Functional Expansion Tally Capability in the MCS Code

Muhammad Imron, Bamidele Ebiwonjumi and Deokjung Lee

CONTACT

Ulsan National Institute of Science and Technology
Address 50 UNIST-gil, Ulju-gun, Ulsan, 44919, Korea
Tel. +82 52 217 0114 **Web.** www.unist.ac.kr

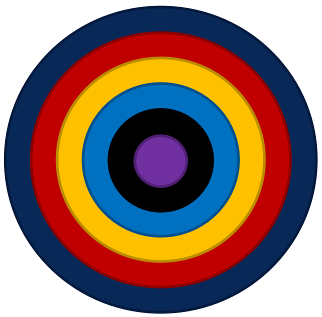
CORE Computational Reactor physics & Experiment lab
Tel. +82 52 217 2940 **Web.** reactorcore.unist.ac.kr

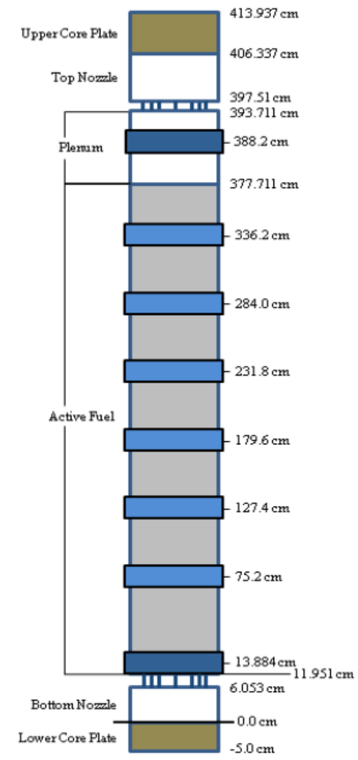
Overview

Introduction

1. Introduction

- **The continuous-energy Monte Carlo (MC) is often considered as the most accurate method to solve particle transport problems.**
- **Despite this advantage, MC solutions suffer from statistical uncertainties due to the nature of the MC method. Especially when the fine-mesh tallies are required: true high-fidelity whole core multi-physics simulations.**
- **This problem could be overcome by increasing number of histories.**
- **However, this straightforward approach would require expensive resources, that makes MC codes less efficient. In this context, the Functional Expansional Tally (FET) can play its role**
- **In this work, the multi-dimensional FET for a cylindrical geometry is implemented into the MCS code [1]**





[1] H. Lee et al., "MCS – A Monte Carlo particle transport code for large-scale power reactor analysis," Ann. Nucl. Energy, vol. 139, p. 107276, May 2020.

Theory

2.1. Functional Expansion Tally (FET)

- **FET [2,3] solutions are obtained by expanding the tally quantity as a linear combination of polynomials $\psi(\vec{\xi})$**

$$f(\vec{\xi}) = \sum_{n=0}^{\infty} \bar{a}_n k_n \psi_n(\vec{\xi})$$

$$\bar{a}_n = \langle f, \psi_n \rangle = \int_{\Gamma} f(\vec{\xi}) \psi_n(\vec{\xi}) \rho(\vec{\xi}) d\vec{\xi}$$

- **where $\overline{a_n}$ is the expansion coefficients, $\vec{\xi}$ is the neutron phase space consisting of $(\vec{r}, \overrightarrow{\Omega}, E)$.**
- **The k_n is the normalization constant which can be calculated according to the choice of the polynomials basis set that is being used**

$$k_n = \frac{1}{\|\psi_n\|^2}$$

$$\|\psi_n\|^2 = \int_{\Gamma} \psi_n^2(\vec{\xi}) \rho(\vec{\xi}) d\,\vec{\xi}$$

- **The $\rho(\vec{\xi})$ is the weighting function that shall be both complete and orthogonal with respect to $\psi_n(\vec{\xi})$.**

