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FUNCTIONAL EXPANSION TALLY-BASED FEATURES IN SERPENT 2

Ana Jambrina

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LUT University

LAPPEENRANTA CAMPUS

- Lappeenranta - South-East Finland
- 230 Km from St. Petersburg and Helsinki
- Campus – Skinnarila district, by Lake Saimaa
- City of Lappeenranta nominated for the European Green Leaf Award 2021
- Carbon negative by 2024

- SMR safety analysis and design framework – national effort towards decarbonisation
- District heating - LUTHER

FEs & FETs

FEs represent underlying data as a set of coefficients to orthogonal functions

FE moment: $a_n = c_n \int_\Gamma \psi_n \rho_\psi F$

FET moment: $\hat{a}_n = c_n V \frac{\sum_{i=0}^{I} s_i w_i \rho_\psi(\zeta_i) \psi_n(\zeta_i)}{\sum_{i=0}^{I} w_i}$

Reconstruction: $F(\zeta) = \sum_{n=0}^{M} \hat{a}_n \rho_\psi(\zeta)\, \psi_n(\zeta)$

Error = approximation + truncation

Jacobi polynomials, $J_n^{\alpha,\beta}(\zeta)$ - Legendre, Zernike, etc.

MOTIVATION

Mesh-free / Non-discretization
(Monte Carlo alignment)

Storage / Memory
Transferral / Performance

Stochastic transformation to
deterministic equivalence (functionals)

OUTLINE

MODELLING

APPLICATIONS

Current status - Serpent 2.1.31

On-going

Coming-next

Future work

MODELLING

MODELLING

CURRENT STATUS SERPENT 2.1.31

Polynomial basis:

- Legendre polynomials: $P_n(x) = \sum_{i=0}^{n} \binom{n}{i} \binom{-n}{-1} i \left(\frac{1-x}{2}\right)^i$ $\quad c_n = \frac{2n+1}{2}$
- Zernike polynomials: $Z_n^m(r,\phi) = \begin{cases} R_n^m(r)\Phi_m(\phi) & m > 0 \\ R_n^0(r) & m = 0 \\ R_n^{|m|}(r)\Phi_m(\phi) & m < 0 \end{cases}$ $\quad c_n^m = \begin{cases} \frac{n+1}{\pi} & m = 0 \\ \frac{2(n+1)}{\pi} \end{cases}$

$$R_n^{|m|}(r) = \sum_{k=0}^{\frac{n-|m|}{2}} (-1)^k \binom{n-k}{k} \binom{n-2k}{\frac{n-|m|}{2}-k} r^{n-2k} \qquad \Phi_m(\phi) = \begin{cases} \cos m\phi & m > 0 \\ 1 & m = 0 \\ \sin|m|\phi & m < 0 \end{cases}$$

Convolution:

- Cartesian geometry: $\psi_c(x,y,z) = \psi_{i,j,k}(x,y,z) = P_i(x)P_j(y)P_k(z)$
- Cylindrical geometry (circle-XS): $\psi_c(r,\phi,z) = \psi_{n,i}^m(r,\phi,z) = Z_n^m(r,\phi)P_i(z)$

MODELLING

CURRENT STATUS SERPENT 2.1.31

Recursion formula:

- Legendre polynomials:

$$\left.\begin{aligned} P_0 &= 1. \\ P_1 &= x. \\ P_n &= \frac{(2n-1)xP_{n-1}(x)-(n-1)P_{n-2}(x)}{n} \end{aligned}\right\}$$

- Zernike polynomials:

$$\left.\begin{aligned} R_n^n(r) &= r^n \\ R_n^{n-2}(r) &= nR_n^n(r) - (n-1)R_{n-2}^{n-2}(r) \\ R_n^{|m|-4}(r) &= H_1 R_n^{|m|}(r) + \left(H_2 + \frac{H_3}{r^2}\right) R_n^{|m|-2}(r) \end{aligned}\right\} R_n^m(0) = \begin{cases} 0 & m \neq 0 \\ -1 & \frac{n}{2} \text{ odd} \\ 1 & \end{cases}.$$

defining

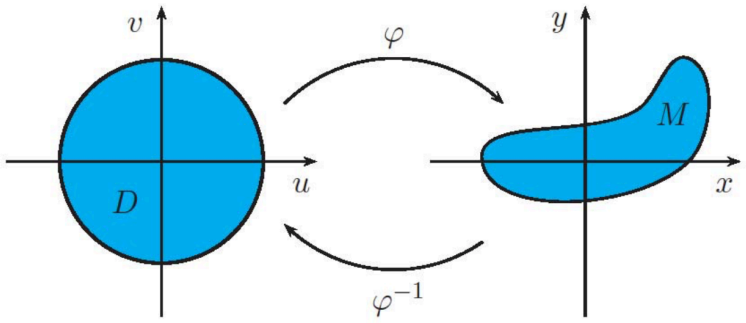
$$\left.\begin{aligned} H_3 &= \frac{-4(|m|-2)(|m|-3)}{(n+|m|-2)(n-|m|+4)} \\ H_2 &= \frac{H_3(n+|m|)(n-|m|+2)}{4(|m|-1)} + (|m|-2) \\ H_1 &= \frac{|m|(|m|-1)}{2} - |m|H_2 + \frac{H_3(n+|m|+2)(n-|m|)}{8} \end{aligned}\right\} \text{Chong's relationship.}$$

