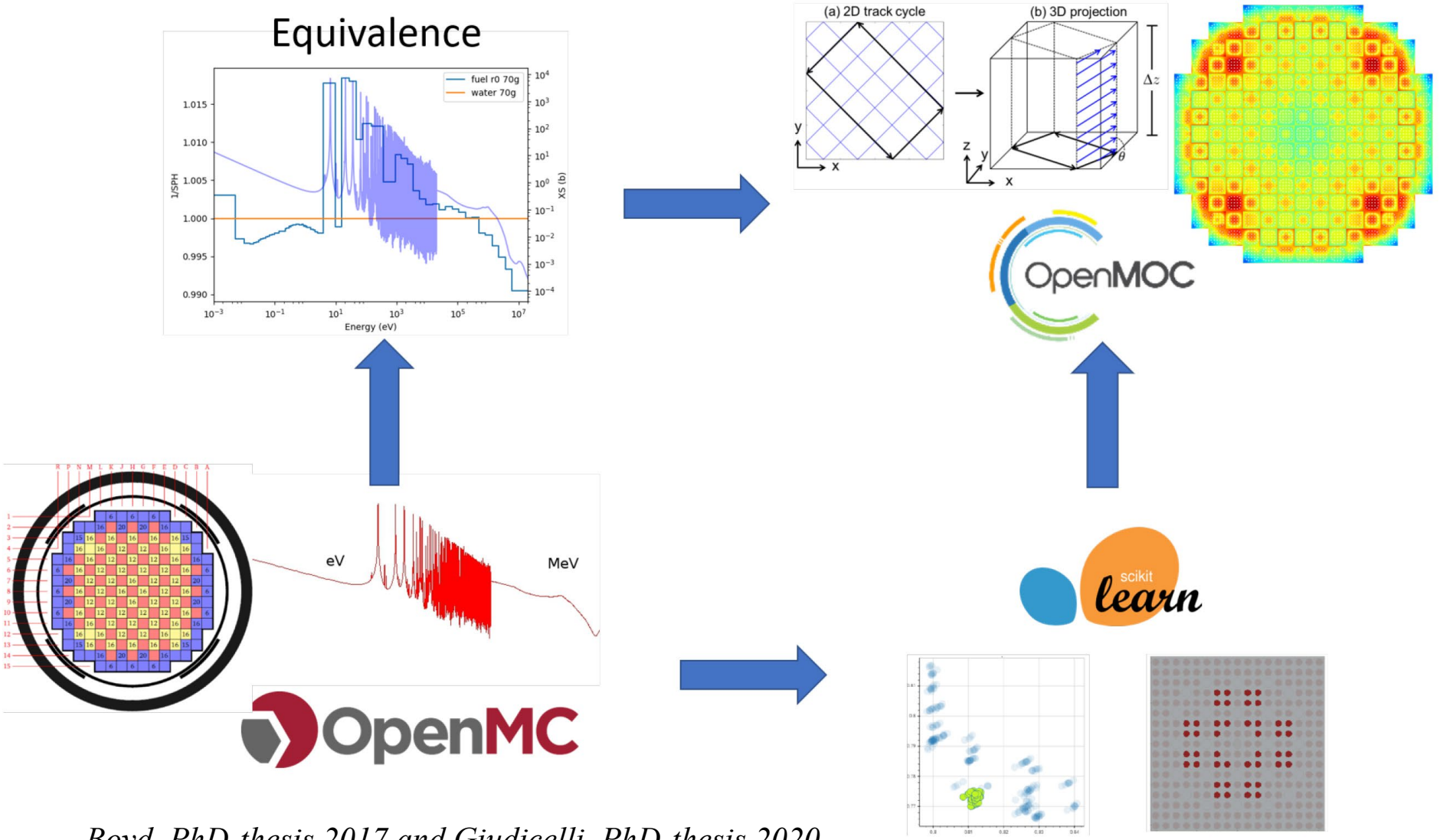
2D BEAVRS

	$\Delta\rho$	$\frac{\Delta RR_{fiss.}}{RR^{ref}_{fiss.}}$		$\frac{\Delta RR_{U238,abs.}}{RR^{ref}_{U238,abs.}}$		Iter.
		RMS	max	RMS	max	
	(pcm)	(%)	(%)	(%)	(%)	5E-4
Homogeneous						
No equivalence	-226	0.36	1.28	1.15	2.85	-
SPH in fuel, per enrichment	-12	0.18	0.96	0.52	3.32	9

Limitations

- Transport cross section creates convergence issues
  - Dampening procedures have been proposed in the literature to alleviate some of these issues
- Transport cross sections are difficult to generate for heterogeneous cases
- Transport cross section accuracy can also be limiting for highly heterogeneous cases
  - High order scattering might be necessary
- SPH factor generation is problem dependent, iterative and sometimes difficult