2.1. Functional Expansion Tally (FET)

- **Fortunately, in MC simulations, the calculations of the expansion coefficients are easily done with collision-based estimator. The unbiased collision-based estimator for coefficients $\overline{a_n}$ of reaction x is defined by [3, 4]**

$$\bar{a}_n = \frac{1}{N}\sum_{i=1}^{N}\sum_{k=1}^{K_i} w_{i,k}\frac{\Sigma_x(\vec{\xi}_{i,k})}{\Sigma_t(\vec{\xi}_{i,k})}\psi_n(\vec{\xi}_{i,k})\rho(\vec{\xi}_{i,k})$$

- **where N is the total number of particles in each batch, K_i is the total number of collisions of particle i, and w_{ik} is the particle i weight at collision k.**
- **In the MCS code, the Legendre polynomials are used for the axial direction and the Zernike polynomials are used for the radial direction in a cylindrical geometry.**

2.2. FET Implementation

- **The multi-dimensional FET implementation in MCS assumes that solutions are separable. For example, in the cylindrical geometry, the solution is assumed separable as follow**

$$f(r, \theta, z) = g(r, \theta)h(z)$$

- **This separability is favored to save computational memory.**
- **A very efficient recursive method [5] to construct the radial parts of the Zernike polynomials is adopted in the MCS**

$$R_m^n(r) = r\left[R_{n-1}^{|m-1|}(r) + R_{n-1}^{m+1}(r)\right] - R_{n-2}^{m}(r)$$

- **where the first few order polynomials can be manually determined.**
- **To our knowledge, this method is applied into FET for the first time.**

[5] B. H. Shakibaei and R. Paramesran, "Recursive Formula to Compute Zernike Radial Polynomials," Opt. Lett. Vol. 38, Issue 14, pp. 2487-2489, Jul. 2013.

2.2. FET Implementation

- **Once the radial parts are calculated, the Zernike polynomials can be calculated in a usual fashion.**

$$Z_n^m(r,\theta) = R_n^m(r)\,cos(m\theta) \text{ for } m > 0$$
$$Z_n^m(r,\theta) = R_n^m(r)\,sin(m\theta) \text{ for } m < 0$$
$$Z_n^m(r,\theta) = R_n^m(r) \text{ for } m = 0$$

- **One of the limitations of FET is due to the fact the polynomials only good when approximating a smooth distribution**
- **But they can become less effective if they are used to expand functions that contain discontinuities.**
- **This issue can be solved by employing a piecewise expansion.**
- **In a piecewise expansion, a single tally region with known discontinuities is divided into two or more smaller tallies that are expected to have continuous solutions.**

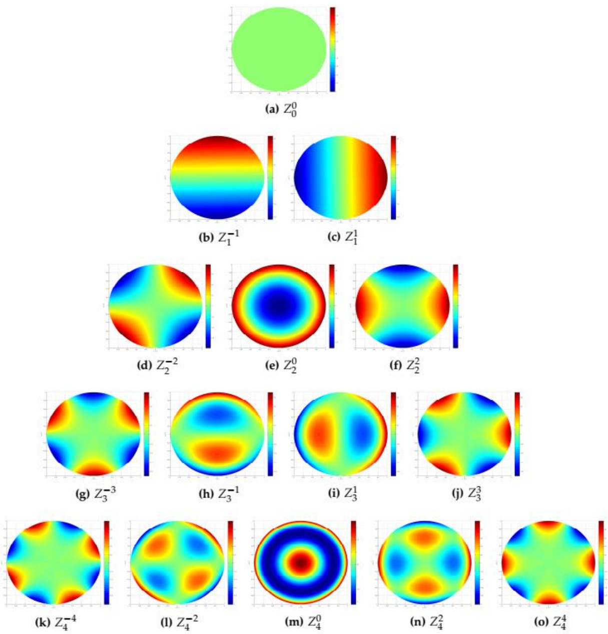
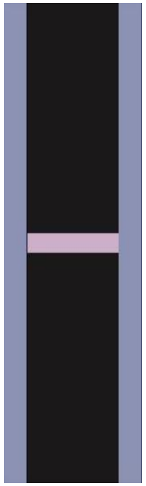


