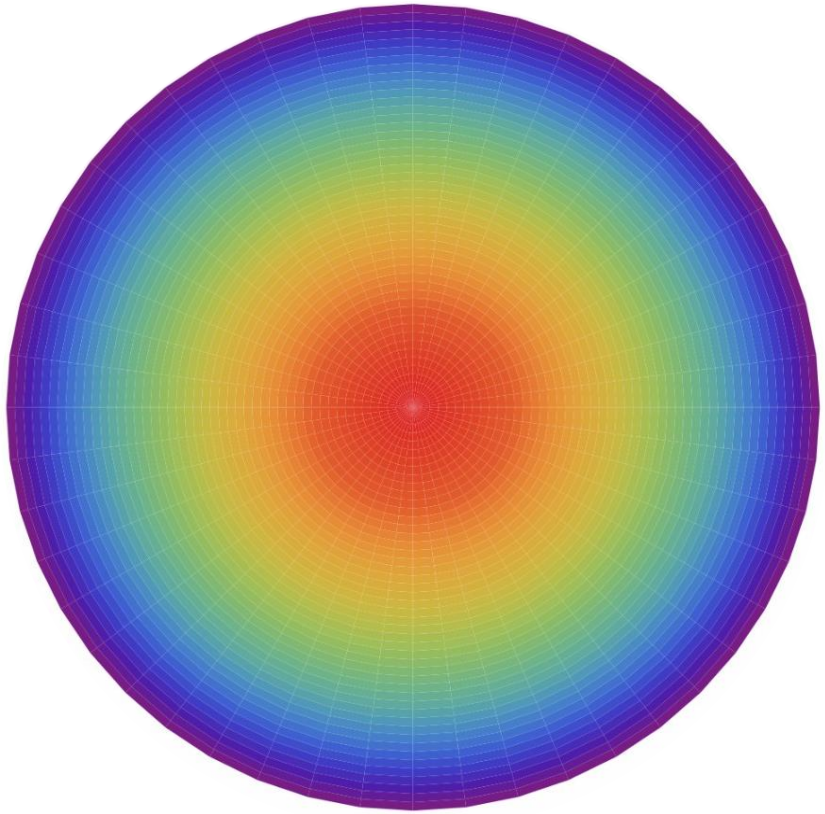
REACTOR PHYSICS & COMPUTATIONAL ANALYSIS LABORATORY



DEVELOPMENT AND VERIFICATION OF A THREE-DIMENSIONAL MULTIGROUP HYBRID FINITE ELEMENT DIFFUSION SOLVER IN CYLINDRICAL GEOMETRY FOR MOLTEN SALT FAST REACTOR ANALYSIS

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Presentation Outline

PRESENTATION OUTLINE

A six-part research roadmap



01 **Motivation & Objectives**
Why this work matters and what we aim to achieve

02 **Theoretical Framework**
Cylindrical HFEM/VNM formulation for multigroup diffusion

03 **Computational Implementation**
Consistent methods and solution strategies

04 **Verification Approach**
Accuracy assessment and reference cases

05 **Results & Discussion**
Performance, robustness, and suitability

06 **Conclusions & Outlook**
Key takeaways and next steps

Motivation and Research Objectives

WHY THIS WORK MATTERS

Accurate multigroup diffusion analysis is essential for MSFR neutronics design.

Cylindrical HFEM/VNM formulations provide a consistent and efficient framework for complex geometries.

The MSFR core is a cylinder: Cartesian nodes staircase its walls, so HFEM is built in r–θ–z, axis included.

Verification builds confidence in our methods and supports credible engineering decisions.

RESEARCH OBJECTIVES

01 Develop cylindrical HFEM/VNM formulations for multigroup diffusion in MSFR systems.

02 Implement and benchmark the methods within a consistent computational framework.

03 Verify accuracy against established analytical solutions and reference cases.

04 Assess performance, robustness, and suitability for engineering applications.

Implementation caveat: HFEM/VNM is a cornerstone method and may be integrated with other solvers (e.g., MOC, SN, or Monte Carlo) as appropriate.

Theoretical Framework: Multigroup Eigenvalue Problem

What is solved: the multiplication factor k and its fundamental-mode flux Φ

MULTIGROUP DIFFUSION, G = 1 … G

$$-\nabla \cdot D_g \nabla \Phi_g + \Sigma_{\mathrm{r},g} \Phi_g = \frac{\chi_g}{k} \sum_{g'} \nu \Sigma_{\mathrm{f},g'} \Phi_{g'} + \sum_{g' \neq g} \Sigma_{\mathrm{s},g' \to g} \Phi_{g'} \qquad (1)$$

LEAKAGE IN R–Θ–Z

$$\nabla \cdot D \nabla \Phi = \frac{1}{r} \partial_r (r D \partial_r \Phi) + \frac{1}{r^2} \partial_\theta (D \partial_\theta \Phi) + \partial_z (D \partial_z \Phi) \qquad (2)$$

OUTER BOUNDARY: MARSHAK VACUUM

$$j^- = \frac{1}{4} \Phi - \frac{1}{2} J_n = 0, \qquad J_n = -D \partial_n \Phi \qquad (3)$$

ALL GROUPS TOGETHER

$$M\Phi = \frac{1}{k} F\Phi, \qquad F = \chi (\nu \Sigma_{\mathrm{f}})^{\mathrm{T}} \qquad (4)$$

THE EIGENVALUE k

neutrons produced per neutron lost in the whole core: the multiplication factor

THE EIGENVECTOR Φ

the fundamental-mode flux of every group in every cell; its fission rate gives the power

HOW IT IS SOLVED

M is never assembled: response matrices invert it group by group, and a power iteration finds k

Multigroup diffusion and its notation: Ott & Bezella, Introductory Nuclear Reactor Statics (1989)

Theoretical Framework: HFEM Weak Form

Flux discontinuous across faces; continuity imposed weakly through a surface multiplier

$$(\nabla\varphi^*, D\nabla\varphi)_D + (\varphi^*, \Sigma_r\varphi)_D - (\chi^*, [\varphi])_\Gamma - ([\varphi^*], \chi)_\Gamma + \frac{1}{2}(\varphi^*, \varphi)_{\partial D} = (\varphi^*, q)_D \tag{5}$$

