

NEW 3D DIFFUSION CODE BASED ON THE NODAL POLYNOMIAL EXPANSION



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Interface current techniques for multidimensional reactor calculations¹

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Abstract

The nodal collision probability method (NCPM) and the nodal expansion method (NEM) can both be used for multidimensional reactor calculations with comparable computational efficiency in their basic versions.

Both methods are based on interface current techniques the difference being, that NCPM is directly derived from integral transport theory whereas NEM relies on diffusion theory. It is shown that NEM which combines interface currents with weighted residual techniques can more easily be extended to achieve high accuracy for very large meshes. In addition, NEM converges rapidly towards the exact solution of the neutron diffusion equation with finer mesh size. It was therefore adopted as solution method for reactor calculations at KWU.

Zusammenfassung

Partialstromverfahren für mehrdimensionale Reaktorrechnungen

Die nodale Stoßwahrscheinlichkeits-(NCPM) und die nodale Entwicklungsmethode (NEM) sind Partialstromverfahren, die in ihren Grundversionen mit vergleichbarer Effizienz für Reaktorrechnungen verwendet werden können. NEM hat jedoch gegenüber NCPM den Vorteil, leichter zu einem auch bei sehr groben Maschen noch genaueren Rechenverfahren ausgebaut werden zu können. Dies wird durch Verknüpfung des Partialstromverfahrens mit der Methode gewichteter Residuen erreicht. NEM hat darüber hinaus die Eigenschaft, mit hoher Ordnung gegen die Lösung der Diffusionsgleichung zu konvergieren. Die Methode wird deshalb bei der KWU in mehrdimensionalen Reaktorrechnungen benutzt.

INIS DESCRIPTORS

COARSE MESH METHOD	SERIES EXPANSION
POWER DISTRIBUTION	ACCURACY
REACTOR LATTICES	MULTIGROUP THEORY
NUMERICAL SOLUTION	COLLISION INTEGRALS
NEUTRON TRANSPORT	NEUTRON DIFFUSION
THEORY	EQUATION

1. Introduction

Nodal methods are the basis for the evaluation of both transient and static power distributions in large LWRs at KWU. Nodal methods are in use for multidimensional reactor calculations for a long time already. The reader is referred to the review paper of A. F. Henry [1] for a detailed discussion of the various approaches possible and approximations necessary in formulating nodal balance equations. One of the main difficulties associated with nodal methods is the determination of spatial coupling coefficients. This problem has severely limited the practical use of nodal methods until recently.

A particular class of nodal methods is characterized by the fact that spatial coupling is expressed in terms of interface currents. Formally exact nodal equations of this type can be

obtained by integrating the multigroup neutron balance equation

$$\vec{\nabla}_u \cdot \vec{\Gamma}_g + \Sigma_{g0} \phi_g = \sum_{g'=1}^G (\Sigma_{g'g} + \frac{\Sigma_{g'g}}{\lambda} v \Sigma_{g'g}) \phi_{g'} \quad (g = 1, 2, \dots, G) \quad (1)$$

over the volume

$$V^m = a_x^m a_y^m a_z^m$$

of a rectangular box

$$\sum_{u=x,y,z} [j_{gu}^+ + j_{gu}^-] - [j_{gu}^- + j_{gu}^+] + \Sigma_{g0}^m \phi_g^m = \sum_{g'=1}^G (\Sigma_{g'g}^m + \frac{\Sigma_{g'g}^m}{\lambda} v \Sigma_{g'g}^m) \phi_{g'}^m \quad (2)$$

The notation is fairly standard and in accordance with previous usage. ϕ_g^m is the average flux of node m and j_{gu}^+ and j_{gu}^- represent average partial currents on the right ($u = r$) or left ($u = l$) surface $A_{gu}^m = a_x^m \cdot a_y^m$ of box m . The subscript u ($u = x, y, z$) denotes dependence of the quantity concerned on the spatial variable u .