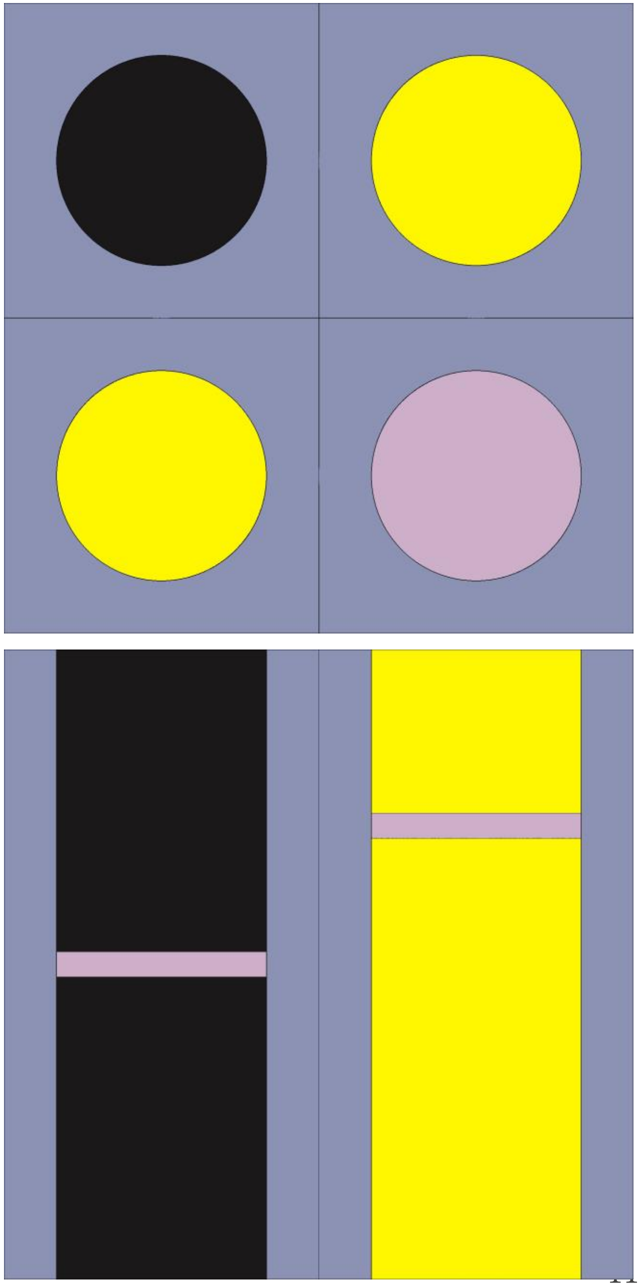
Figure from Ref [4]



Results

3.1. Problem Description

- To demonstrate FET capability in MCS, we developed a hypothetical 2x2 three-dimensional lattice problem
- Pin radius = 2 cm. Pitch = 3 cm.
  - Black: Fuel 3.1% wt
  - Yellow: Fuel 2.1% wt
  - Pink: Boron
- Height spanned from -25 cm to 25 cm.
- Axially, 2 cm thick Boron is located at the axial center of the 3.1% wt fuel.
- And other 2 cm thick Boron is located at the 10 cm above axial center of the 2.1% wt fuel.
- Only tally for 3.1% wt fuel is calculated.



