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

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IAEA Workshop on
Computational Nuclear Science and Engineering
May 23, 2022

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**

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

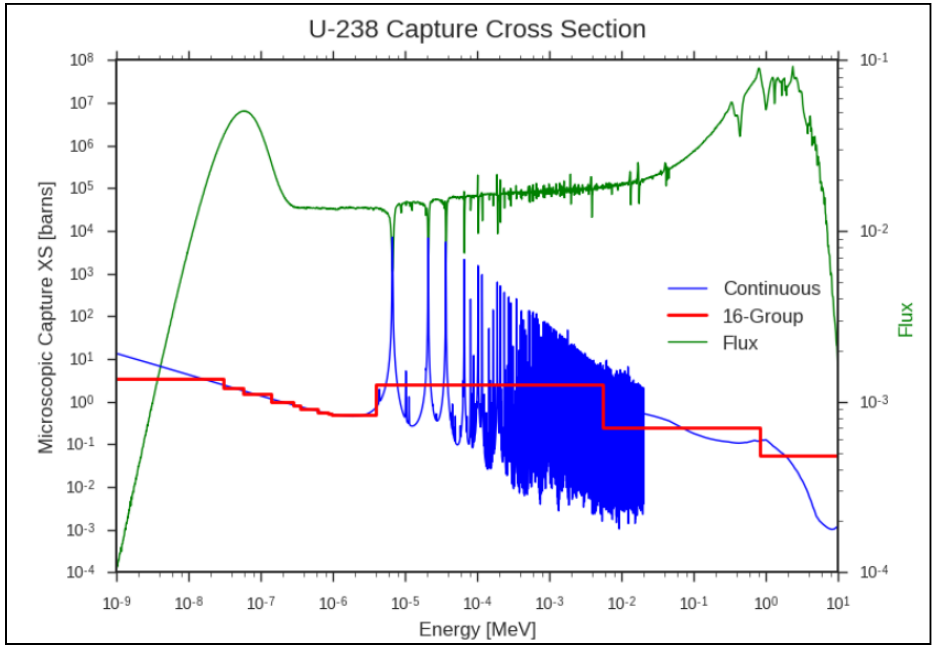
Why do we need high-fidelity deterministic codes?

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

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



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

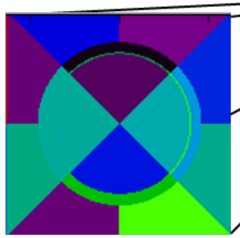
- Energy condensation introduces angular dependence to the multigroup cross-section, so we apply the following approximation

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

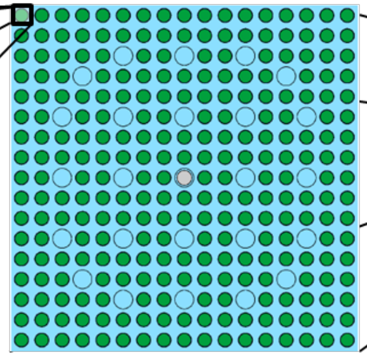
Approximation 2

Curse of Dimensionality

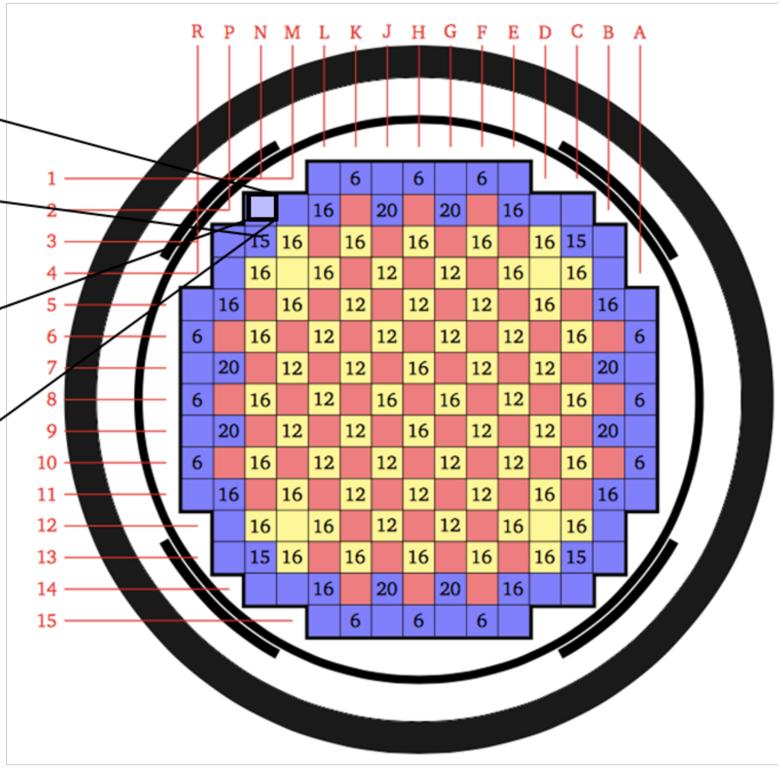
70 groups per source region



24 source regions / pin-cell



57800 (17x17x200) pin-cells / assembly



17 x 17 assembly regions

≈10 billion scalar fluxes

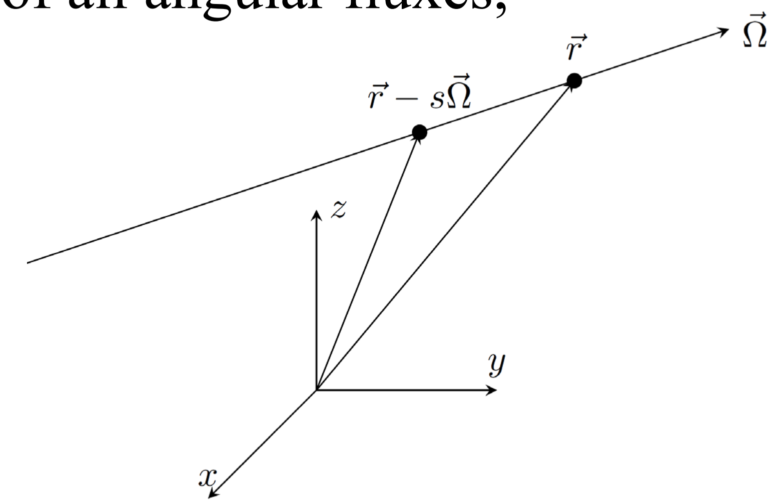
≈100 trillion angular fluxes

10 billion unknowns in double precision is ~75GB

Storing angular fluxes is very costly and should be avoided!