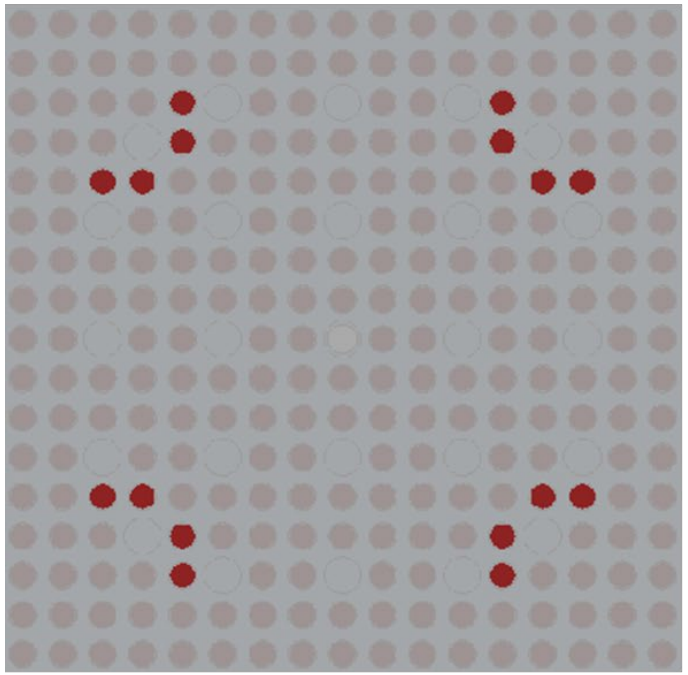
Opportunities – Can we learn multigroup cross sections?



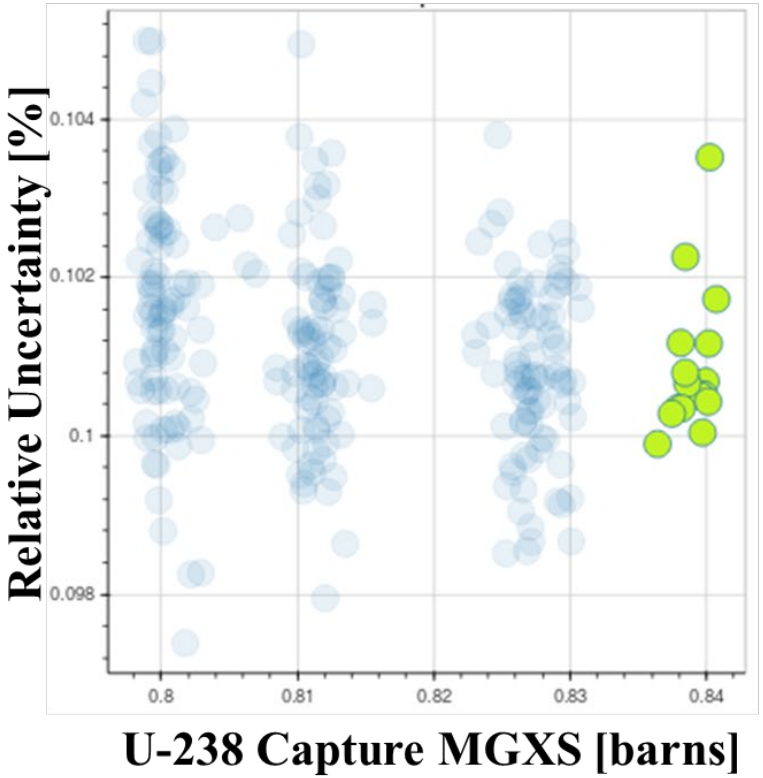
Boyd, PhD-thesis 2017 and Giudicelli, PhD-thesis 2020

Statistical Clustering – Assembly Example

- By observing noisy Monte Carlo results, we can see clusters emerge
  - Similar spatial locations are exposed to a similar spectrum and should yield the same value
  - Clustering can be used "to accelerate" the statistical convergence of Monte Carlo by identifying which clusters to combine without user input