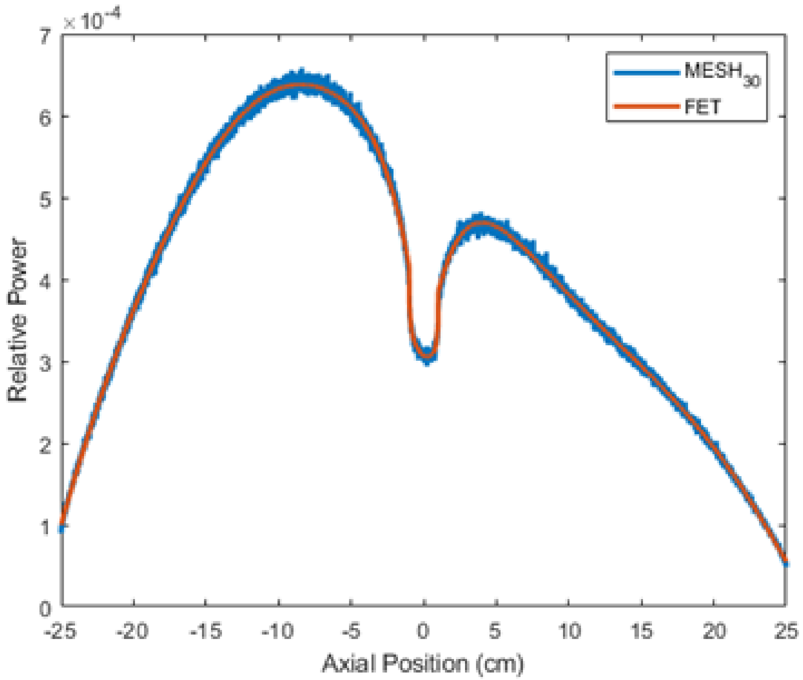
3.1. Problem Description

- **Cases**

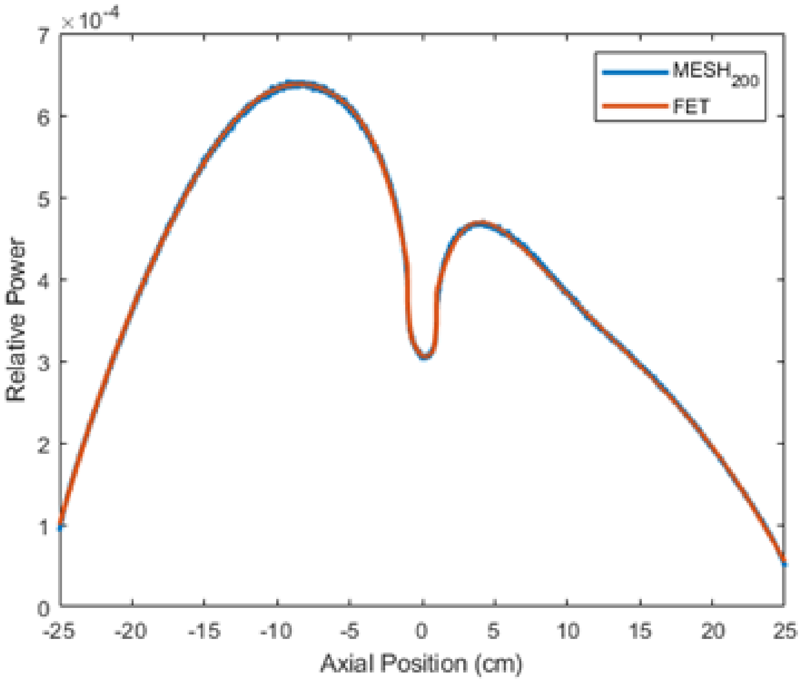
Cases	Tally Type	Number of Histories/batch
FET	FET	300,000
MESH_30	Normal Mesh Tally	300,000
MESH_200	Normal Mesh Tally	2,000,000

- **All cases use 25 inactive and 150 active batches**
- **For axial flux tally, the problem is divided into 10,000 mesh axially**
- **Mesh division for radial flux tally**
  - **Radial : 40**
  - **Azimuthal : 72**
  - **Axial : 50**
- **FET used 7th order of Legendre polynomials and 11th order of Zernike Polynomials (total 102 coefficients were stored – 32 for each material regions)**