Method of Characteristic – In a nutshell

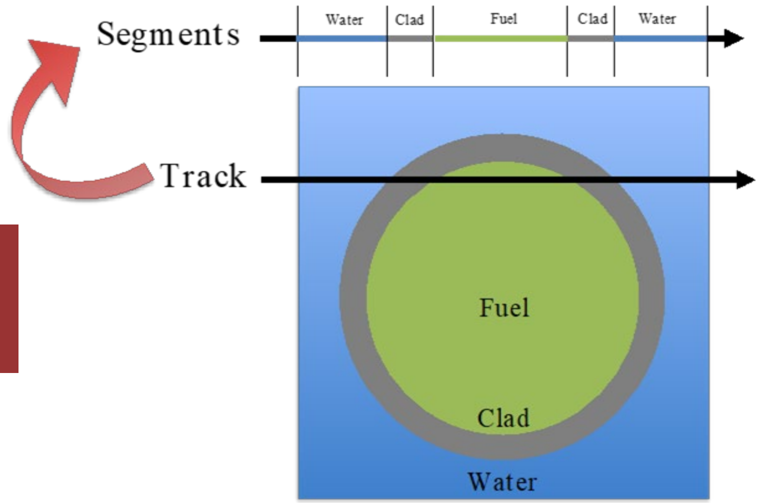
- Many common solution techniques do not require storage of all angular fluxes, they instead rely on sweeping across discrete angles.



$$\vec{\Omega} \cdot \nabla \psi_g(\vec{r}, \vec{\Omega}) + \Sigma_{t,g}(\vec{r})\psi_g(\vec{r}, \vec{\Omega}) = Q_g(\vec{r}, \vec{\Omega})$$

$$\frac{d\psi_g(\vec{r} - \vec{\Omega}s, \vec{\Omega})}{ds} + \Sigma_{t,g}(\vec{r} - \vec{\Omega}s)\psi_g(\vec{r} - \vec{\Omega}s, \vec{\Omega}) = Q_g(\vec{r} - \vec{\Omega}s, \vec{\Omega})$$

$$\psi_g^{out}(\vec{r}, \vec{\Omega}) = \psi_g^{in}(\vec{r}, \vec{\Omega})e^{-\Sigma_{t,g}s} + \frac{Q_g(\vec{r}, \vec{\Omega})}{\Sigma_{t,g}}(1 - e^{-\Sigma_{t,g}s})$$



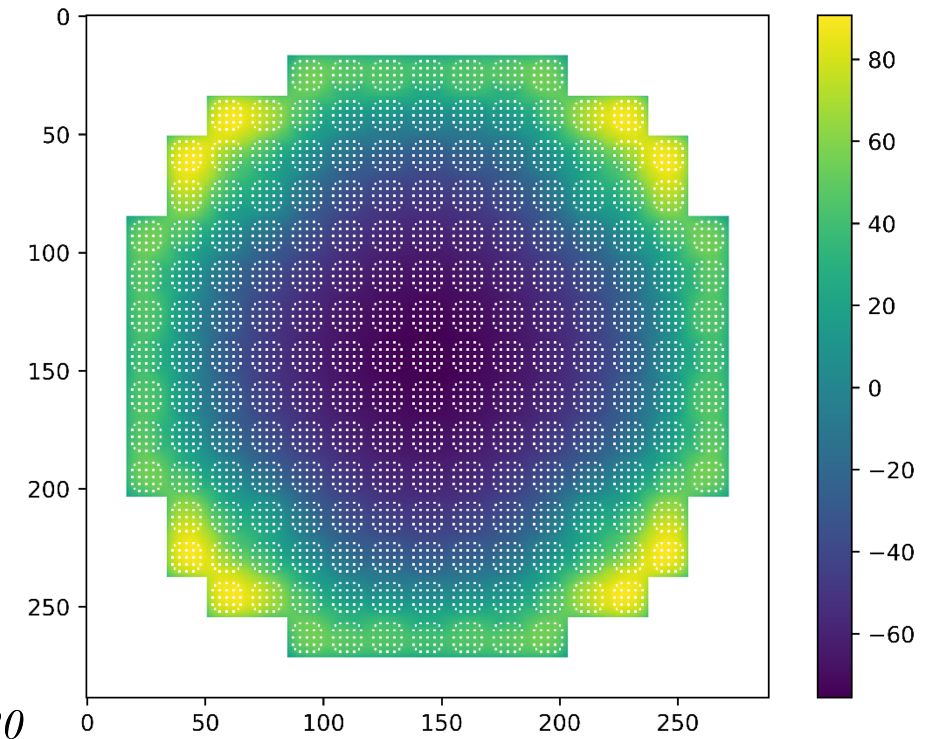
As we sweep through each segment we can compute the contribution of each angle to the scalar flux and never store the angular flux.

What if we also assume an isotropic source?

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



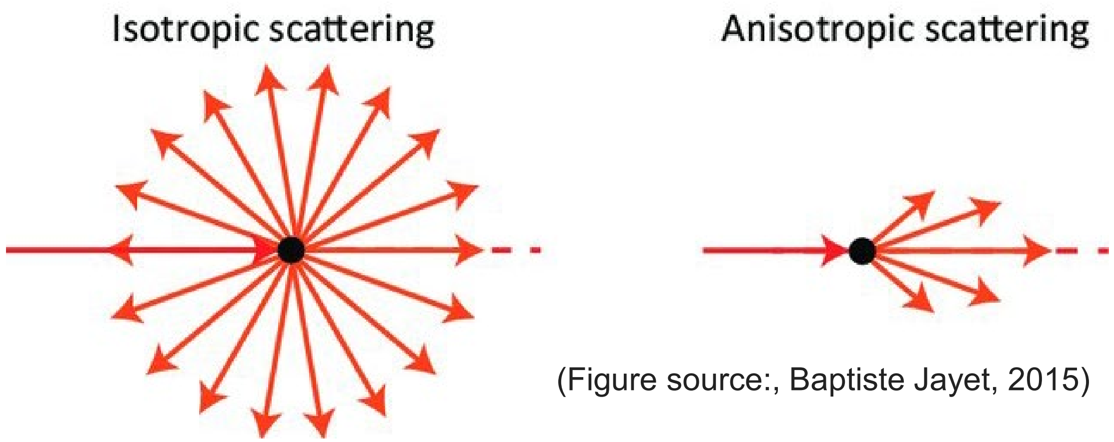
Liu, PhD thesis, 2020

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

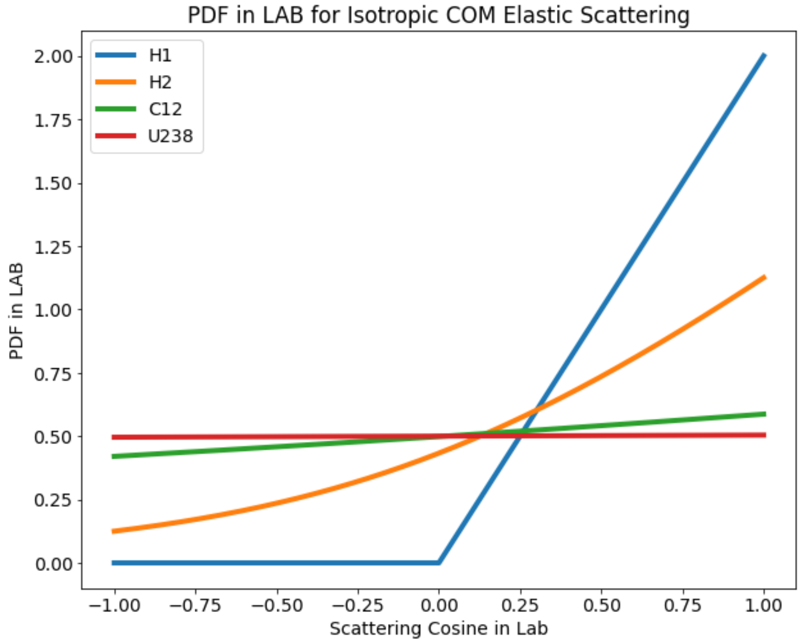
But in reality scattering is very anisotropic

Especially for H-1!