φ, χ	flux, discontinuous across faces; multiplier on each internal face, equal to the net current there	**φ*, χ***	the corresponding test functions
D	diffusion coefficient, $D = 1/(3\Sigma_{tr})$: Serpent's INF_DIFFCOEF	**Σ_r**	removal, which contains the within-group scattering
q	fission source $\chi_g/k\ \Sigma\ \nu\Sigma_f\varphi$ plus in-scatter from the other groups	**$(\cdot,\cdot)_D$, $(\cdot,\cdot)_\Gamma$**	integrals over the element volumes and the internal faces
[f]	jump across a face, $f^+ - f^-$	**$\frac{1}{2}(\varphi^*, \varphi)_{\partial D}$**	Marshak vacuum condition on the outer boundary

Varying φ* inside one element gives its exact balance: the method is conservative in every node, at every order.

Jung et al., Ann. Nucl. Energy 214 (2025) 111128 · Zhang & Li, Nucl. Eng. Technol. 54 (2022) 3181

Computational Implementation: Cylindrical HFEM Solver

From the deck to k: each element is built once, then two nested loops find the face currents and the eigenvalue

1 INPUT

Serpent constants for every ring: D, Σ_r, Σ_s, $\nu\Sigma_f$, χ in 33 groups, condensed to 25 / 24 few groups

2 MESH

the deck's zones cut into cells, $\Delta r \times \Delta\theta \times \Delta z$; every face interior, on the boundary or on the axis

3 BASIS

complete monomials of degree p_v in the volume and p_s on each face, orthonormalised per node

rank condition: $p_s \le p_v - 2$

4 ELEMENT MATRICES

$$E_{ij} = \int b_i b_j \mathrm{d}V$$
$$S_{r,ij} = \int \partial_r b_i \partial_r b_j \mathrm{d}V$$
$$S_{\theta,ij} = \int r^{-2} \partial_\theta b_i \partial_\theta b_j \mathrm{d}V$$
$$S_{z,ij} = \int \partial_z b_i \partial_z b_j \mathrm{d}V$$

dV = r dr dθ dz; exact moments on the parent element; S_θ: a Gauss rule, converged off the axis and fixed on it

5 RESPONSE MATRICES

$$A = \Sigma_r E + D(S_r + S_\theta + S_z)$$
$$T = E_s^{-1} M^{\mathrm{T}}, \qquad K = \frac{1}{2} T A^{-1} M$$
$$R = (K + I)^{-1}(K - I)$$
$$B = (K + I)^{-1} \frac{1}{2} T A^{-1}$$
$$j^+ = R j^- + B E s$$

E_s: face mass, M: volume–face coupling; built once per distinct element

OUTER · POWER ITERATION

INNER · k FIXED · GROUPS 1 → G

6 GLOBAL CURRENT SYSTEM

$$(I - R\Pi) j^+ = BEs + Rc$$

direct LU (SuperLU), factorised once per group; GMRES and red–black give the same k

face	incoming j^-
interior, to n	j^+ of the matching face of n
vacuum (Marshak)	0
reflecting	j^+
zero flux	$-j^+$
axis, centre	none: the face has zero area

currents of every group

new k, next outer

7 RECOVER THE FLUX

$$\Phi = A^{-1}\left(Es - M(j^+ - j^-)\right)$$

8 FISSION SOURCE

$$F = \sum_g \nu\Sigma_{f,g}\Phi_g$$

9 UPDATE k

$$k^{(n+1)} = k^{(n)} \frac{\langle \nu\Sigma_f, \Phi^{(n+1)} \rangle}{\langle \nu\Sigma_f, \Phi^{(n)} \rangle}$$

ε_F below 10^{-8} to 10^{-11}: k, Φ and the power; nodal balance 9.1×10^{-17} to 4.7×10^{-15}

Fig. 1. Flowchart of the solver; GMRES [7], SuperLU [8], power iteration [6]

