Functional expansion tallies in Serpent

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Motivation

FETs ?

- FEs represent underlying data as a set of coefficients of a polynomial function
- FETs reconstruct a series approximation of discrete events to the true continuous distribution with respect to (an orthogonal) set of basis functions.

FETs in Serpent ?

- No (spatial) discretization. Monte Carlo intrinsic geometry modelling
- Storage and Memory. Data transferral and Performance
- Stochastic transformation to deterministic equivalence (functional-form)

Original implementation in Serpent 2.1.31 based on B. Wendt work [1-2]

[1] B. Wendt, L. Kerby, A. Tumulak, and J. Leppänen, "Advancement of functional expansion capabilities: Implementation and optimization in Serpent 2". Annals of Nuclear Energy 334 pp. 138-153, 2018.

[2] B. Wendt, "Generalized Data Representation and Transfer Solutions in Multiphysics Simulations through the Characterization and Advancement of Functional Expansion Implementations". PhD Thesis. Idaho State University, 2018.

FETs in Serpent 2.2.0

Funtional expansion (FE):

$F(x) \approx \sum_{m=0}^{M} a_m k_m \psi_m(x) \rho(x)$

where

$a_m = \int F(x) \psi_m(x) \rho(x) dx$

Surface cell-based Tallies (FETs)

for $n \leftarrow$ neutron particles **do**

$\hat{a}_m = \frac{1}{N} \sum_{n=1}^{N} \sum_{k=1}^{K} \omega_{n,k} \psi_m(x_{n,k})$

Collision cell-based Tallies (FETs)

for $n \leftarrow$ neutron particles **do**

$\hat{a}_m = \frac{1}{N} \sum_{n=1}^{N} \sum_{k=1}^{K} \frac{\omega_{n,k} \psi_m(x_{n,k})}{\Sigma_t(x_{n,k})}$

Legendre FE-basis (1D):

$\hat{F}_m(\tilde{x}) = \sum_{m=0}^{M} \hat{a}_m k'_m P_m(\tilde{x})$

$\rightarrow \tilde{x} \in [-1, 1]$ Legendre sub-space

where

$\tilde{x} = 2\frac{x - x_{min}}{x_{max} - x_{min}} - 1$

$k'_m = \frac{2m+1}{x_{max} - x_{min}}$

$P_m(\tilde{x}) = \sum_{i=0}^{m} \binom{m}{i} \binom{m}{1} i \left(\frac{\tilde{x}-1}{2}\right)^i$

Zernike FE-basis (2D):

$\hat{F}_n^m(\tilde{r}, \tilde{\phi}) = \sum_{n=0}^{N} \sum_{n=0}^{M} \hat{a}_n^m k'^m_n Z_n^m(\tilde{r}, \tilde{\phi})$

$\rightarrow \tilde{r} \in [0, 1], \quad \tilde{\phi} \in [0, 2\pi)$ Zernike sub-space

where

$\tilde{r} = \frac{\sqrt{(x-x_0)^2 + (y-y_0)^2}}{r} \qquad \tilde{\phi} = \phi$

for $n - m$ is even , $n \geqslant |m| \geqslant 0$ **do**

$$Z_n^m(\tilde{r}, \tilde{\phi}) = \begin{cases} R_n^m(\tilde{r}) \Phi_m(\tilde{\phi}) & m > 0 \\ R_n^0(\tilde{r}) & m = 0 \\ R_n^{|m|}(\tilde{r}) \Phi_m(\tilde{\phi}) & m < 0 \end{cases}$$

$$R_n^{|m|}(\tilde{r}) = \sum_{k=0}^{\frac{n-|m|}{2}} (-1)^k \binom{n-k}{k} \binom{n-2k}{\frac{n-|m|}{2}-k} r^{n-2k}$$

$$\Phi_{|m|}(\tilde{\phi}) = \begin{cases} \cos(|m|\tilde{\phi}) & m > 0 \\ 1 & m = 0 \\ \sin(|m|\tilde{\phi}) & m < 0 \end{cases}$$

$$k'_m = \begin{cases} \frac{n+1}{\pi} & m = 0 \\ \frac{2(n+1)}{\pi} & \text{otherwise} \end{cases}$$