- For most nuclide in the energy range of nuclear reactors, elastic scattering can be assumed to be isotropic in the center-of-mass.
- This however translates to very anisotropic scattering in the laboratory reference frame
  - For H-1, neutrons always scatter forward in the laboratory system



(Figure source:, Baptiste Jayet, 2015)



High order scattering is needed

- Scattering source

$$Q_{g,scat}(\vec{r},\vec{\Omega}) = \sum_{g'=1}^{G}\sum_{l=0}^{L}\frac{2l+1}{4\pi}\Sigma_{s,l,g'\to g}(\vec{r})\sum_{j=-l}^{l}R_l^j(\vec{\Omega})\psi_{g',l}^{j}(\vec{r})$$

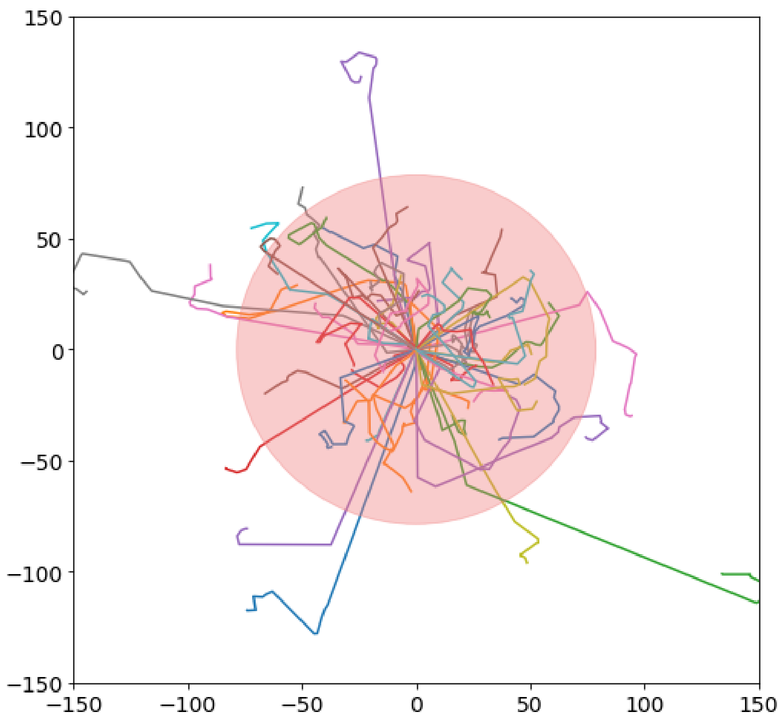
where the scattering cross-section is expanded using Legendre polynomials and the angular flux in spherical harmonics

$$\psi_{g',l}^{j}(\vec{r}) = \int_{4\pi} d^2\Omega' R_l^j(\vec{\Omega}')\psi_{g'}(\vec{r},\vec{\Omega}')$$

- 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)

But is it really needed for reactor applications?

- While each neutron path in H-1 may be anisotropic, the overall source will still look very isotropic in a nuclear reactor since neutrons are coming from everywhere
  - Initial neutron flights are very forward peaked, but then start looking isotropic after many collisions



Path of neutrons slowing down in H-1 from an isotropic fission source

We can thus approximate the scattering source as being isotropic, but we must preserve the distance travelled by these neutrons, a term we call migration.

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

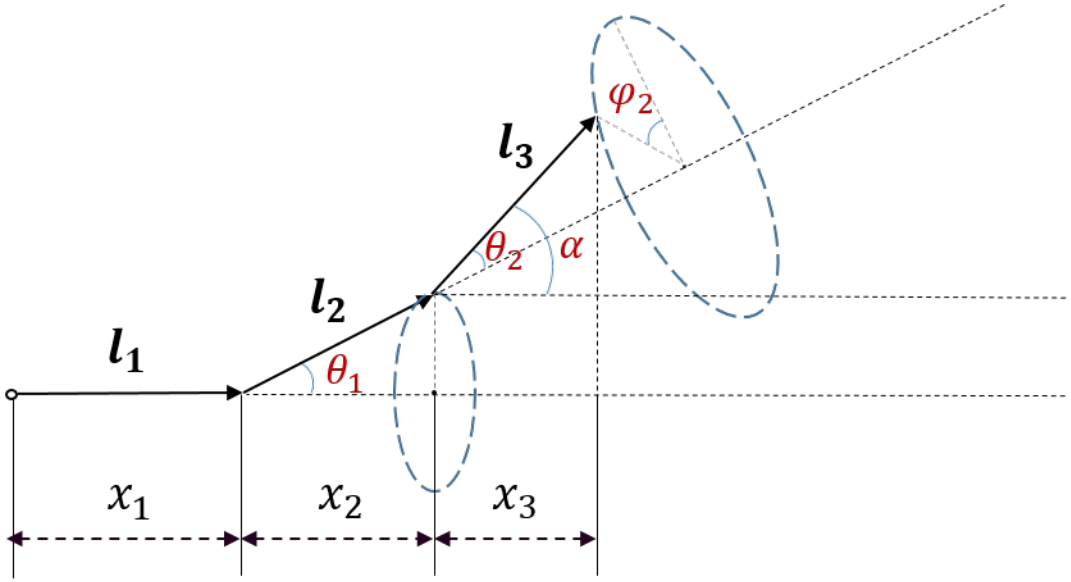
$$\vec{\Omega} \cdot \nabla\psi(\vec{r}, \vec{\Omega}, E) + \Sigma_{tr}(\vec{r}, E)\psi(\vec{r}, \vec{\Omega}, E) = \frac{Q^*(\vec{r}, E)}{4\pi}$$

- 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
  - λ_{tr} is the transport mean free path once the asymptotic is reached
  - The larger μ-bar, the more collisions needed to reach that asymptotic



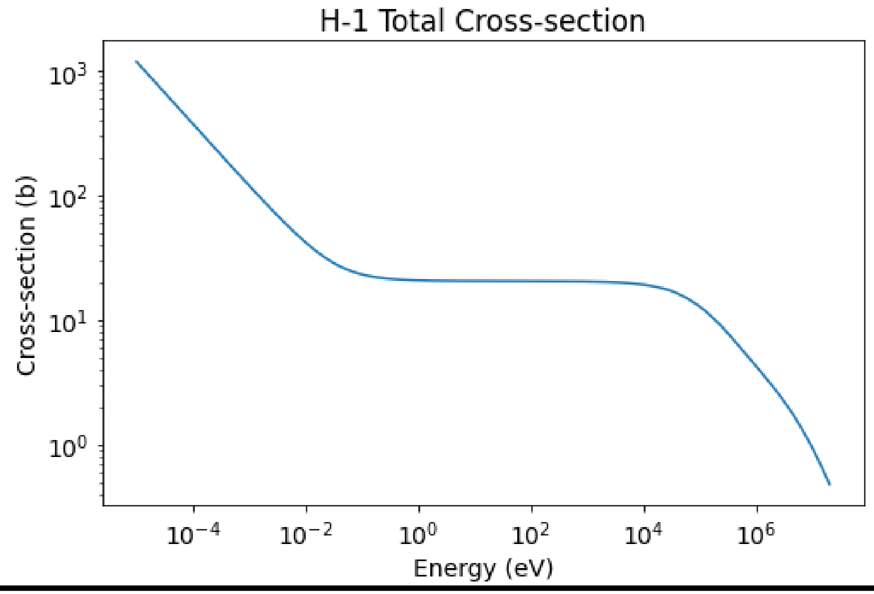
$$\lambda_{tr} = \lambda_t + \lambda_t\bar{\mu} + \lambda_t\bar{\mu}^2 + \cdots$$