Benchmark Problem: MSFR Design and Fuel Circuit

Right half of the r–z section, to scale, in the Serpent model's colours

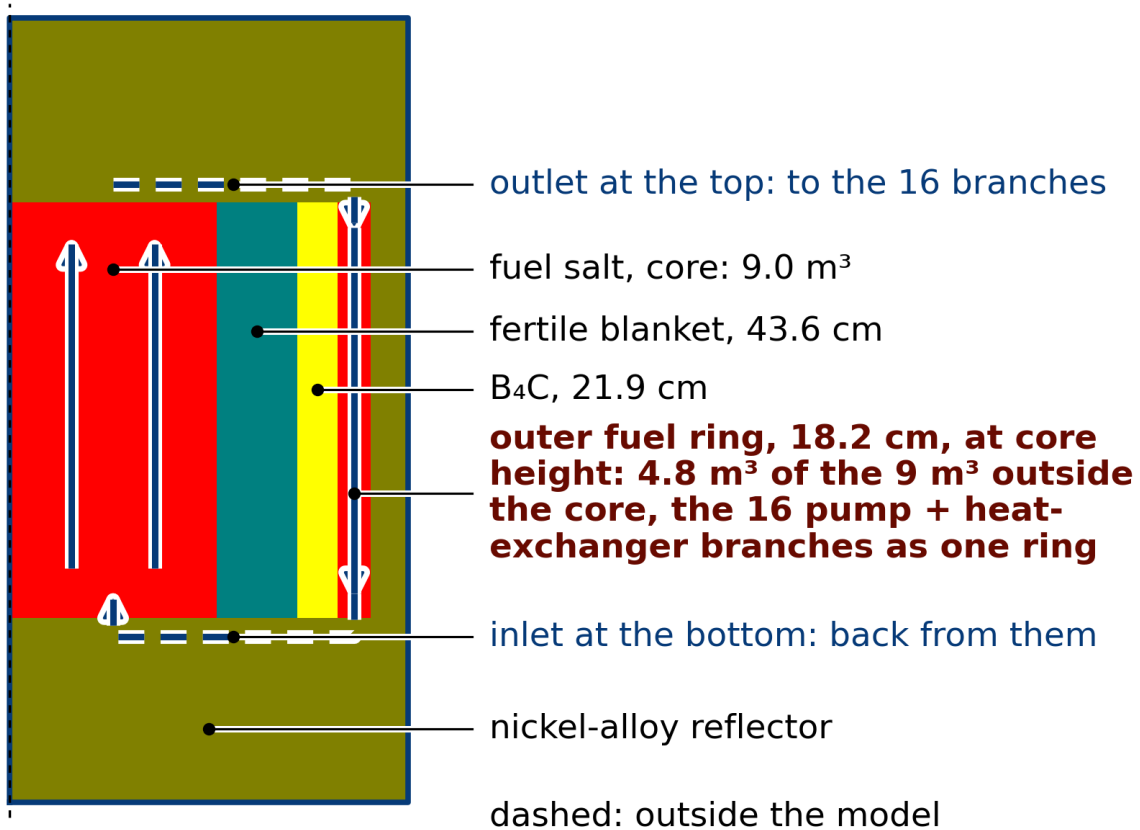


Fig. 2. Right half of the MSFR r–z section with the fuel circuit

THE DESIGN [1, 3]

Power 3000 MW_{th}, fast spectrum, no moderator

Core a cylinder, H = D = 2.255 m; 18 m³ of salt, half in the core

Loop 16 branches, each a pump and a heat exchanger of 187 MW

Flow 650 °C in at the bottom, 750 °C out at the top; 4.5 m³/s, 4.0 s around the circuit

THE OUTER FUEL RING

What the salt of the 16 branches, outside the blanket and the B_4C, kept as one ring at core height [9]

Why there 43.6 cm of fertile salt and 21.9 cm of B_4C shield the heat exchangers: the flux from the core is negligible against the delayed neutrons emitted in them [9]

In k it is fuel, with its own constants, in every calculation

[1] ANL/NSE-20/7, App. A · [3] Jaradat et al. (2021) · [9] EVOL D2.2 (2013), Fig. 3.1 and Sec. 3.1.1

Benchmark Problem: Reference Data

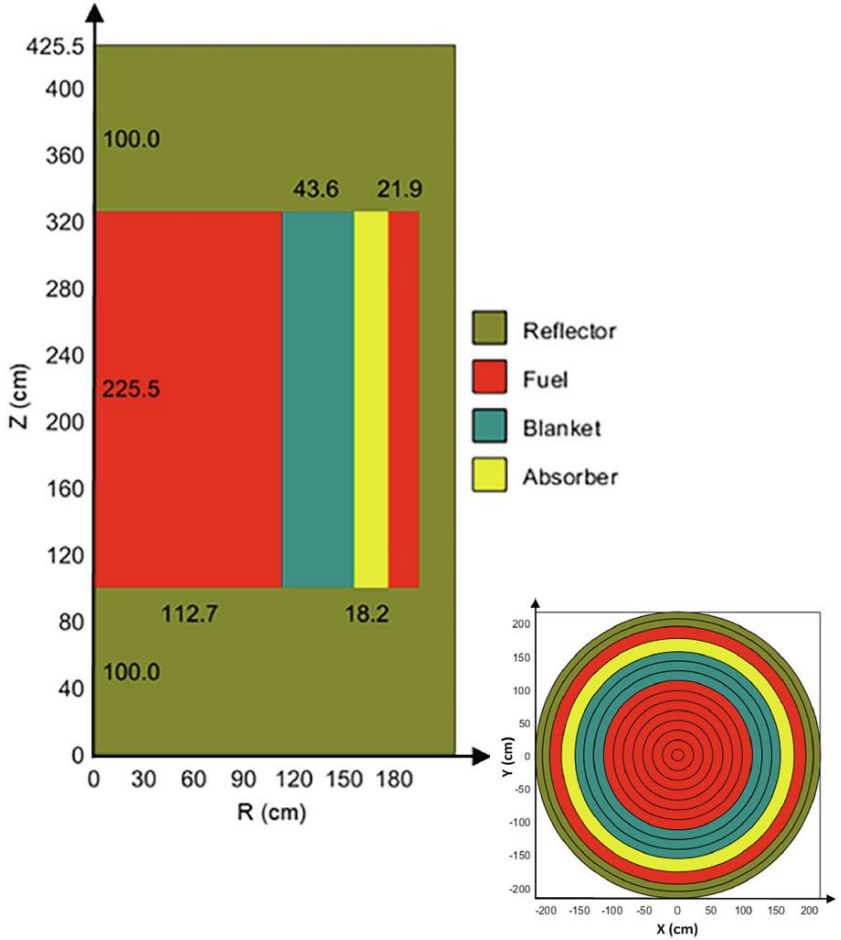


Fig. 3. Benchmark geometry: r–z section, radial plane

Table I: Characteristics of the Molten Salt Fast Reactor*

Characteristic	Value
Thermal / electric power	3 000 MWth / 1 300 MWe
Fuel composition	$LiF–ThF_4–^{233}UF_4$, $LiF–ThF_4–(TRU)F_3$
Fuel inlet / outlet temperature	650 °C / 750 °C
Core height / core radius	**2.255 m / 1.1275 m**
Fuel salt volume	18 m³
Total fuel salt transit time	4.0 s
Flow rate	4.5 m³/s
Density [kg/m³]	ρ = 4094 − 0.882 (T[K] − 1008)
Kinematic viscosity [m²/s]	v = 5.54 × 10^{-8} · e^(3689 / T[K])
Dynamic viscosity [Pa·s]	μ = [2.268 − 4.886 × 10^{-4} (T[K] − 1008)] × 10^{-4} · e^(3689 / T[K])
Thermal conductivity [W/m·K]	k = 0.928 + 8.397 × 10^{-5} T[K]
Specific heat [J/kg·K]	c_p = −1111 + 2.78 T[K]

ANL/NSE-20/7: M. K. Jaradat, G. Yang, H. Park, W. S. Yang, C. H. Lee and Y. S. Jung, "*Multiphysics Coupling of PROTEUS-NODAL and SAM for Molten Salt Reactor Simulation*," Argonne National Laboratory, 28 February 2020.