Introducing spatial coupling coefficients γ_{gu}^m as quotients of partial currents and average fluxes the "conventional" nonlinear form of (2) is obtained

$$\sum_{u=x,y,z} \frac{1}{\phi_g^m} (\gamma_{gu}^m \phi_g^m - \gamma_{gu}^{m'}) \phi_g^m + \Sigma_{g0}^m \phi_g^m = \sum_{g'=1}^G (\Sigma_{g'g}^m + \frac{\Sigma_{g'g}^m}{\lambda} v \Sigma_{g'g}^m) \phi_{g'}^m \quad (3)$$

Of course, the formal operations leading to (3) are not very useful, unless a prescription for calculating coupling coefficients is given. Various attempts to solve this problem are reported in [1; 2]. The methods discussed in this paper are both based on the linear form (2) of the nodal balance equation. Obviously, in order that (2) be a useful relationship an additional set of equations for the calculation of interface currents is necessary.

2. Nodal collision probability method (NCPM)

The interface current technique has been used by many authors for reactor cell calculations [3-6]. As shown in [7; 8] the method can also be used to solve multidimensional reactor problems with a coarse mesh. To this end, the integral transport equation is transformed into an equivalent partial current equation

$$j_{gs}^m = v^m \sum_{g'=1}^G (\Sigma_{g's}^m + \frac{\Sigma_{g's}^m}{\lambda} v \Sigma_{g's}^m) \phi_{g'}^m + \sum_{s'=1}^6 P_{gs'}^m j_{gs'}^m \quad (4)$$

where s now denotes one of the six surfaces of a rectangular parallelepiped. Eq. (4) states that the outgoing current through one of the six surfaces is equal to the sum of contribution from volume sources and from uncollided neutrons penetrating the cell from each of the other bounding surfaces. The coefficients P denote escape and transmission probabilities for the contributing neutrons. In this equation each node i directly coupled both through flux and current terms to its six nearest neighbours. Eqs. (2) and (4), together with suitable albedo or symmetry boundary conditions form a consistent set of homogeneous equations which are sufficient to determine the complete set of fluxes and currents describing the entire neutron field of the reactor.

The basic equations (2), (4) are exact provided that the correct collision probabilities are known. Obviously, the latter depend in a very complicated way on the unknown spatial distribution of the sources both in- and outside the cell. Therefore the most important step of the approximation is the proper choice of effective collision probabilities that retain essential effects and still are simple enough to be precalculated. Experience has shown that the sole use of first-flight collision probabilities for flat isotropic sources leads to insufficient accuracy. Much better results are obtained if, in addition, collision probabilities for isotropic linearly space-dependent source distributions are included. Source gradient and curv-

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ENGINEERING → TRANSPORT or DIFFUSION?

MAINFRAMES or PERSONAL COMPUTERS?

FINE MESH or COARSE MESH?