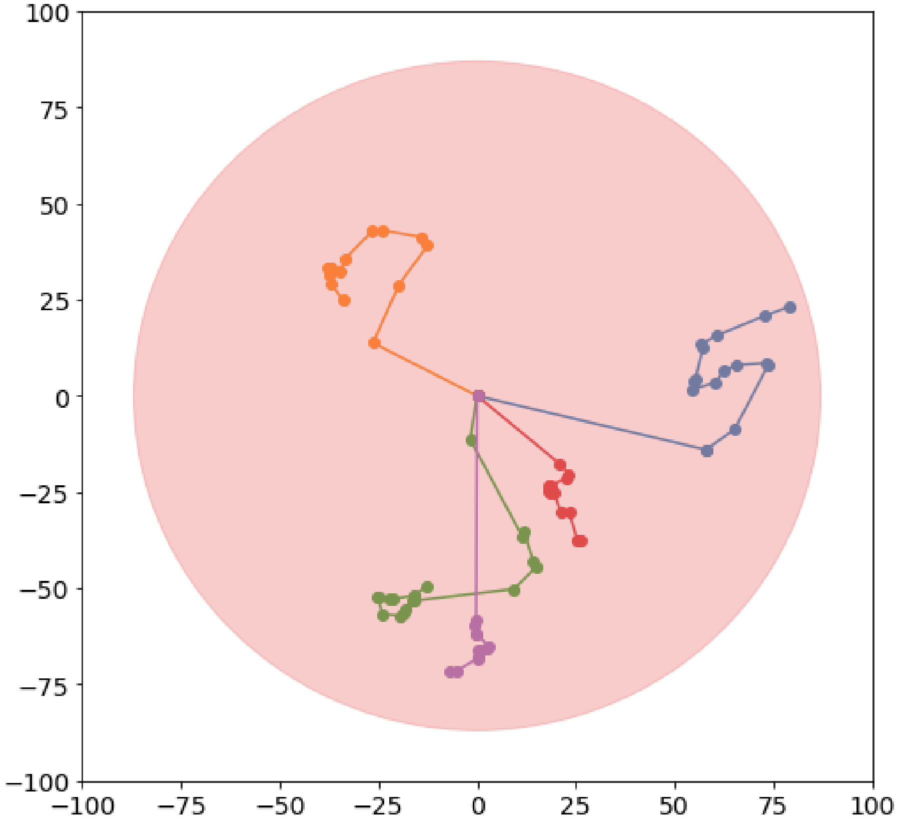
$$= \frac{\lambda_t}{1-\bar{\mu}}$$

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

But the energy dependence is strong!

- Fast neutrons tend to travel greater distances and are the main cause of the migration of neutrons
  - Cause in large part by the cross-section of H-1
- After many collisions, neutrons travel lesser distances and migrate less from their origin
  - They reach their asymptotic value





Path of neutrons slowing down in H-1 from an isotropic fission source

Borrowing from Diffusion Theory

- The concept of migration of neutron is at the heart of the diffusion coefficient used in diffusion theory. If we take the first moment of the transport equation after expansion

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

which is interpreted as Fick's law

$$J(\vec{r},E) = -D(\vec{r},E)\nabla\phi(\vec{r},E)$$

for which D is defined as

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

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

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

  - flux-limited approximation

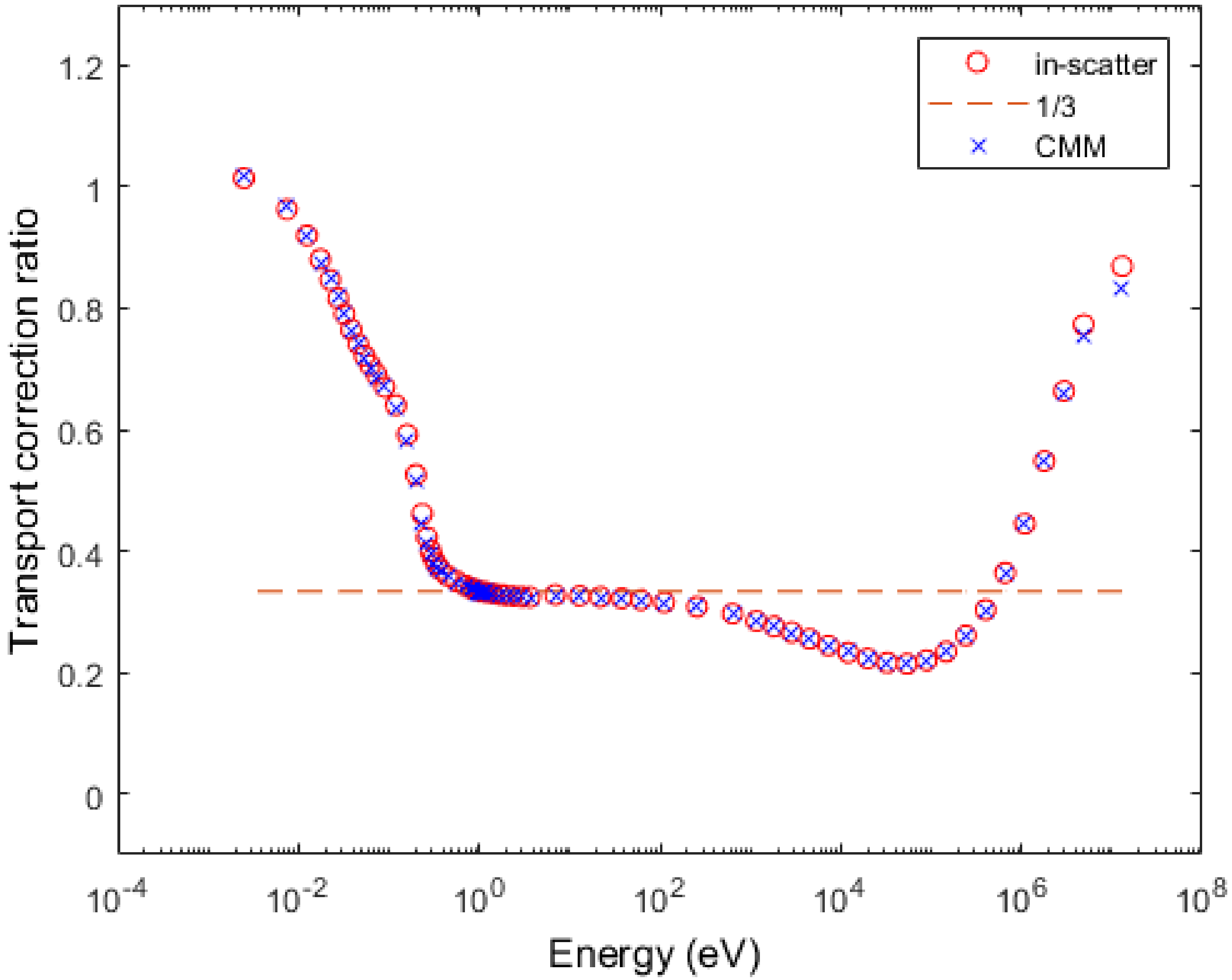
$$\Sigma_{tr,g}^{fl} = \Sigma_{t,g} - \sum_{g'=1}^{G} \frac{\Sigma_{s1,g' \rightarrow g} \phi_{g'}}{\phi_g}$$