***** Jaradat, Park, Yang, and Lee, "**Development and validation of PROTEUS-NODAL transient analyses capabilities for molten salt reactors**," Ann. Nucl. Energy 160 (2021) 108402, Table 1.

Benchmark Problem: Model Specification

The two Serpent models that supply the constants: 2-D r–θ, axially infinite, and 3-D r–θ–z between axial reflectors

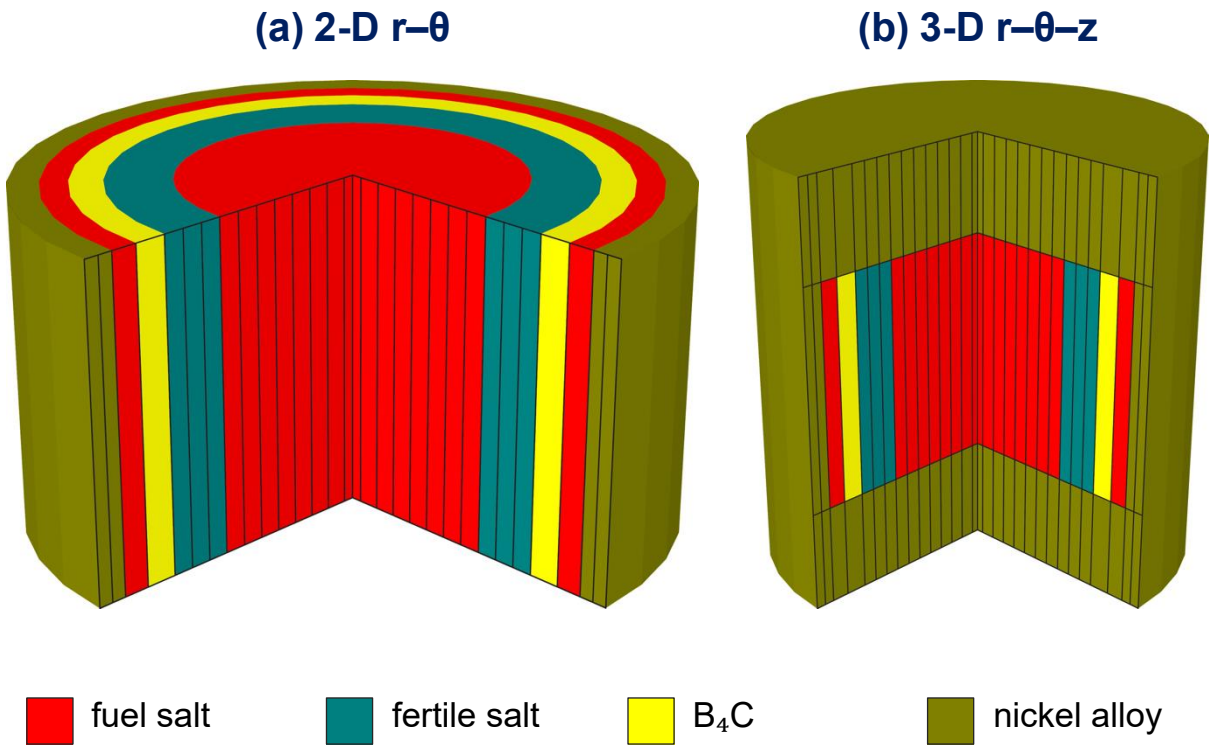


Fig. 4. Cutaways of the two Serpent models, in the Serpent colours

Table II: Specification of the two Serpent models

	2-D r–θ	3-D r–θ–z
outer radius	216.76 cm	216.76 cm
active core height	225.50 cm	225.50 cm
modelled height	axially infinite	425.50 cm
radial zones	15	15
homogenisation regions	15	15 + 1 reflector
det cards in the deck	22	24
few groups solved	25 of 33 delivered	24 of 33 delivered
group structure	33_groups_anl	33_groups_anl
library	ENDF/B-VII.1	ENDF/B-VII.1
statistics	800 000 × 500	800 000 × 500
Serpent ANA_KEFF	**0.99679 ± 7 pcm**	**0.97177 ± 7 pcm**

[1] ANL/NSE-20/7, Fig. 2.1 · Serpent 2, ENDF/B-VII.1; statistics are neutrons × active cycles

Discretization: p-Refinement in 2-D

p_v and p_s raised on one fixed mesh, 30 × 8, 25 few groups

Table III: 2-D, 30 × 8; reference: Serpent k = 0.99679 ± 7 pcm

Volume / Side (p_v/p_s)	k_{eff} (error)	power RMS (%)	power max (%)
1 / 0	0.99744 (+65)	0.1687	0.4925
3 / 1	0.99754 (+75)	0.0033	0.0061
4 / 1	0.99754 (+75)	0.0016	0.0030
5 / 2	0.99755 (+75)	0.0006	0.0012
6 / 1	0.99755 (+75)	0.0000	0.0000
6 / 2	0.99755 (+75)	0.0000	0.0000