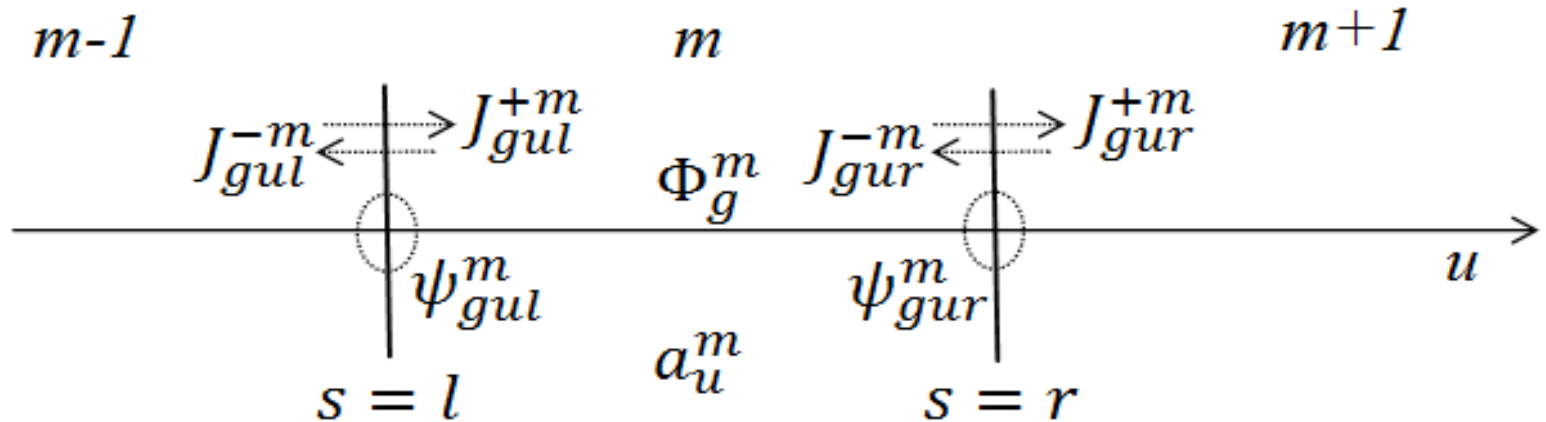
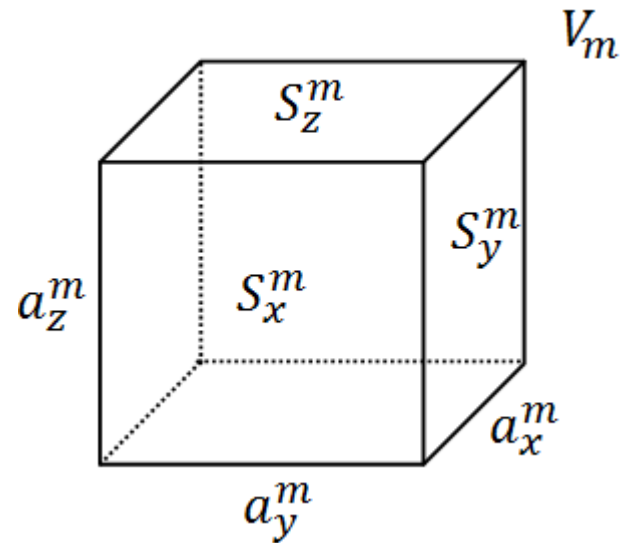
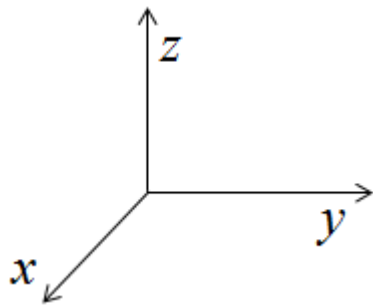
METHOD **NODAL (NEM)**

- Higher Order Finite Difference,
- Finite Element, **FORTRAN → NEM3D**
- Nodal: NCPM, NEM, NAM, FEM.

BENCHMARK TEST IAEA 3D -LWR

SUMMARY OF THE METHOD

$$(J_{\text{out}} - J_{\text{in}}) + (L - P) = 0$$



METHOD DEVELOPMENT

$$\vec{\nabla} \cdot D_g(\vec{r})\vec{\nabla}\phi_g(\vec{r}) - \Sigma_{tg}(\vec{r})\phi_g(\vec{r}) + \sum_{g'} [\Sigma_{gg'}(\vec{r}) + \frac{1}{\lambda}\chi_g\nu\Sigma_{fg'}(\vec{r})]\phi_{g'}(\vec{r}) = 0$$

$$\vec{J}_g(\vec{r}) = -D_g(\vec{r})\vec{\nabla}\phi_g(\vec{r})$$

$$\vec{\nabla} \cdot \vec{J}(\vec{r}) + \Sigma_{tg}(\vec{r})\phi_g(\vec{r}) = \sum_{g'} [\Sigma_{gg'}(\vec{r}) + \frac{1}{\lambda}\chi_g\nu\Sigma_{fg'}(\vec{r})]\phi_{g'}(\vec{r})$$