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

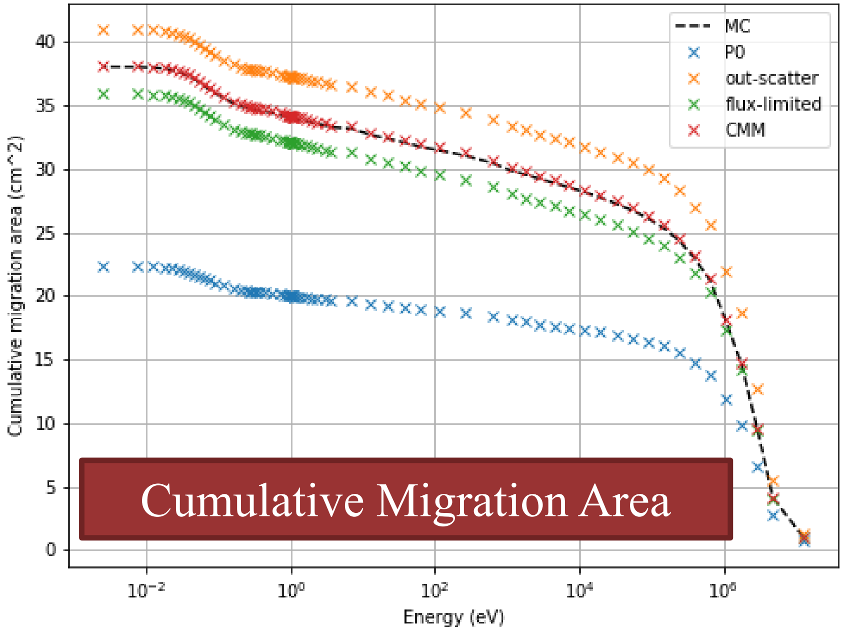
- Many collisions are needed to reach the asymptotic value
  - In H-1 this comes with a large change in energy
  - Poor energy resolution can lead to large errors in the fast leakage