Convolution (3D):

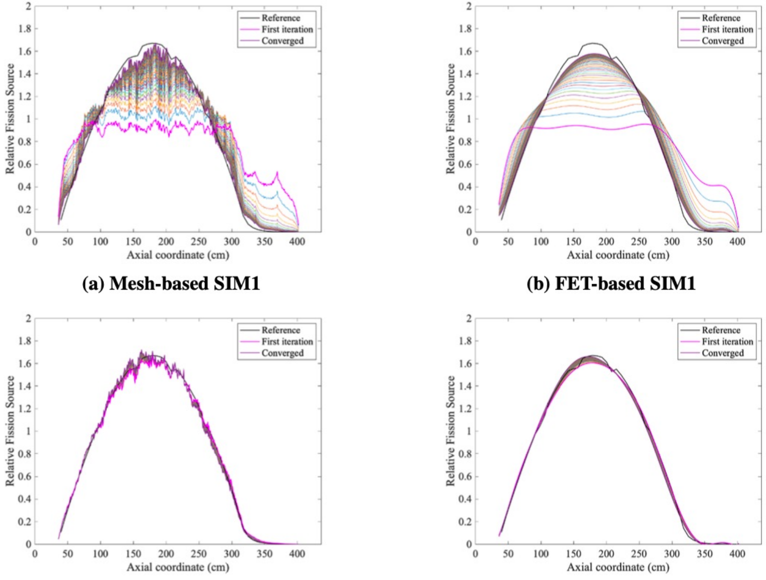
$\hat{F}_c(\Lambda) = \sum_{c=0}^{C} \hat{a}_c k'_c \psi_c(\Lambda) \quad \Lambda \in \mathbb{R}^3$

where

$\hat{F}(\tilde{x}, \tilde{y}, \tilde{z}) = \sum^{I,J,K} \hat{a}_{i,j,k} k'_{i,j,k} P_i(\tilde{x}) P_j(\tilde{y}) P_k(\tilde{z})$

$\hat{F}(\tilde{r}, \tilde{\phi}, \tilde{z}) = \sum^{N,M,I} \hat{a}_{n,i}^m k'^m_{n,i} Z_n^m(\tilde{r}, \tilde{\phi}) P_i(\tilde{z})$

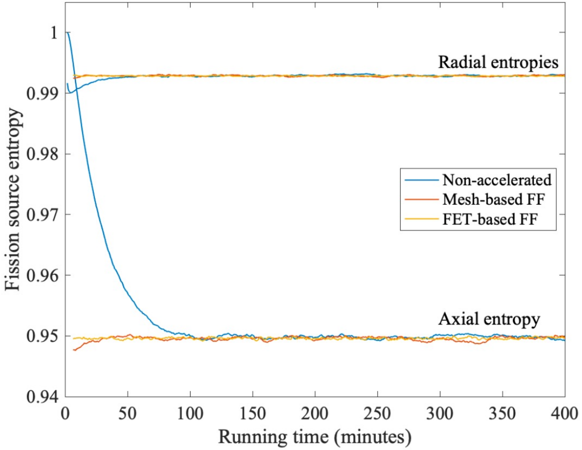
Previous work: modelling and applications



(a) Mesh-based SIM1 (b) FET-based SIM1 (c) Mesh-based SIM2 (d) FET-based SIM2

3D convolution of (collision) FETs for the reconstruction of the form factors, inward currents and sources, within the built-in response matrix solver to accelerate the convergence of the fission source when evaluating the forward solution to the *k*-eigenvalue criticality source [3]