INTEGRATING IN A VOLUME V_m :

$$\int_{V_m} \vec{\nabla} \cdot \vec{J} dV + \int_{V_m} \Sigma_{tg}\phi_g dV = \sum_{g'=1}^G \int_{V_m} \Sigma_{gg'}\phi_{g'} dV + \sum_{g'=1}^G \int_{V_m} \frac{1}{\lambda}\chi_g\nu\Sigma_{fg'}\phi_{g'} dV$$

$$\Phi_g^m \equiv \frac{\int_{V_m} \phi_g(x, y, z) dV}{\int_{V_m} dV} = \frac{1}{V_m} \int_{V_m} \phi_g(x, y, z) dV$$

$$\int_{V_m} \Sigma \chi_g \phi_g(x, y, z) dV = \Sigma \chi_g^m \Phi_g^m V_m$$

$$\int_{V_m} \vec{\nabla} \cdot \vec{J}(x, y, z) dV + \Sigma_{tg}^m \Phi_g^m V_m = \sum_{g'=1}^G [\Sigma_{gg'}^m + \frac{1}{\lambda} \chi_g^m \nu \Sigma_{fg'}] \Phi_{g'}^m V_m$$

$$\sum_{u=x,y,z} \frac{1}{a_u^m} [(J_{gur}^{+m} - J_{gur}^{-m}) - (J_{gul}^{+m} - J_{gul}^{-m})] + \Sigma_{tg}^m \Phi_g^m = \sum_{g'=1}^G [\Sigma_{gg'}^m + \frac{1}{\lambda} \chi_g^m \nu \Sigma_{fg'}] \Phi_{g'}^m$$



BOUNDARY CONDITIONS

$$J_{gus}^{+m} - J_{gus}^{-m} \cong -D_{gus}^m \frac{d}{du} \psi_{gu}^m(u) \Big|_{us};$$
$$2(J_{gus}^{+m} + J_{gus}^{-m}) \cong \psi_{gu}^m(u) \Big|_{us}.$$

Where,

$$\psi_{gu}^m \equiv \frac{1}{A_u^m} \int_{A_u^m} \phi_g(x, y, z) dS_v.$$

$$\phi_g^m \equiv \frac{1}{a_u^m} \int_0^{a_u^m} \psi_{gu}^m(u) du.$$

POLINOMIAL FORMULATION

$$\psi_{gu}^m(u) \cong \psi_{gu}^{m(N)}(u) = \sum_{n=0}^N c_{un,g}^m h_n \left(\frac{u}{a_u^m} \right)$$

$$h_n \left(\frac{u}{a_u^m} \right) = \sum_{i=0}^n b_{ni} \left(\frac{u}{a_u^m} \right)^i$$

BENCHMARK

Table 1: Nuclear data for IAEA benchmark (ANT 7416 1977)