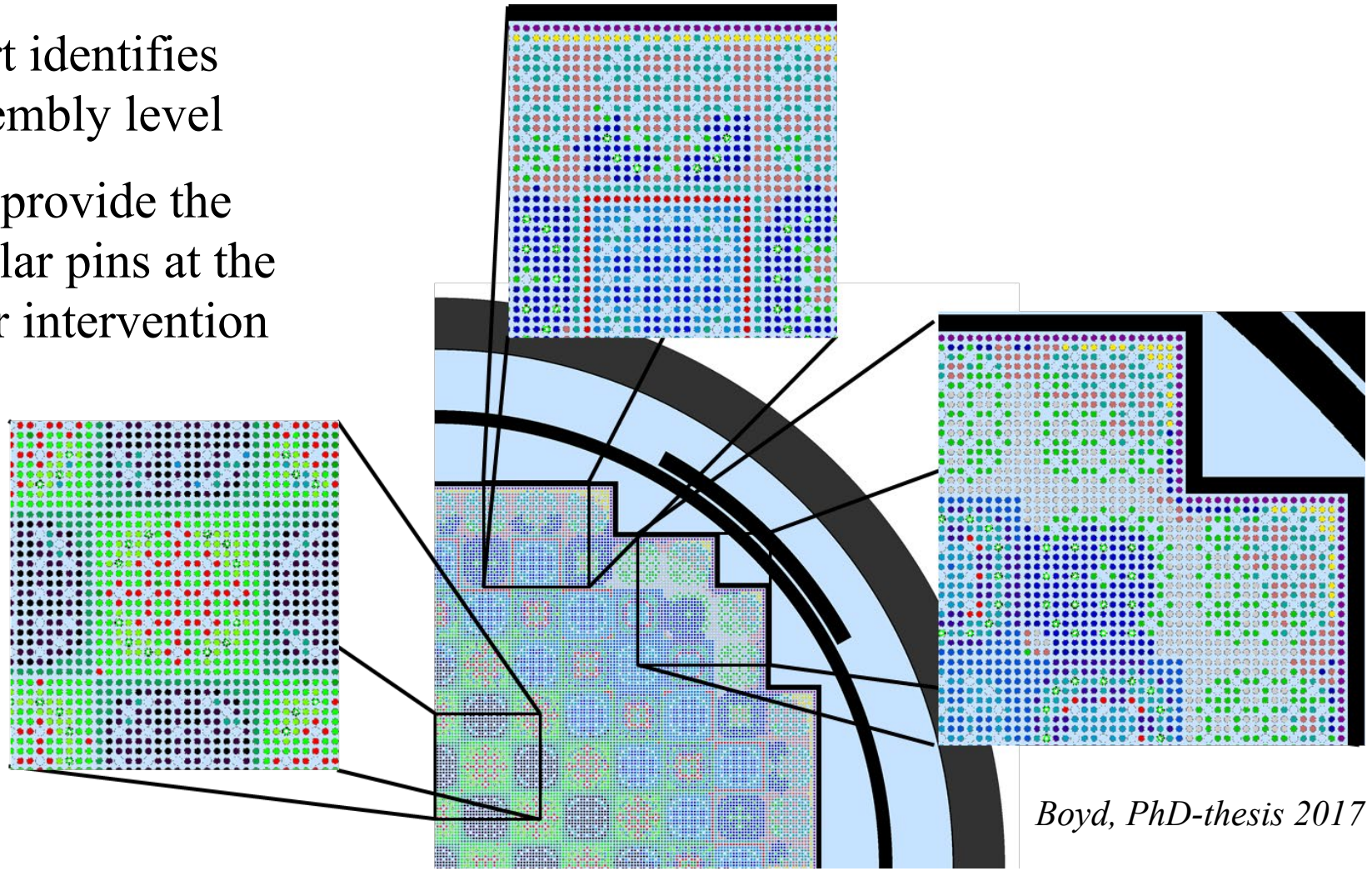


Boyd, PhD-thesis 2017



At the core level

- Current state-of-the-art identifies similar pins at the assembly level
- Clustering techniques provide the ability to identify similar pins at the core level with no user intervention



Boyd, PhD-thesis 2017

Summary - Deterministic

- High-fidelity deterministic transport can provide accurate results at a fraction of the cost of Monte Carlo methods.
  - Necessary for high fidelity transient analysis.
- High order scattering is necessary to properly represent the movement of neutrons in the presence of light nuclei
- Transport correction allows to preserve most of the effect of anisotropy at a fraction of the cost
  - Strong energy dependence that must be captured appropriately.
  - Not all approximations work well for H-1.
  - Always condense $1/\Sigma_{tr}$ in energy if further condensation is desired.
- If angular dependence of the cross-sections is not preserved, additional equivalence factors are needed.

Summary - Stochastic

- High fidelity Monte Carlo simulations require large amounts of nuclear data, especially in coupled simulations where temperature must be accounted for
  - Many techniques exist that can accurately capture the temperature effects in the resolved resonance range
- Random access of nuclear data can hinder performance on modern computing architectures
- By default, most general Monte Carlo simulations tools still neglect some important temperature phenomena
  - Resonance upscattering
  - Thermal scattering

Acknowledgements