1: **Iteration scheme:**
2: **for** $k \leftarrow$ outer iterations **do**
3: $\cdots$
4: **for** $n \leftarrow$ mesh cells **do**
5: **for** $c \leftarrow$ FE-th coefficients **do**
6: $$\hat{f}_i^c = \frac{\hat{R}_i^c}{J_i^{in}}$$
7: $$\hat{f}_s^c = \frac{\hat{R}_s^c}{S}$$



[3] A. Jambrina, J. Leppänen and H. Suikkanen ”Enhancing the Performance of Fission Source Convergence with Functional expansion tallies in Serpent 2 Monte Carlo Code”. The European Physical Journal Web of Conferences, 247(1):04001, 2021

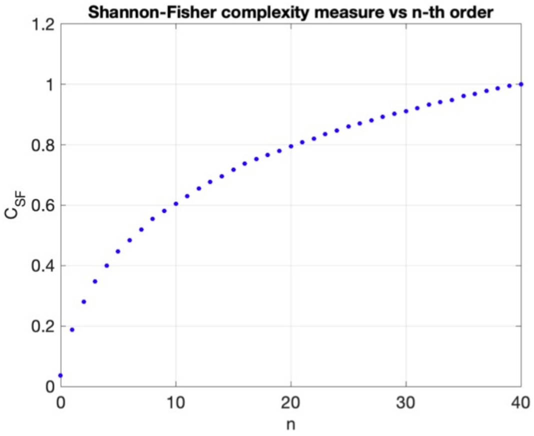
Previous work: modelling and applications

FET-based formulation of the Shannon-Fisher Complexity Metric for global and local stationary diagnosis of the fission source [4]

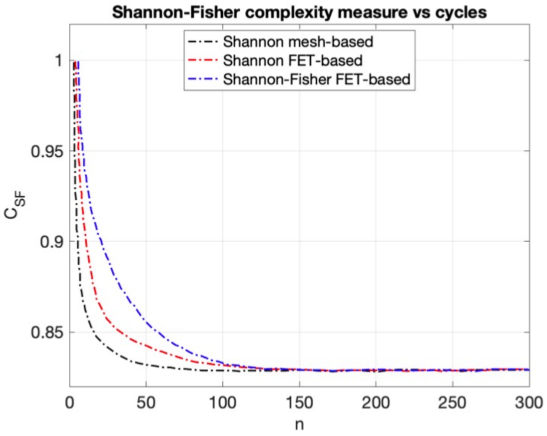
$$C_{SF} = F\left[\rho\left(x\right)\right] \times \frac{1}{2\pi e} e^{2S[\rho(x)]} = \frac{1}{2\pi e} F\left[\rho\left(x\right)\right]$$

$$F\left[\rho\left(x\right)\right] = \int_{\Gamma} \frac{\left(\frac{d}{dx}\rho\left(x\right)\right)^2}{\rho\left(x\right)} dx$$

$$S\left[\rho\left(x\right)\right] = -\int_{\Gamma} \rho\left(x\right) \log \rho\left(x\right) dx$$