3.2. Tally Results (Axial)



FET axial flux vs MESH_30
(Fuel 3.1% wt)



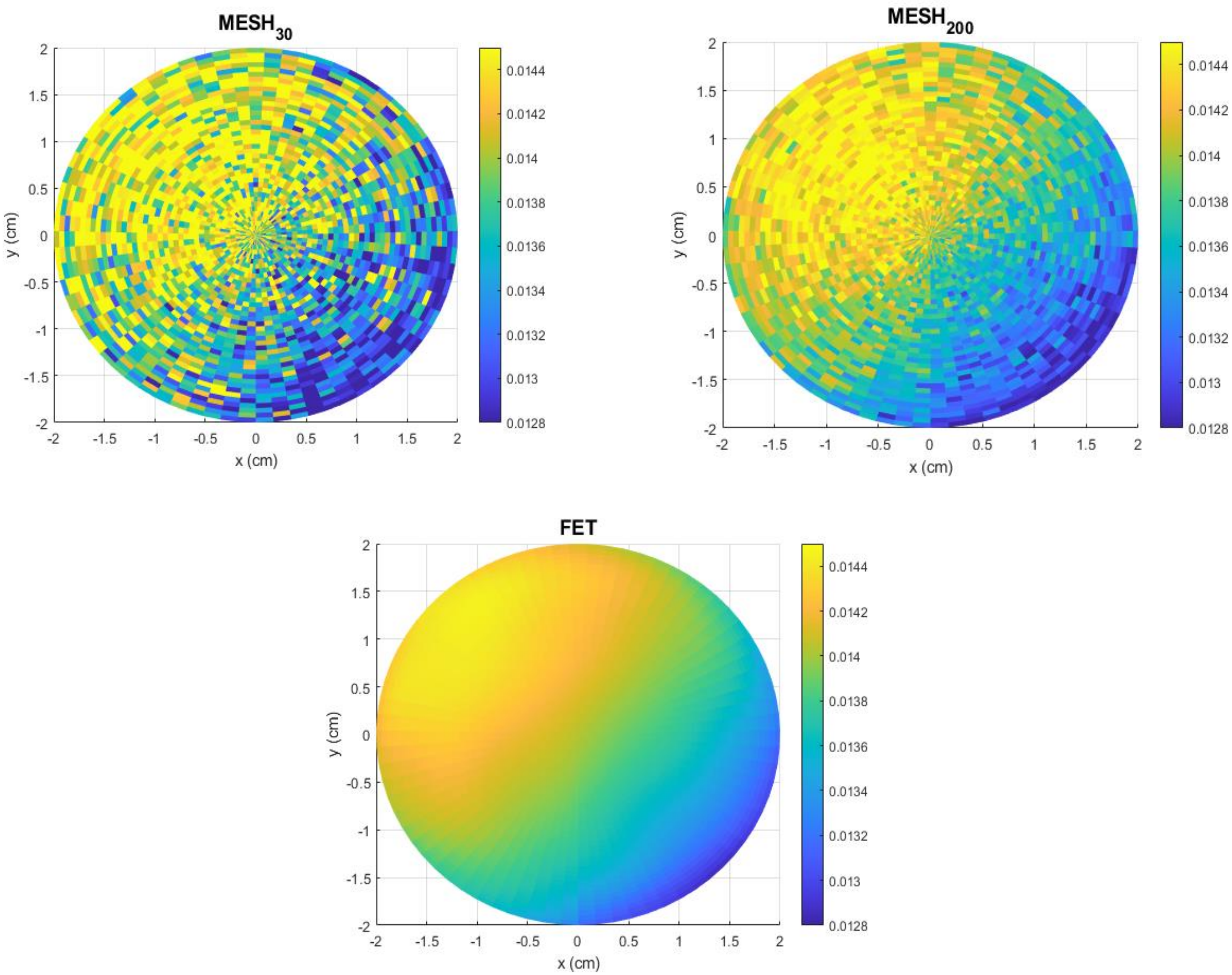
FET axial flux vs MESH_200
(Fuel 3.1% wt)