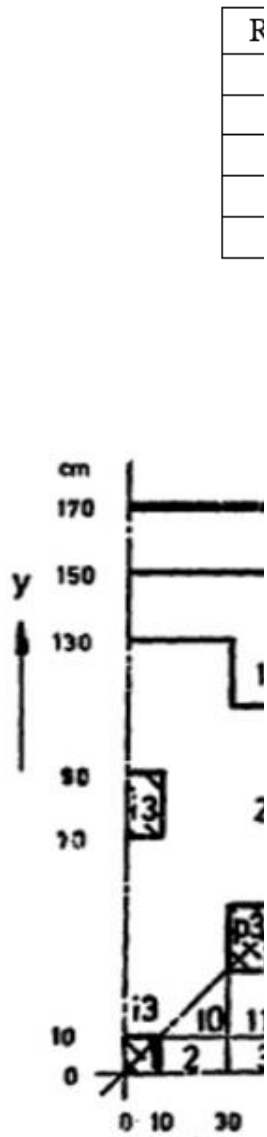


Figure 4: The c

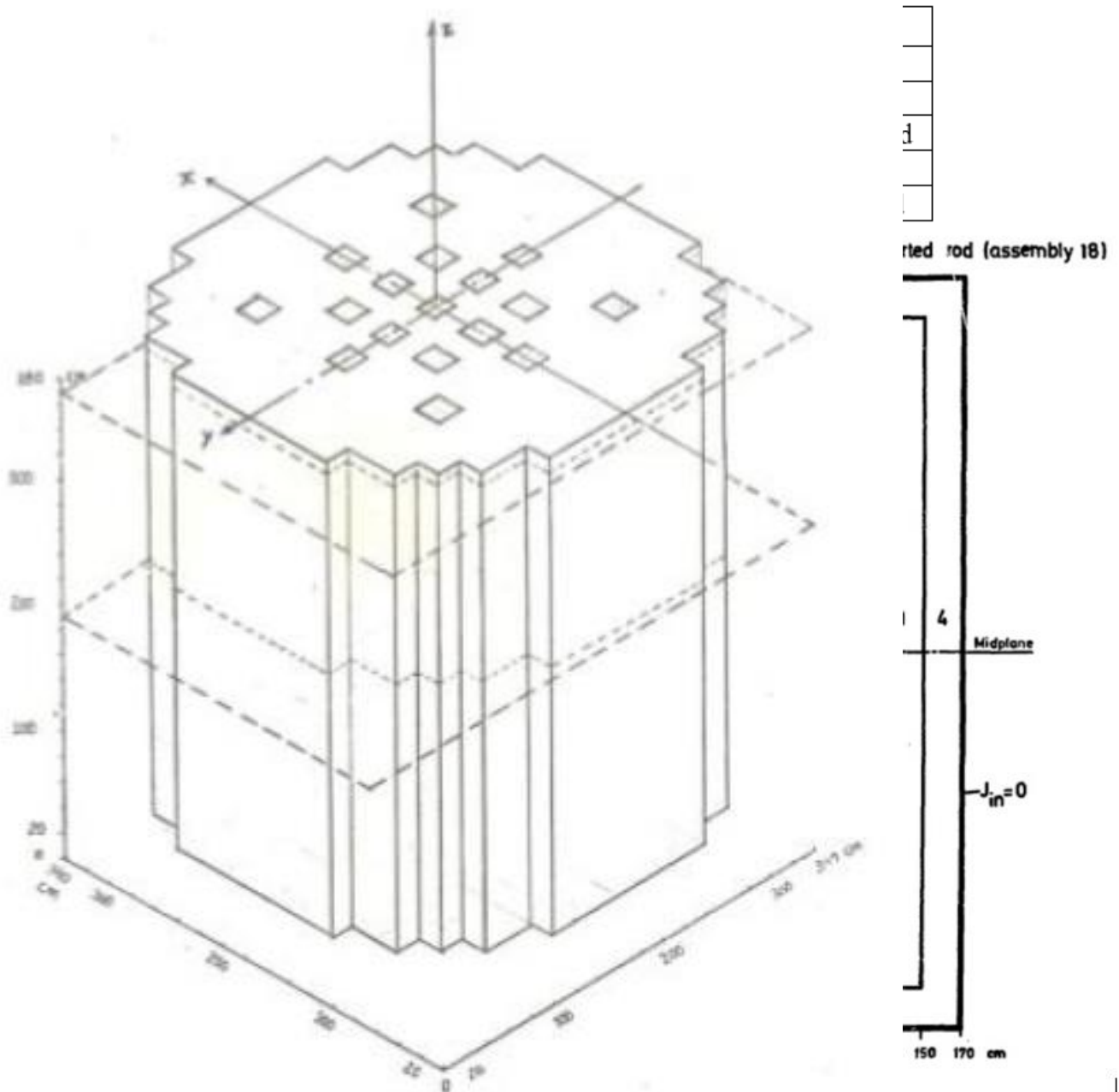


Figure 5: The core longitudinal cross section with control rods.