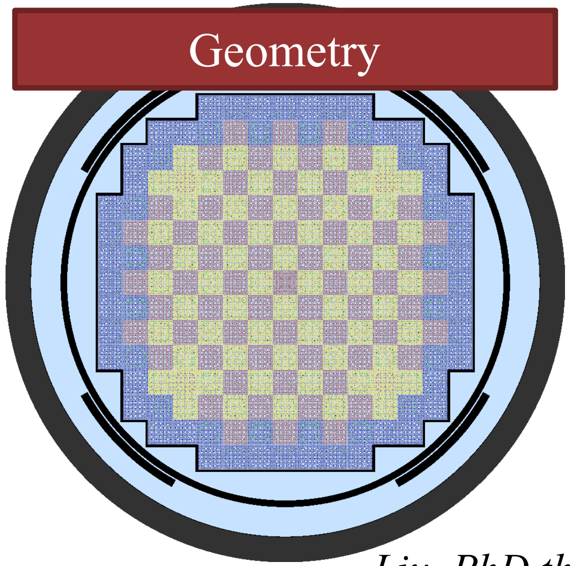
H-1 Transport correction ratio

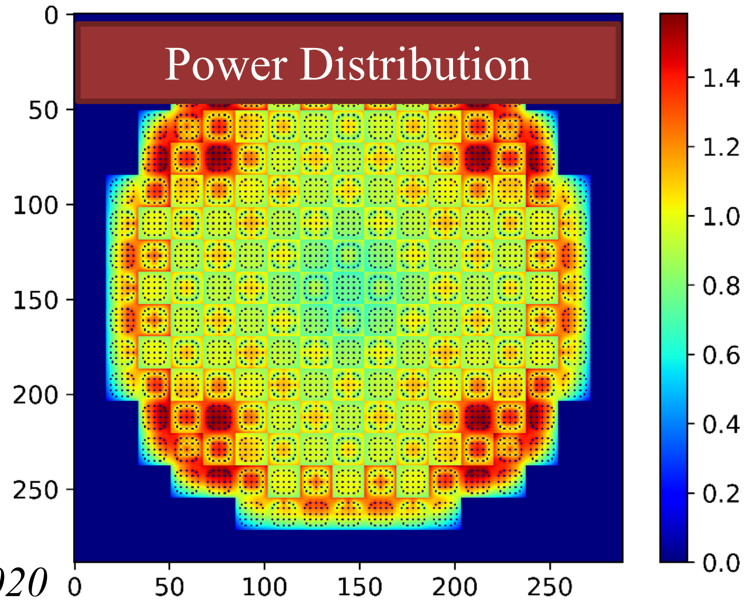


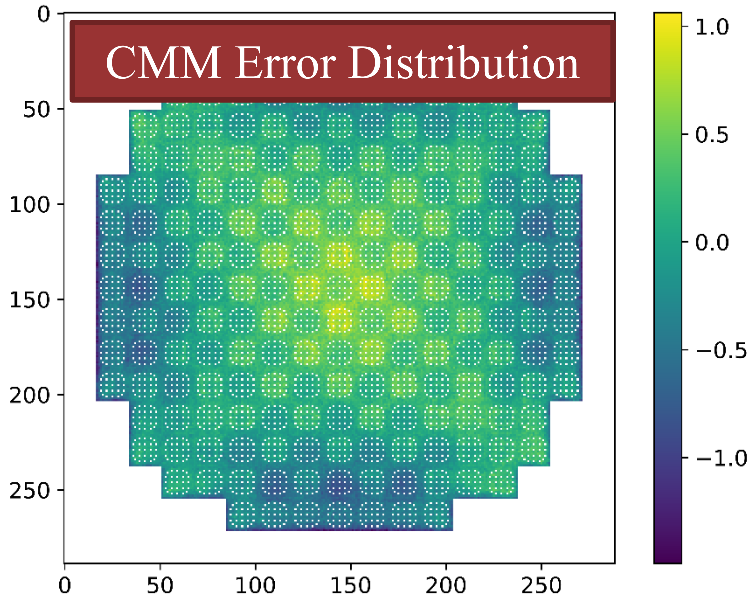
Transport cross-section

	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%







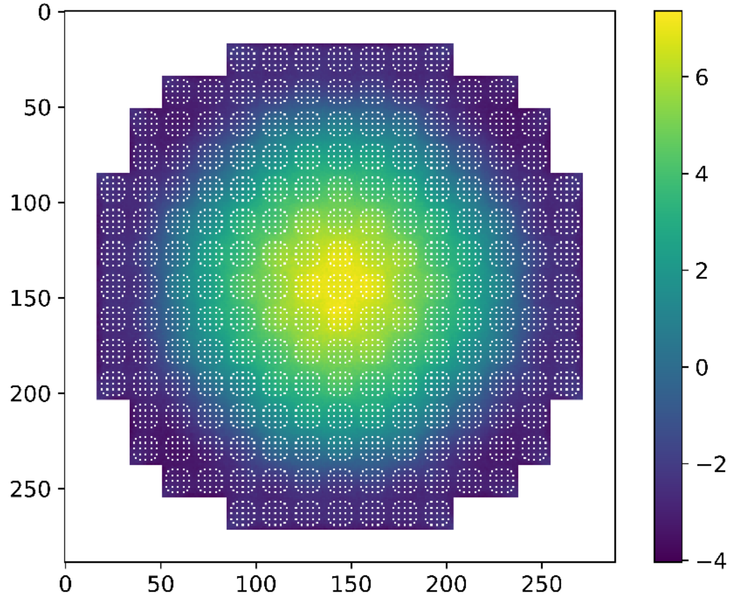


Liu, PhD thesis, 2020

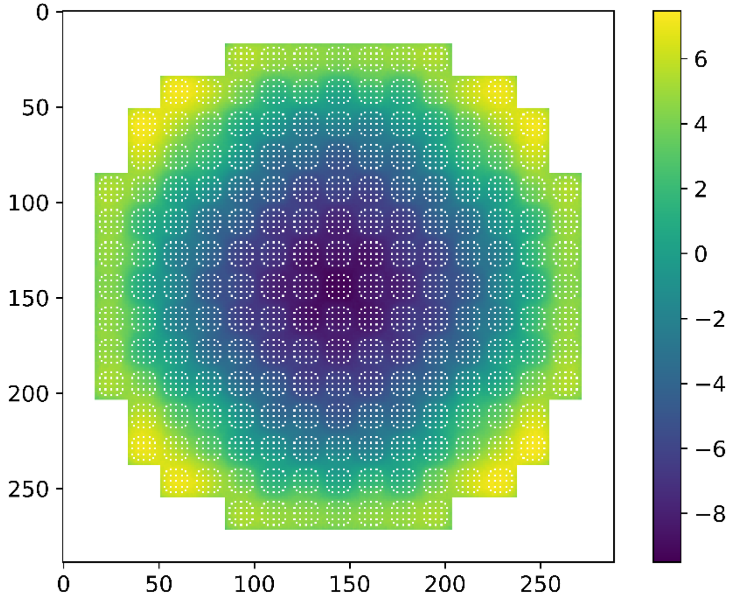
Migration area is key!

Liu, PhD thesis, 2020

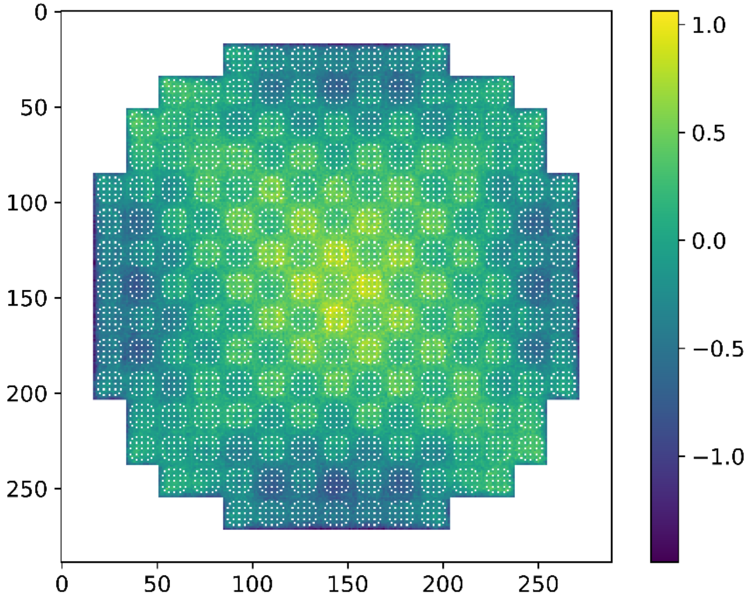
Out-scatter Error Distribution



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**

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.

$$\Sigma_{tr,g} = \frac{\int\int\int \Sigma_{tr}(E)\psi(\vec{r},\vec{\Omega},E)dEdVd\Omega}{\int\int\int \psi(\vec{r},\vec{\Omega},E)dEdVd\Omega} = \frac{\int\int\int s\Sigma_{tr}(E)\psi(\Omega,E)e^{-\Sigma_{tr}s}dEdsd\Omega}{\int\int\int s\psi(\Omega,E)e^{-\Sigma_{tr}s}dEdsd\Omega}$$

$$\Sigma_{tr,g} = \frac{\int\int s\Sigma_{tr}(E)\phi(E)e^{-\Sigma_{tr}s}dEds}{\int\int s\phi(E)e^{-\Sigma_{tr}s}dEds}$$

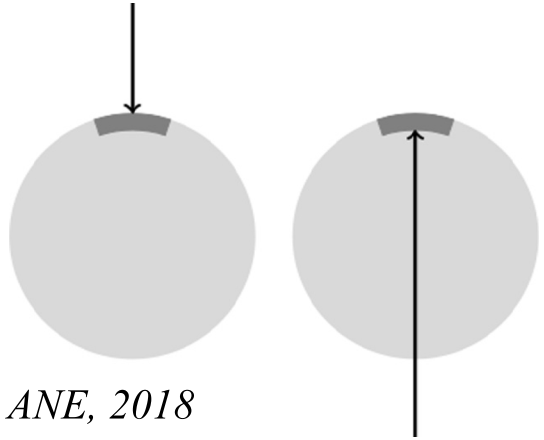
if we note that

$$\int s\Sigma_{tr}e^{-\Sigma_{tr}s}ds = \frac{1}{\Sigma_{tr}} = \lambda_{tr} \qquad \int se^{-\Sigma_{tr}s}ds = \frac{1}{\Sigma_{tr}^2}$$

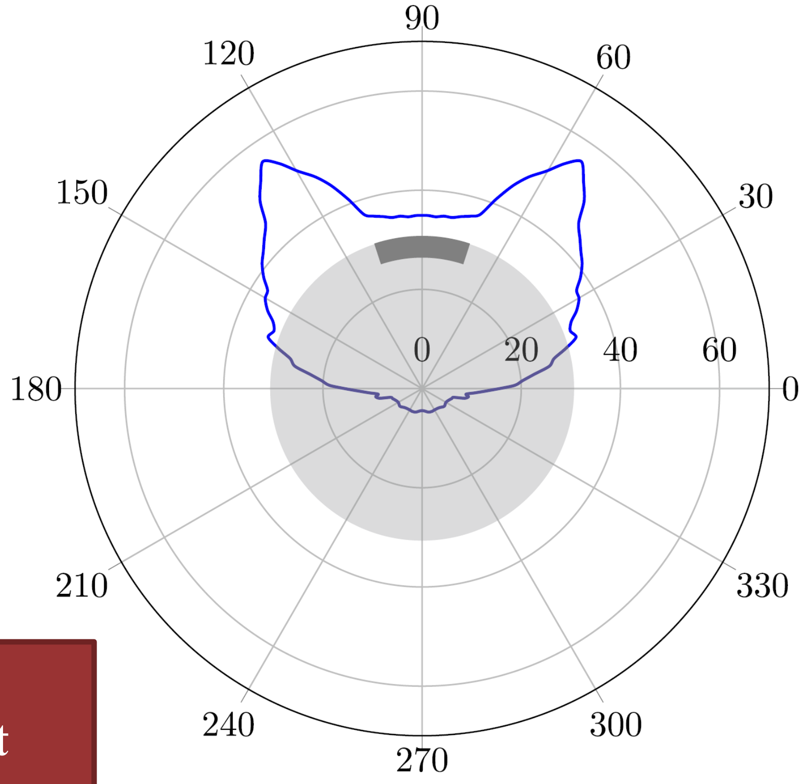
$$\frac{1}{\Sigma_{tr,g}} = \frac{\int_{E_g}^{E_{g-1}} \lambda_{tr}(E)\phi(E)dE}{\phi_g}$$