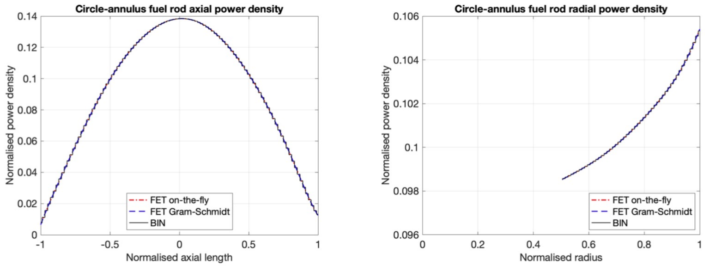
(a) Complexity vs n-th polynomial



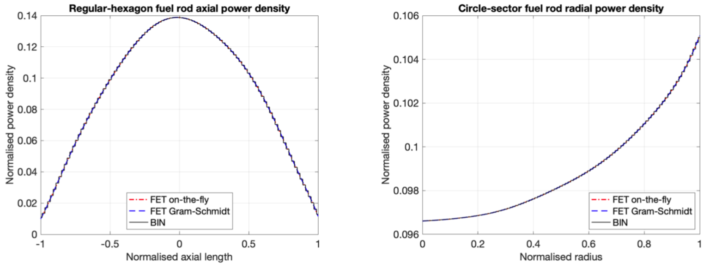
(b) Complexity vs cycles

[4] A. Jambrina and J. Leppänen, "Functional Expansion Tally-based Shannon-Fisher Complexity Metric for Fission Source Convergence Analysis in Serpent 2 Monte Carlo Code". In proceedings of M&C 2021 ANS-conference, Raleigh, NC, USA. Oct 3-7, 2021.

Previous work: modelling and applications



(a) Axial distributions **(b) Radial distributions**

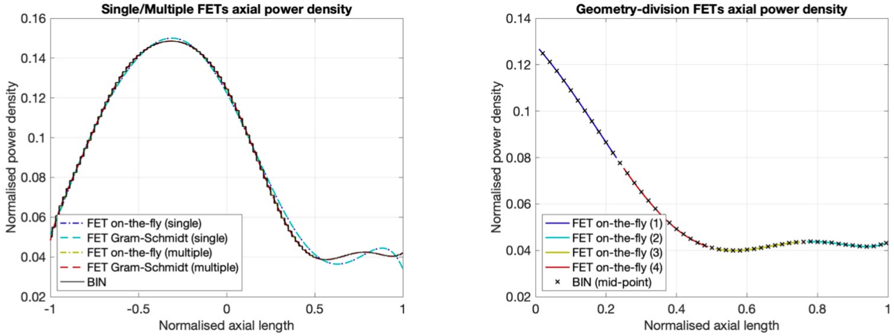


(a) Axial distributions **(b) Radial distributions**

Generalization of the 2D Zernike polynomials subspace onto circle partitions and deformations for FET application [5]

$$tr : D \to S \subset \mathbb{R}^2 \quad | \quad \vec{r} = (x, y) = tr\,(x', y') = (x\,(x', y')\,, y\,(x', y'))$$

$$\delta_{i,j} = \frac{1}{\pi} \iint_D Z_i\,(x', y')\, Z_j\,(x', y')\, dx'dy' = \frac{1}{\pi} \iint_S Z_i\left(tr^{-1}(x, y)\right) Z_j\left(tr^{-1}(x, y)\right) |J\,(x, y)|\, dxdy$$



(a) Continuous/Piece-Wise FETs **(b) Piece-Wise FETs**

[5] A. Jambrina and J. Leppänen, ”General Formulation of Functional Expansion Tallies for Regular 2D Geometries in Serpent 2 Monte Carlo Code”. In proceedings of M&C 2021 ANS-conference, Raleigh, NC, USA. Oct 3-7, 2021.

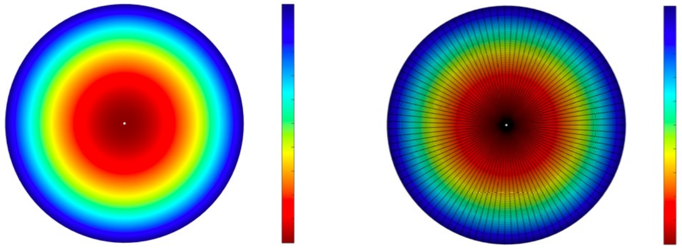
Previous work: modelling and applications

FET-based formulation for spherical geometries based on 3D Zernike polynomials [6]

$$Z_{nl}^{m}(r,\theta,\phi) = R_{nl}(r)\,Y_{l}^{m}(\theta,\phi)$$

$$Y_{l}^{m}(\theta,\phi) = N_{l}^{m} P_{l}^{m}(\cos\theta)\,e^{im\phi} \qquad N_{l}^{m} = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}$$

$$r\eta = r\left(\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\phi\right)^{T}.$$