 **IQSBOX (FINNEMANN, 1975) – Nodal Expansion Method**

FEM-3D (MISFELDT, 1975) – Finite Element Method

VENTURE (VONDY et al., 1977) – Finite Difference Method

VANCER (VONDY and FOWLER, 1978) – Finite Element Method

Ph.D. Thesis (CHRISTENSEN, 1985) – Nodal Expansion Method

ARROTA (EISENHART, 1991) – Analitic Nodal Method

NESTLE (TURINSKY et al., 1994) – Nodal Expansion Method

 **PARCS (DOWNAR et al., 2002) – Analitic Nodal Method**

RESULTS COMPARISON

CODE	$a_x \times a_y \times a_z(\text{cm}^3)$	k_{eff}	$\Delta k_{eff}(\%)$
VENTURE	Extrap.	1.02903	-
VENTURE	$10 \times 10 \times 10$	1.02864	0.03790
VANCER	$10 \times 10 \times 10$	1.02949	0.04470
FEM-3D	$10 \times 10 \times 10$	1.02920	0.01652
IQSBOX	$20 \times 20 \times 20$	1.02911	0.00777
NEM3D-1A	$20 \times 20 \times 20$	1.02901	0.00194
Christensen	$20 \times 20 \times 20$	1.02896	0.00680
ARROTA	$20 \times 20 \times 20$	1.02899	0.00389
NESTLE	$20 \times 20 \times 20$	1.02899	0.00389
PARCS	$20 \times 20 \times 20$	1.02909	0.00641