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

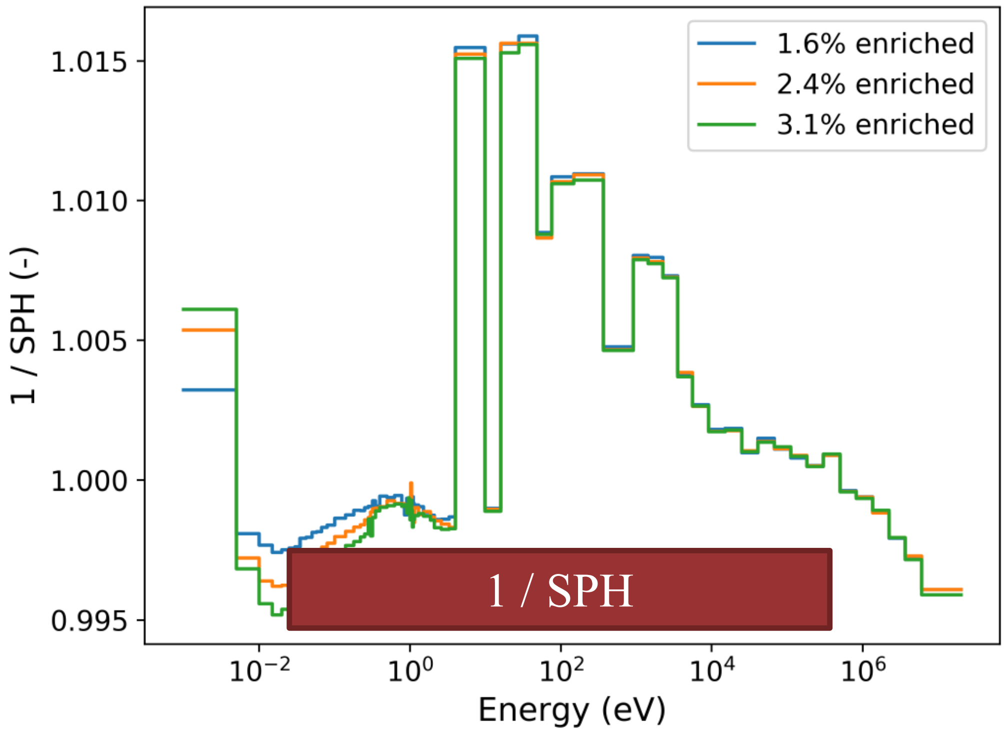
Approximation 2 will always lead to a minus 200-300 pcm error in coarse group structures (for LWRs), regardless of the scattering order or transport cross-section. Adding more groups >5000's will eventually eliminate this error.

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
      - $\Sigma^* = \Sigma \times f$
      - 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
  - It can also hide poorly converged solutions and should be handle with care

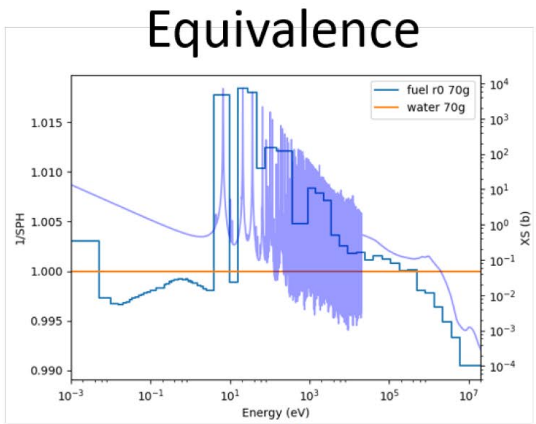
Full core performance of 3D OpenMOC vs OpenMC

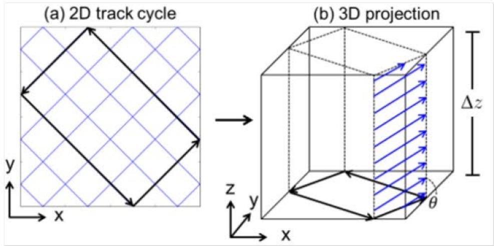
	Machine	CPU-hours	Method
Gunow – PhD – 2017	Mira[4]	800,000[1]	3D MOC extruded geometry
Tramm – PhD – 2018	Theta[4]	220,000[2]	3D MOC Random Ray
Gaston – PhD – 2019	Lemhi[4]	200,000[3]	3D MOC Unstructured mesh
Giudicelli – PhD - 2020	Lemhi[4]	6,000	3D MOC extruded geometry

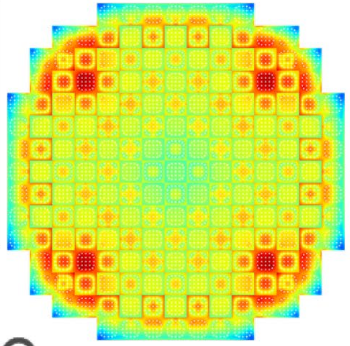
1: Estimated at 200,000 CPU hrs on Lemhi
2: Simplified geometry
3: Estimated
4: Theta is a Xeon Phi system, Lemhi is a Xeon Skylake system, Mira is POWERPC8 system

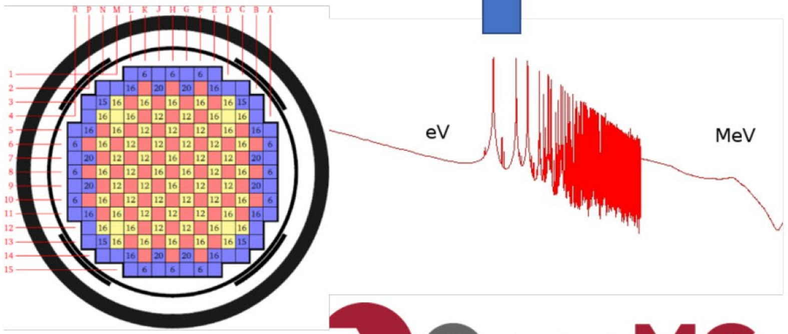
- Monte Carlo (OpenMC) Full core PWR with pin powers
  - 1% statistical accuracy in each pellet
  - ~100,000 CPU-hours on Lemhi-like system
  - Very difficult for transients due to time scales
    - Prompt neutrons of ~10^{-5} s and delayed neutrons ~1 s

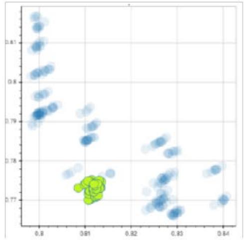
Opportunities – Can we learn multigroup cross sections?