MODELLING

ON-GOING

Geometry generalisation (regular) 2D/1D:

- Zernike-based polynomials (derived from unit circle).
- Approaches:
  1. Gram-Schmidt orthogonalization process.
     - Pre-calculated polynomial term – non-recursive formula.
     - Geometrical/domain dependency.
     - Prone to numerical error – integral.
  2. Diffeomorphism/conformal mapping – variable transformation.
     - On-the-fly coefficient calculation – recursive formula.
     - General methodology for regular 2D/1D.
- Proof-of-concept:
  1. Angular/radial transformation.
  2. Continuous/piece-wise transformation.
     - Annulus, sector and hexagon.



MODELLING

COMING-NEXT

Geometry generalisation (regular) 3D.

- Spherical harmonics: $K_l^m(r,\phi,\varphi) = R_l^{|m|}(r) Y_l^m(\phi,\varphi)$ $\left.\begin{matrix} l-m \text{ even} \\ l \geq |m| \geq 0 \end{matrix}\right\}$

$$R_l^{|m|}(r) = N_l \sum_{n=0}^{\frac{l-|m|}{2}} (-1)^n \binom{l-n+\frac{1}{2}}{n} \binom{l-2n+\frac{1}{2}}{\frac{l-|m|}{2}-n} r^{l-2n} \qquad N_l = \sqrt{2l+3}$$

$$Y_l^m(\phi,\varphi) = \begin{cases} \sqrt{2} N_l^{|m|} P_l^m(\cos\phi)\cos m\varphi & m > 0 \\ N_l^{|m|} P_l^m(\cos\phi) & m = 0 \\ \sqrt{2} N_l^{|m|} P_l^{|m|}(\cos\phi)\sin|m|\varphi & m < 0 \end{cases} \qquad N_l^{|m|} = \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-|m|)!}{(l+|m|)!}}$$

- Spherical convolution: $\psi_c(r,\phi,\varphi) = \psi_{l,l'}^{m,m'}(r,\phi,\varphi) = R_l^{|m|}(r) Y_{l'}^{m'}(\phi,\varphi)$
- Spherical-harmonics-based: variable transformation (regular 3D geometry).

MODELLING

FUTURE WORK

STL geometry.

- Spherical harmonics generalisation + geometrical moments (voxel-like) – using existing *N-tree* search.

Modelling heterogeneities

- FE orthogonal: smooth functions - independent coefficients.
- Approaches:
  1. Adaptive mesh: refinement (sampling) or coarseness (coefficient variance).
  2. Filtering / regularisation: weighting coefficients – breaking orthogonality.

APPLICATIONS

APPLICATIONS

CURRENT STATUS SERPENT 2.1.31

Detectors (dfet)

- Collision (volume) tally.
- Single reaction / energy / time / mesh-bin (non-subdivisions).

Interface (ifc – type 3 → 31/32)

APPLICATIONS

ON-GOING

Fission source acceleration.

- Enhance initial guess: FETs + response matrix solver.
  1. FET-based coupling coefficients (response & source-to-response) reconstruction.
  2. Response matrix solver runs based on FETs moments variance.
  3. Stopping criteria tolerance-based.

Alternative metric to Shannon entropy.

- Super-imposed FETs (mesh-free).
- FETs coefficients and moments track over generations – variance analysis.
  1. Lo-/Hi- order (avoid noise).
  2. Polynomial basis dependent.
- Fission source reconstruction – high dominance ratio.

APPLICATIONS

COMING-NEXT

Detector options.

- Multiple reaction / energy / time.
- Surface & super-impose track length tally.

FET-based fission source convergency stopping criteria.

- Based on FETs coefficients establish a stopping criteria between inactive / active cycles.
- Possible coupled system with response matrix solver.

FET-based Xenon reconstruction.

- Scoring Xe-135 / I-135 reaction rates with FETs and solving Bateman equations.
- Expansion to other nuclides.

APPLICATIONS

FUTURE WORK

FET-based burnup calculations.

- FE nuclide densities.
- Solution coupled system.

FET-based time-dependent calculations.

- Temporal / temporal + spatial FE – alternative polynomial basis.

FET-based diffusion coefficients (group constant generation).

UNDER CONSTRUCTION

- Wiki page
- Tutorial case
- Post-processing script (serpentTools ?)

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THANKS FOR YOUR ATTENTION!

Ana.Jambrina@lut.fi

LUT University