Relative Difference Against FET

Cases	Max Rel Diff	Min Rel Diff	RMS
MESH_30	13.70%	-10.43	1.56%
MESH_200	13.58%	-4.45	0.91%

UNIST CORE

3.2. Tally Results (Radial)



Radial flux Distribution at z = -10 cm
(Fuel 3.1% wt)

UNIST CORE

3.2. Tally Results (Radial)

Relative Difference Against FET for Radial
Flux at z= -10 cm

Cases	Max Rel Diff	Min Rel Diff	RMS
MESH_30	20.18%	-15.33	5.04%
MESH_200	7.49%	-7.45	2.13%

Running Time Relative to FET

Cases	Running Time Relative to FET
FET	1
MESH_30	0.96
MESH_200	8.34

For the same given number of histories, the running time of FET is slightly slower due to the calculation Legendre and Zernike polynomials for every collision -> **Compensated by smoother tallies!**

3.3. Standard Deviation

- **The FET standard deviation calculations require the calculations of the covariance matrix of the individual coefficients' standard deviation. This is because their standard deviations are correlated.**
- **However, the calculations of covariance matrix during MC simulations are computationally expensive; thus, this approach is counterproductive to the objective of the FET.**
- **Therefore, only for purpose of this test, we ran an identical problem 30 times in MCS using different random number seeds to calculate the real standard deviations of the tallied quantities.**
- **The same lattice problem will be used and the standard deviation for the axial power of the 3.1% enriched fuel pin will be calculated.**