(a) FET-based

(b) Mesh-based (reference)

$$Z_{nl}^{m}(\mathbf{x}) = \sum_{\nu=0}^{k} q_{kl}^{\nu} |\mathbf{x}|^{2\nu} e_{l}^{m}(\mathbf{x})$$

$$q_{kl}^{\nu} = \frac{(-1)^{k}}{2^{2k}}\sqrt{\frac{2l+4k+3}{3}}\binom{2k}{k}(-1)^{\nu}\frac{\binom{k}{\nu}\binom{2(k+l+\nu)+1}{2k}}{\binom{k+l+\nu}{k}}$$

$$e_{l}^{m}(\mathbf{x}) = r^{l}Y_{l}^{m}(\theta,\phi) = c_{l}^{m} r^{l}\left(\frac{ix-y}{2}\right)^{2} z^{l-m}\sum_{\mu=0}^{\lfloor\frac{l-m}{2}\rfloor}\binom{l}{\mu}\binom{l-\nu}{m+\mu}\left(-\frac{x^{2}+y^{2}}{4z^{2}}\right)^{\mu}$$

$$c_{l}^{m} = c_{l}^{-m} = \frac{\sqrt{(2l+1)(l+m)!(l-m)!}}{l!}$$

$$Z_{nl}^{m}(\mathbf{x}) = \sum_{r+s+t\leq n}\chi_{nlm}^{rst}x^{r}y^{s}z^{t}$$

$$\downarrow$$

$$\Omega_{nl}^{m} = \frac{3}{4\pi}\sum_{r+s+t\leq n}\overline{\chi_{nlm}^{rst}}M_{rst}$$

$$\chi_{nlm}^{rst} = c_{l}^{m}2^{-m}\sum_{\nu=0}^{k}q_{kl}^{\nu}\sum_{\alpha=0}^{\nu}\binom{\nu-\alpha}{\beta}\sum_{u=0}^{m}(-1)^{m-u}\binom{m}{u}i^{u}\sum_{\mu=0}^{\lfloor\frac{l-m}{2}\rfloor}(-1)^{\mu}2^{-2\mu}\binom{l}{\mu}\binom{l-\mu}{m+\mu}\sum_{\nu=0}^{\mu}\binom{\mu}{\nu}$$

$$M_{rst} = \int_{|\mathbf{x}|\leq 1} f(\mathbf{x})\,x^{r}y^{s}z^{t}\,d\mathbf{x}$$

[6] A. Jambrina and J. ”3D Spherical Functional Expansion Tallies in Serpent 2 Monte Carlo Code”. In proceedings of PHYSOR 2022 ANS-conference, Pittsburgh, PA, USA. May 15-20, 2022.

FETs framework

FETs implementation

- Modular scheme
- Common detector structure: discrete vs continuous representation

FETs basis library

- Pre-computed orthonormal coefficients
- Recursive formulation
- User-defined basis
- On-the-fly domain re-definition (geometry/function based approach)

FETs estimators

- Collision flux estimator (implicit/analog)
- Track-length estimator

Validation

Performance

FETs features

Detectors

Multi-physics interface

Built-in features

- Reconstruction form factors response-matrix solver (acceleration fission source convergence)
- Reconstruction eigenmodes fission matrix
- Stationary diagnosis (Shannon entropy/Shannon-Fisher complexity metric)
- Poison equilibrium axial/radial distribution
- […]

FETs features

	Space	Time	Direction
Detectors	$F(x,y,z)$	$F(t)$	$F(u,v,w)$

Multi-physics interface

$F(x,y,z,t)$ $F(x,y,z,u,v,w)$

$F(\ \ )$ = analytical function

Integrate + Differentiate

Built-in features

Monte Carlo ⟷ **MC angular flux** ⟷ **Deterministic**

Hi/Lo: group constants (diffusion coefficients, scattering matrixes)

Feedback
Questions
[...]

Thank you!

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