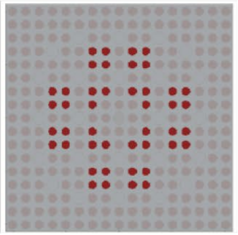








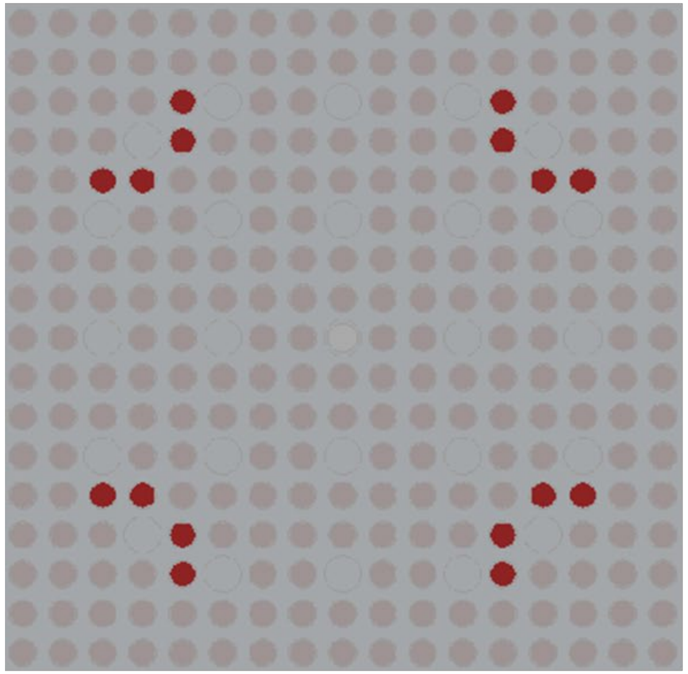




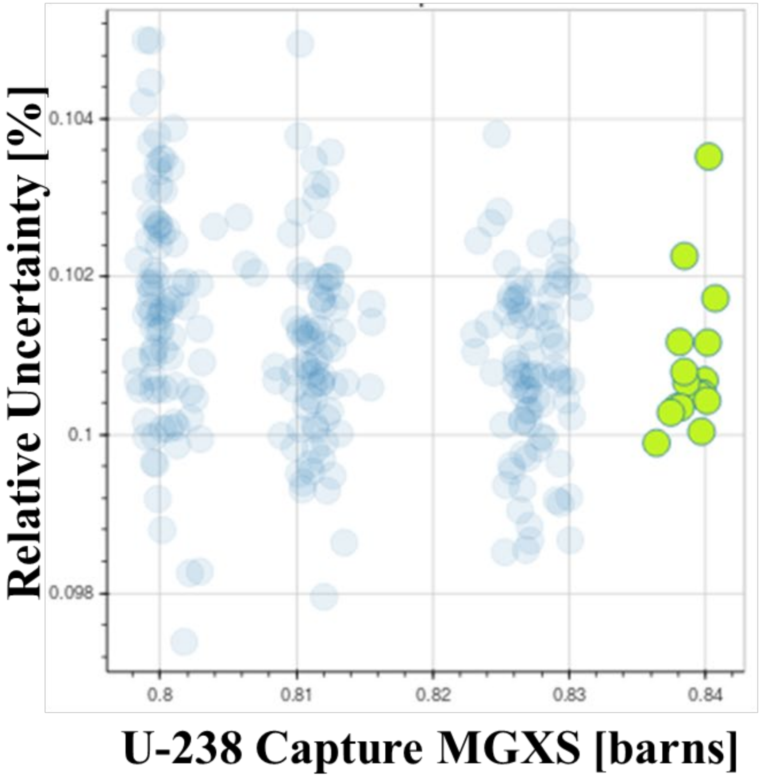
Boyd, PhD-thesis 2017 and Giudicelli, PhD-thesis 2020

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

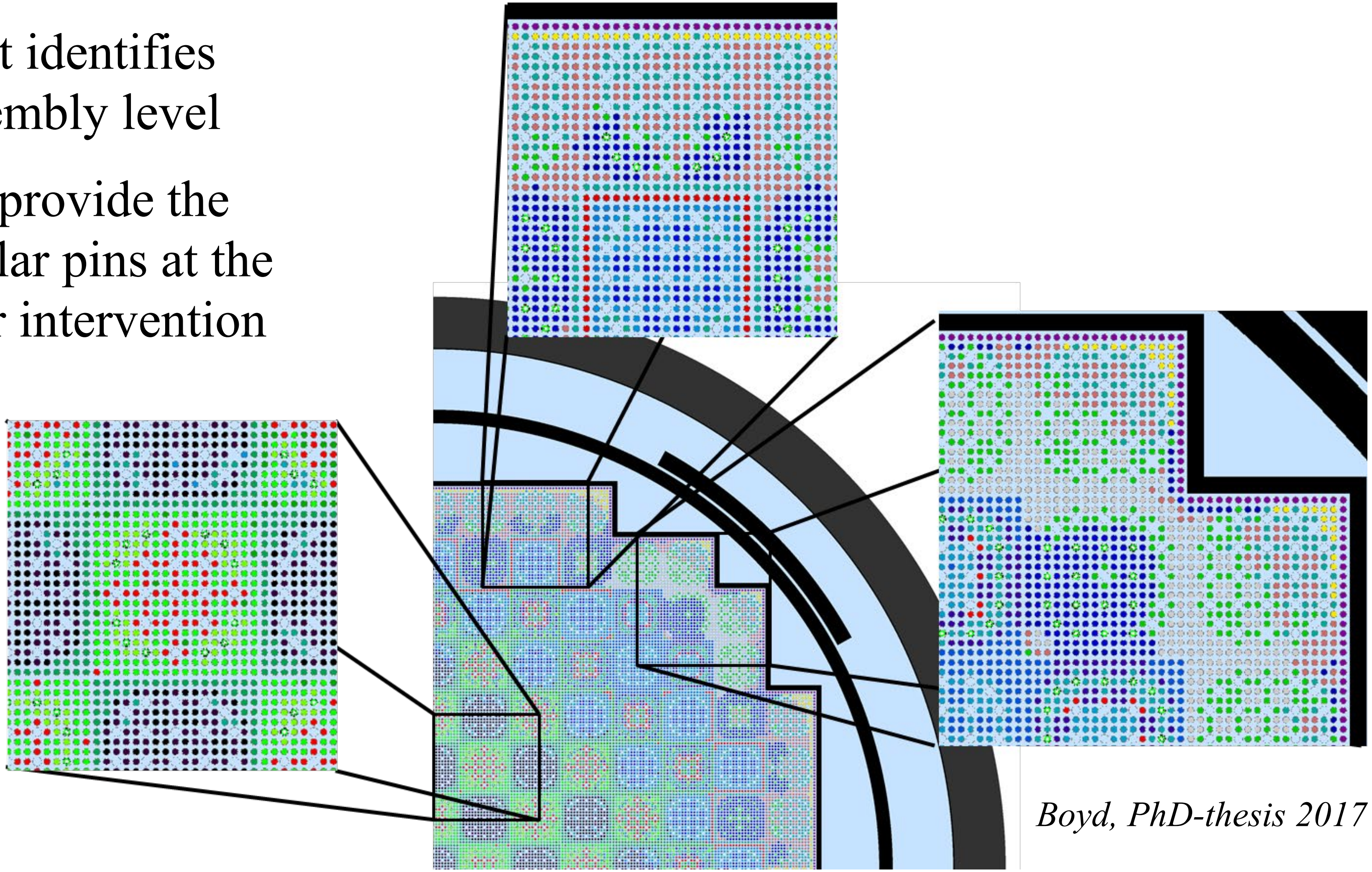


Boyd, PhD-thesis 2017



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.

Acknowledgements

CASL

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Questions?