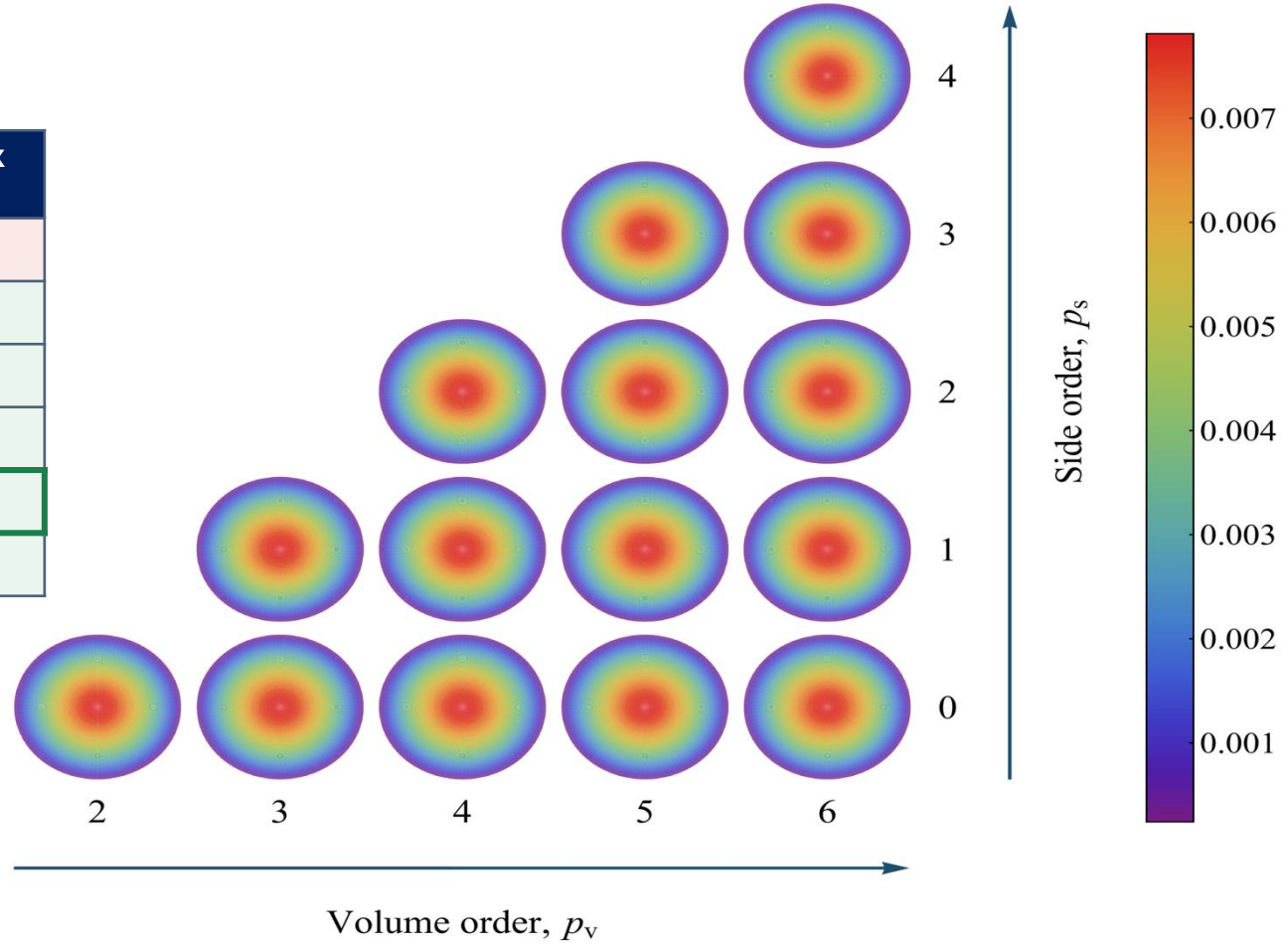


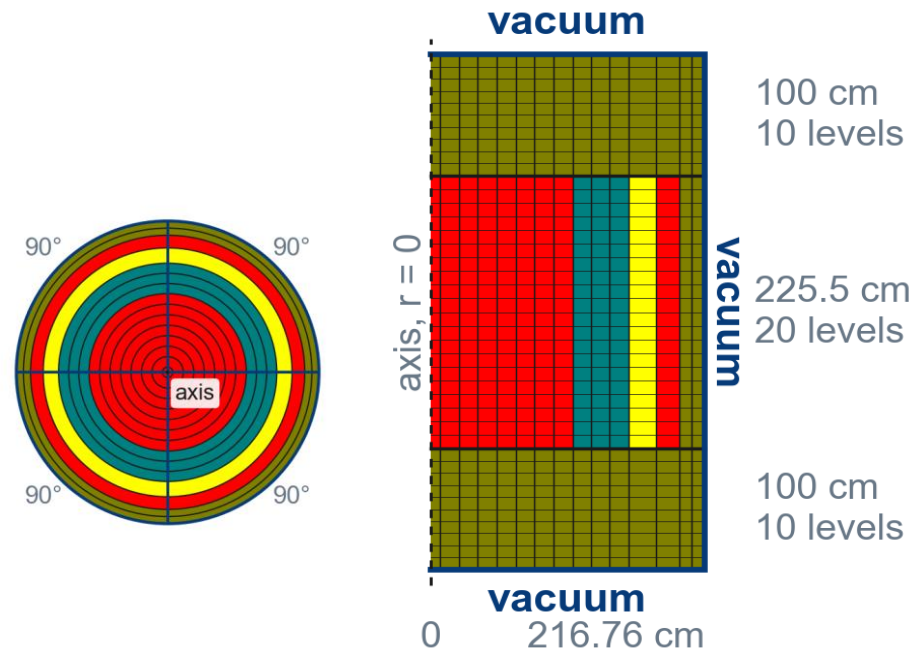
Fig. 5. Fuel-region flux at every order p_v/p_s on the 30 × 8 mesh

Discretization: p-Refinement in 3-D

p_v and p_s raised on one fixed mesh, 15 × 4 × 40, 24 few groups

Table IV: 3-D, 15 × 4 × 40; reference: Serpent k = 0.97177 ± 7 pcm

Volume / Side (p_v/p_s)	k_{eff} (error)	power RMS (%)	power max (%)
1 / 0	0.97130 (−47)	1.1744	4.3683
3 / 1	0.97199 (+23)	0.0142	0.0574
4 / 1	0.97200 (+23)	0.0048	0.0173
5 / 1	0.97200 (+23)	0.0074	0.0335
6 / 1	0.97200 (+23)	0.0000	0.0000



one plane: 15 × 4 = 60 cells r–z: 10 + 20 + 10 = 40 levels

Fig. 6. The 3-D mesh: one radial plane and the r–z section

Discretization: h-Refinement

Radial rings and axial levels refined at fixed order 3/1

Table V: 2-D rings, 3/1; reference: Serpent k = 0.99679 ± 7 pcm

rings	mesh	k_{eff} (error)
30	30 × 8	0.99754 (+75)
60	60 × 8	0.99754 (+75)
120	120 × 8	0.99755 (+75)
240	240 × 8	0.99755 (+76)