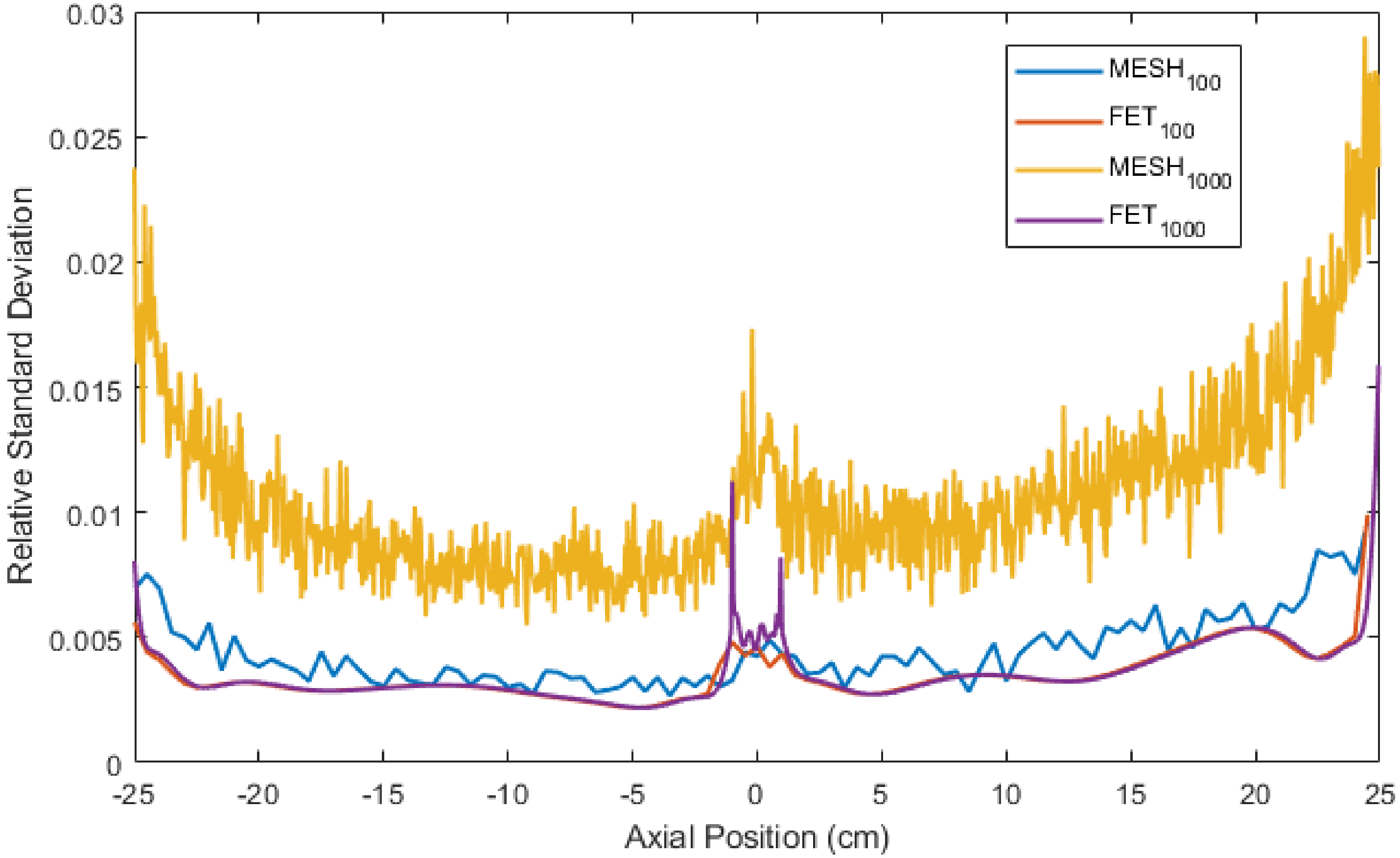
3.3. Standard Deviation

- **Cases**

Cases		Number of axial division
FET_100	FET	100
FET_1000	FET	1000
MESH_100	Normal Mesh Tally	100
MESH_1000	Traditional Mesh Tally	1000

- **All cases use 25 inactive and 150 active batches, and 50,000 histories per batch.**
- **The standard deviations were calculated from 30 simulations using different random number seeds.**

3.3. Standard Deviation



Axial flux standard deviations for each case

UNIST CORE

Conclusions

5. Conclusions

- FET is suitable for problems that require fine mesh tallies: whole core high fidelity multi-physics simulations
- FET uncertainties are insensitive to the mesh sizes.
- Conversely, the conventional mesh tally standard deviation highly depends on the mesh size.
- In that perspective, FET also can be seen as a variance reduction method.
- Now we will attempt to further implement FET for true high-fidelity multi-physics simulations.
- Challenges:
  - Cannot use surface-based tracking -> need to adopt continuously varying material tracking (CVMT).
  - Many material discontinuity in the axial direction: spacer grids -> need to store numerous expansion coefficients

UNIST CORE

References

[1] H. Lee et al., “MCS – A Monte Carlo particle transport code for large-scale power reactor analysis,” Ann. Nucl. Energy, vol. 139, p. 107276, May 2020.

[2] W. L. Chadsey, C. W. Wilson, V. W. Pine, W. L. Chadsey, C. W. Wilson, and V. W. Pine, “X-ray photoemission calculations,” IEEE Trans. Nucl. Sci., vol. 22, no. 6, pp. 2345–2350, Dec. 1975, doi: 10.1109/TNS.1975.4328131

[3] D. P. Griesheimer, “Functional Expansion Tallies for Monte Carlo Simulations,” PhD thesis, The University of Michigan, 2005.

[4] M. S. Ellis, “Methods for Including Multiphysics Feedback in Monte Carlo Reactor Physics Calculations,” PhD thesis, Massachusetts Institute of Technology, 2012.

[5] B. H. Shakibaei and R. Paramesran, “Recursive Formula to Compute Zernike Radial Polynomials,” Opt. Lett. Vol. 38, Issue 14, pp. 2487-2489, Jul. 2013.