$$k_{eff}^{IAEA-3D} = 1.02903$$

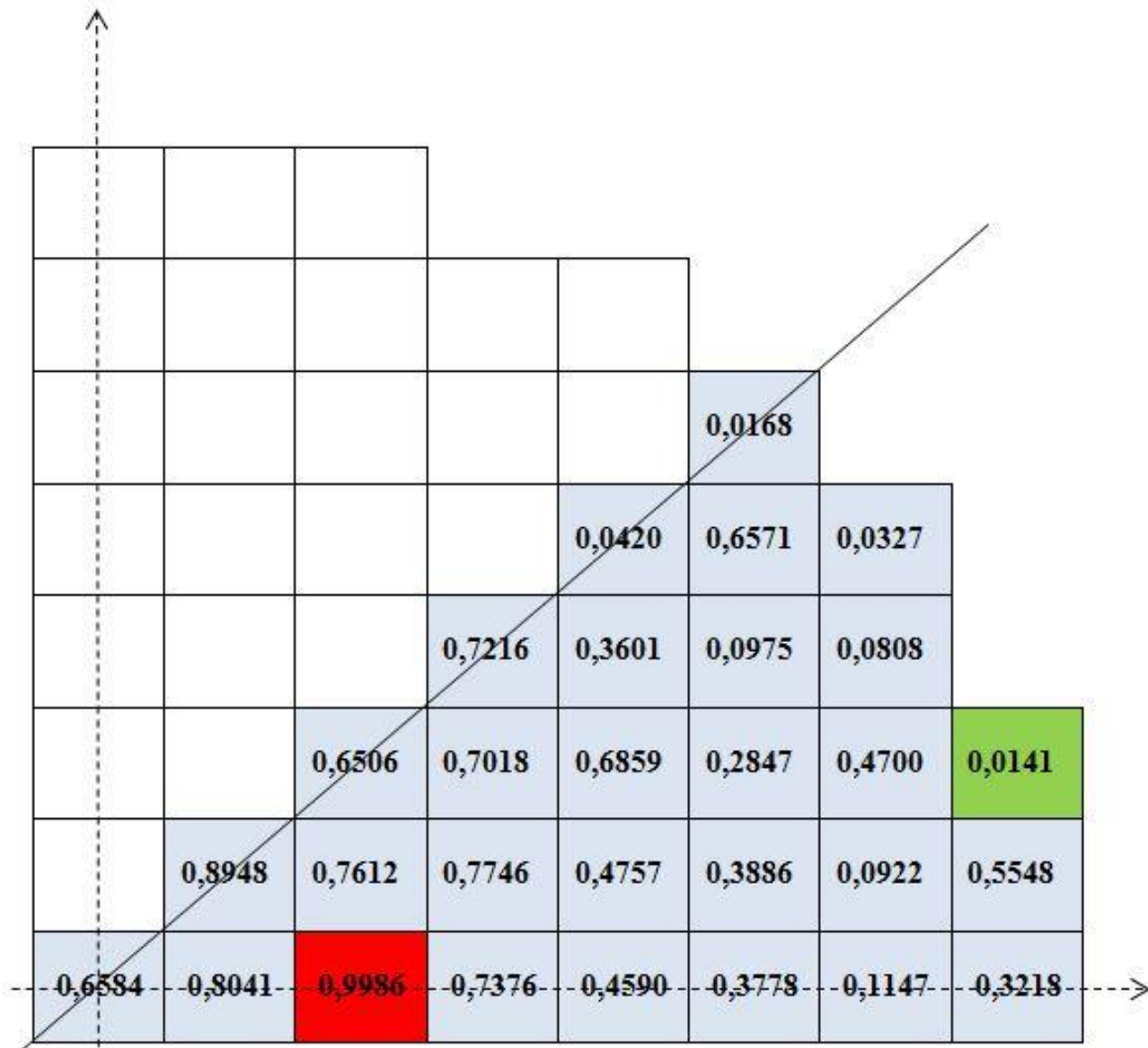


Figure 7: The NEM3D-1A mean radial power distribution deviation.

CONCLUDING REMARKS

- *THE PROPOSED WORK WAS SUCCESSFUL;*
- *NEM IS AN IMPORTANT TOOL FOR COARSE MESH CALCULATIONS IN LWR;*
- *NEM3D-1A WAS ABLE TO PREDICT THE k_{eff} WITH A GOOD ACCURACY;*
- *NEM3D-1A IS ALSO SIMPLE AND FAST;*
- *NEM3D-1A PROGRAM INDICATED STABILITY AND CONVERGENCE OF THE METHOD TO THE EXPECTED SOLUTION;*

REFERENCES

1. "A Consistent Nodal Method for the Analysis of Space-Time Effects in Large LWR's," <https://www.oecd-nea.org/nsd/docs/1975/csni75-5.pdf> (1975).
2. J. J. Dorning, Modern coarse-mesh methods — a development of the '70's. Proc. Topl. Mtg. Computational Methods of Nuclear Engineering, *American Nuclear Society*, Williamsburg Virginia, 23–25 April, Vol. 1, pp. 1-3 (1979).
3. H. Finnemann, F. Bennewitz, M. R. Wagner, "Interface Current Techniques for Multidimensional Reactor Calculations," *Atomkenergie*, Erlangen Germany, Vol. 30, pp.123-125 (1977).
4. J. J. Duderstadt, L. J. Hamilton, *Nuclear Reactor Analysis*, John Wiley & Sons, New York USA (1976).
5. "Argonne code center: benchmark problem book," <https://www.osti.gov/servlets/purl/5037820> (1977).
6. "Solution of the multigroup neutron diffusion equations by finite element method," https://orbit.dtu.dk/files/56550414/RIS_M_1809.pdf (1975).
7. "Static Three-Dimensional ARROTA Benchmarking," <https://www.osti.gov/servlets/purl/527546> (1985).
8. "Test of the Diffusion Theory Difference in Slab Geometry (Computer Code VANCER)," <https://www.osti.gov/servlets/purl/6805732> (1978).
9. "Three-Dimensional Static and Dynamic Reactor Calculations by the Nodal Expansion Method," <https://orbit.dtu.dk/files/170742623/RISOR496.pdf> (1985).
10. T. J. Downar, D. Xu, W. Lee, T. Kozlowski, PARCS: Purdue Advanced Reactor Core Simulator, International Conference on the New Frontiers of Nuclear Technology: Reactor Physics, Safety and High-Performance Computing, PHYSOR, Seoul, Korea, (2002).
11. "Validation of NESTLE Against Static Reactor Benchmark Problems," <https://www.osti.gov/servlets/purl/527546> (1995).
12. "VENTURE: A Code Block for Solving Multigroup Neutronics Problems Applying the Finite-Difference Diffusion-Theory Approximation to Neutron Transport," <https://www.osti.gov/servlets/purl/4158202> (1975).

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