Table VI: 3-D rings, 3/1; reference: Serpent k = 0.97177 ± 7 pcm

rings	mesh	k_{eff} (error)
15	15 × 1 × 40	0.97199 (+23)
18	18 × 1 × 40	0.97200 (+23)
27	27 × 1 × 40	0.97200 (+23)
31	31 × 1 × 40	0.97200 (+23)

Table VII: 3-D axial core levels, 3/1; reference: Serpent k = 0.97177 ± 7 pcm

core levels	mesh (r × θ × z)	cells	level (cm)	k_{eff} (error)
1	15 × 1 × (10+1+10)	315	225.500	0.97459 (+283)
2	15 × 1 × (10+2+10)	330	112.750	0.97216 (+39)
5	15 × 1 × (10+5+10)	375	45.100	0.97200 (+23)
10	15 × 1 × (10+10+10)	450	22.550	0.97199 (+23)
20	15 × 1 × (10+20+10)	600	11.275	0.97199 (+23)
40	15 × 1 × (10+40+10)	900	5.638	0.97199 (+23)

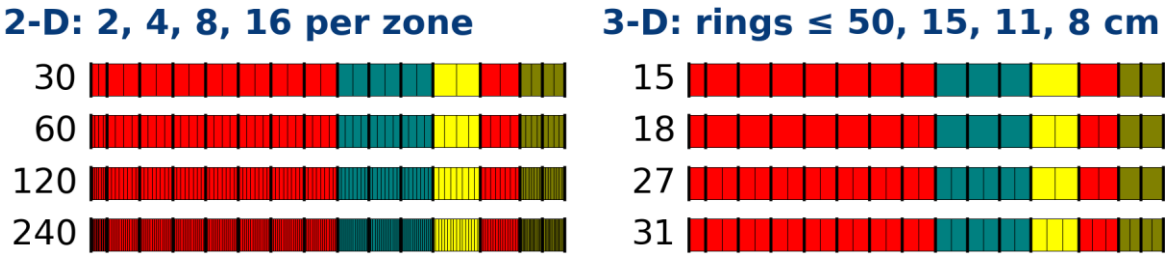


Fig. 7. The refined radial meshes, in the Serpent colours

Results: Fuel Power Distribution

Absolute error in per cent of the core average; reference: the Serpent power tally on the benchmark's fuel node

Table VIII: Fuel power distribution against the Serpent tally

model	Volume / Side (p_v/p_s)	$P_{Serpent}$	P_{HFEM}	RMS (%)	max (%)	largest at
2-D, ring	1/0	1.4142	1.4186	0.234	0.442	ring 1
	3/1	0.3643	0.3615	0.157	0.287	ring 8
	4/1	0.3643	0.3615	0.156	0.285	ring 8
	5/2	0.3643	0.3615	0.155	0.283	ring 8
	6/2	0.3643	0.3615	0.155	0.283	ring 8
	6/1	0.3643	0.3615	**0.155**	0.283	ring 8
3-D, (ring, level)	1/0	1.8313	1.8694	1.503	3.814	ring 1, level 8
	3/1	0.5897	0.5754	0.629	1.432	ring 1, level 1
	4/1	0.5897	0.5754	0.626	1.434	ring 1, level 1
	5/1	0.5897	0.5754	0.625	1.432	ring 1, level 1
	6/1	0.5897	0.5754	**0.625**	1.433	ring 1, level 1

Verification: IAEA LWR Benchmark in r–θ–z

Prinsloo & Tomašević (2008) [10]: the 3-D IAEA PWR benchmark recast in r–θ–z, two groups, diffusion

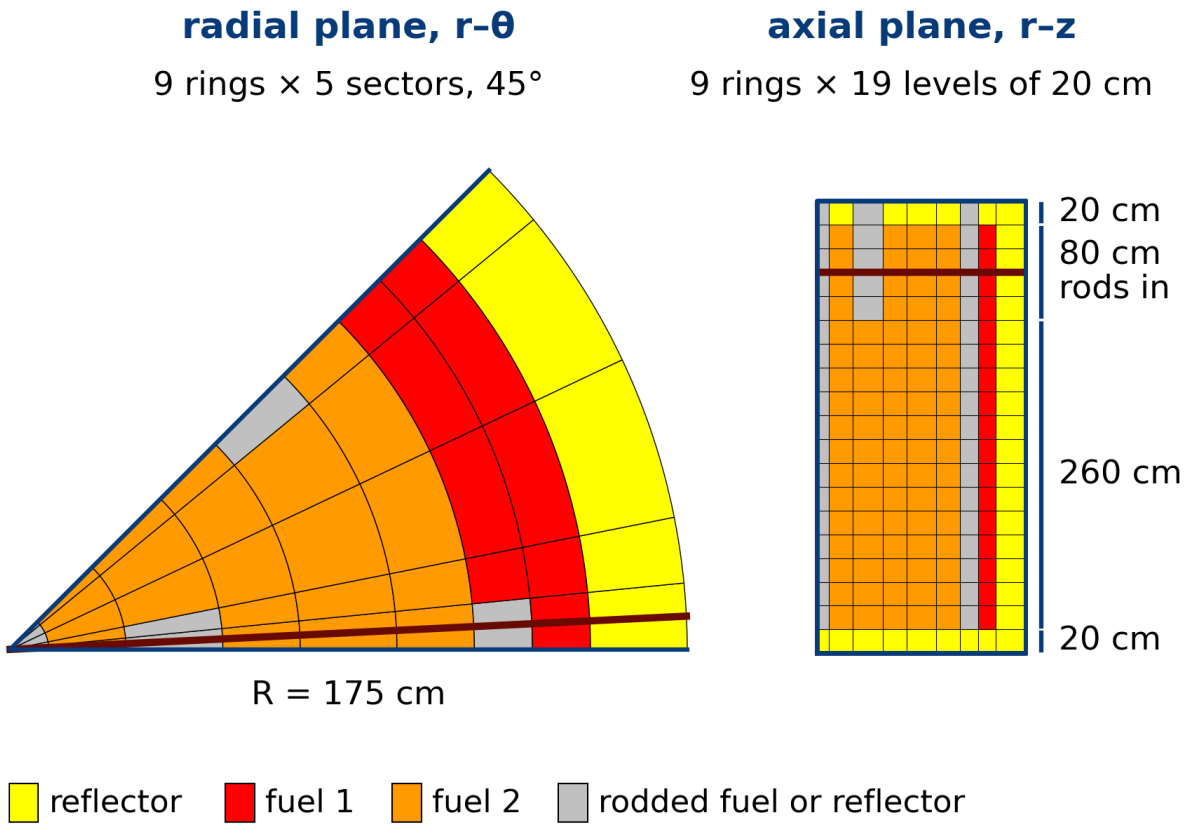


Fig. 8. The IAEA problem in r–θ–z: radial and axial planes

Table IX: Specification of the IAEA problem

item	value
geometry	45° segment; R 175 cm, H 380 cm
materials	two fuels, rodded fuel, reflector, rodded reflector
constants	two groups, Table 1 of [10]
mesh	9 × 5 × 19 = 855 elements
boundary	segment sides reflecting; outside zero flux
reference	k = 1.03353 (Table 4); power of 34 fuel blocks (Fig. 12)

[10] Prinsloo & Tomašević (2008): Table 1, Fig. 5, Sec. 8 · Mahogany: where the other plane cuts

Verification: IAEA LWR Eigenvalue and Power

Absolute error in per cent of the mean block power; reference: Prinsloo & Tomašević (2008) [10], zero-flux boundary

Table X: IAEA eigenvalue and block power against the published reference

model	case	k_{eff} (error)	RMS (%)	max (%)
HFEM	3/1	1.03371 (+18)	1.430	2.751
	4/1	1.03354 (+1)	**0.067**	**0.164**
	5/1	1.03353 (0)	0.093	0.193
	6/1	1.03353 (0)	0.103	0.240
Prinsloo & Tomašević [10]	FD 70 × 32 × 76	1.03343 (−10)	—	—
	FD 105 × 48 × 114	1.03348 (−5)	—	—
	analytic nodal	1.03354 (+1)	0.625	1.063

855 elements, direct inner solve · k error in pcm against k = 1.03353 (Table 4) · nodal: Fig. 13 |relative| × P_{ref} · FD: published relative only

Conclusions

Refinement changes k by under 1 pcm; what remains against Serpent is attributed mainly to the model.

Against Serpent

k at 6/1: +75 pcm (2-D) and +23 pcm (3-D); fuel power RMS 0.155 % and 0.625 %.

IAEA benchmark

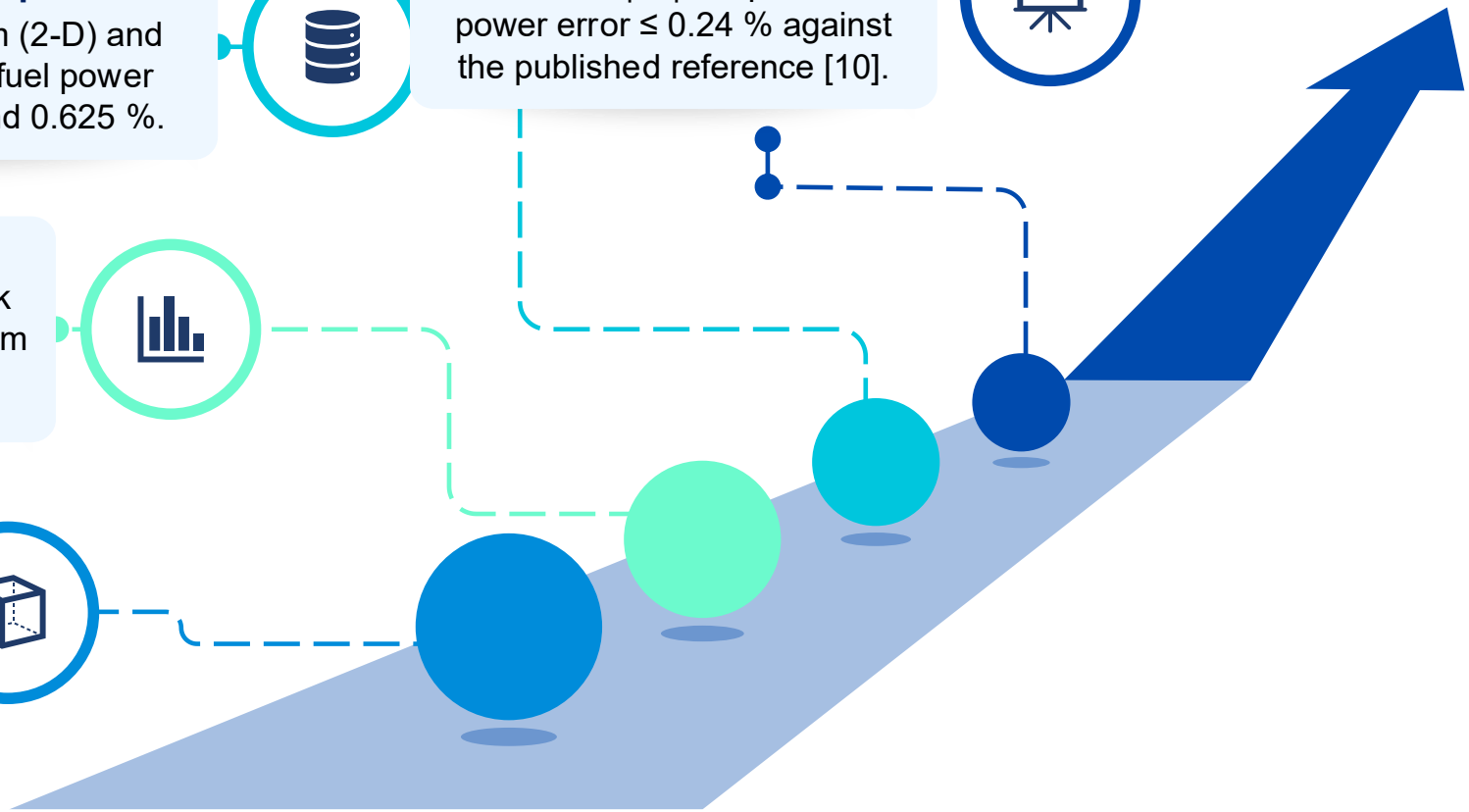
From 4/1, $|\Delta k| \leq 1$ pcm and power error ≤ 0.24 % against the published reference [10].

Convergence

Refinement in order moves k by 0.22 pcm (2-D) and 0.6 pcm (3-D); in mesh, by under 1 pcm.

Method

r–θ and r–θ–z, the 1/r inside the element; balance residual at most 4.7×10^{-15} at every order.



Future Work: Multi-Physics, Multi-Scale Research Roadmap

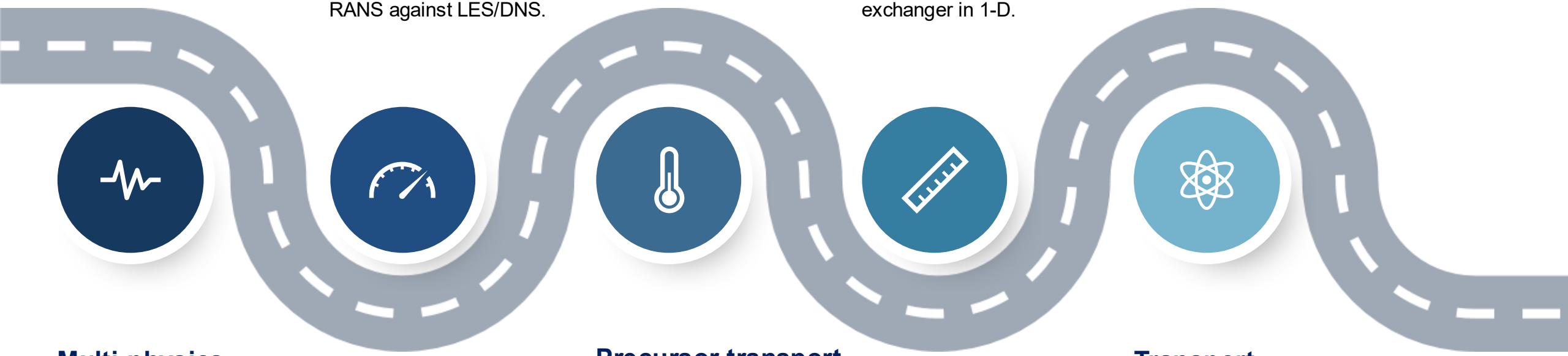
Vision: a verified multi-physics, multi-scale transient analysis of the MSFR, built from simple to complex

3-D core flow

3-D stagnation and recirculation; RANS against LES/DNS.

Multi-scale coupling

3-D core; loop and heat exchanger in 1-D.



Multi-physics coupling

HFEM within CUPID, with Doppler and density feedback; the ANE 160 transients under way.

Precursor transport

Non-uniform 3-D precursor and decay-heat fields in the transient response.

Transport extension

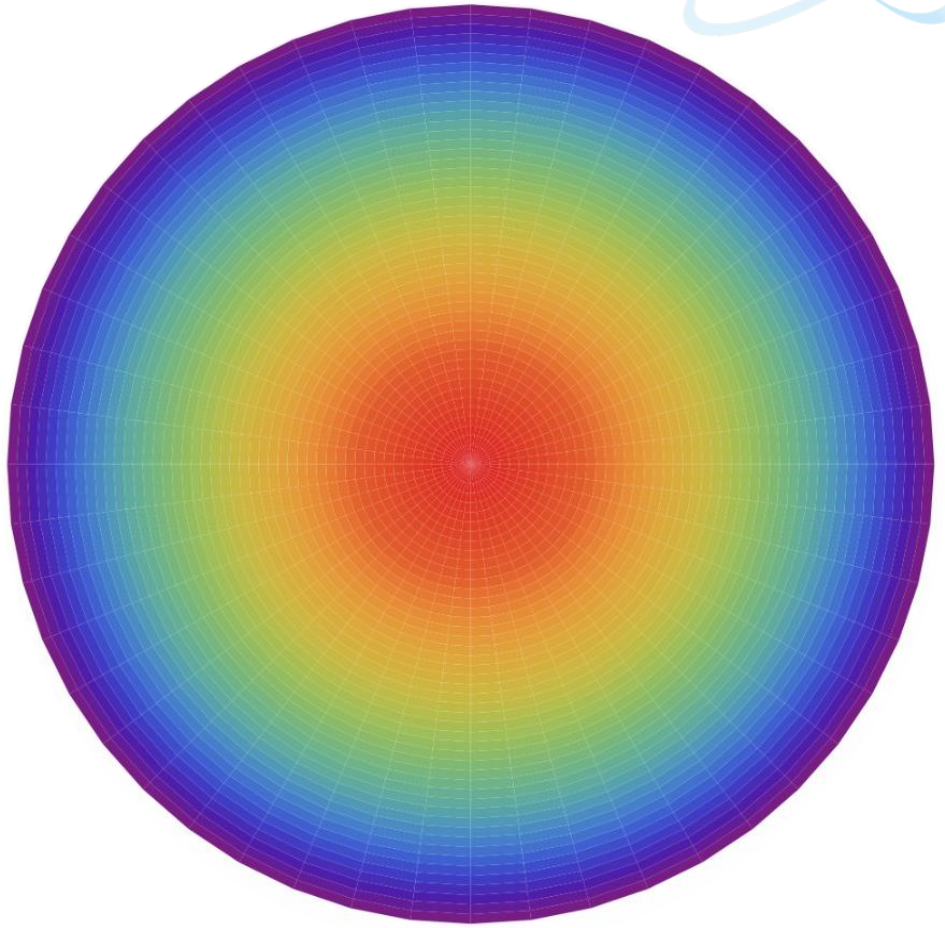
Even-parity P_N within the same HFEM framework.

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Thank you for your attention!



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