



## Development and verification of a higher-order mathematical adjoint nodal diffusion solver



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### ABSTRACT

In this paper, we derive a mathematical formulation of the higher order adjoint NEM-M2B2 equations by preconditioning the nodal interface neutron currents equations of the forward equations system, and by using the Lagrangian Multipliers analysis method. In the NEM-M2B2 system of equations, the quadratic transverse leakage approximation is used to model the leakage of neutrons between each node in the system. The solution of the adjoint equation can be used to perform adjoint-based predictive sensitivity/perturbation analysis. As an example, we use the mathematical adjoint solution as sensitivity weighting for predicting the response of the IAEA-3D benchmark's eigenvalue to a perturbation in the independent parameters of the system (i.e., cross-sections). We also derive perturbation equations associated with the particular NEM-M2B2 model we are using. These perturbation-equations are used in predicting the model eigenvalue change without resorting to recalculating the forward NEM-M2B2 system of equations again (labeled as exact calculations). They also enabled construction of a reactivity sensitivity map showing the importance of each calculation node of the benchmark depending on its spatial and spectral coordinates. Perturbations were imposed on both the absorption cross-sections (fast and thermal) and the scattering cross-section of the IAEA-3D benchmark problem. Several verification steps were taken to ensure that the developed mathematical adjoint solver is adequate for adjoint analysis (e.g., commutativity checks, and comparison against exact calculations).

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### 1. Introduction

Since its development in the 1970s, the Nodal Expansion Method (NEM) has been a standard concept widely used for reactor physics calculations of nuclear reactors (e.g., eigenvalue calculation, 3D power shape computation, whole core loading patterns optimizations, etc.). It has now become the standard tool for industrial nuclear reactor core neutronics calculations due to its speed compared to other methods, and due to the good accuracy that it enables. In NEM, either polynomials or analytical solution of the neutron diffusion equation defined within each node of the system are used to approximate the face averaged surface intranodal fluxes (Lawrence, 1986). Nodal methods can also be used and applied to higher order neutron transport equations rather than the neutron diffusion equation (e.g.,  $P_N$ ,  $SP_N$ ,  $S_N$ ) (Lawrence, 1986).

The neutronics equations formulation in this paper follows the rigorous form of NEM that was put forward by Finnemann et al. (1977). A detailed derivation of the forward model can be found

in the referenced paper and it will not be replicated here. We will be using the NEM-M2B2 equations variant of the NEM. In this variant, a quartic polynomial and the moments weighting method is used to approximate the average nodal surface fluxes and to calculate the weighted residuals of the equations, respectively (Finnemann et al., 1977). Quadratic transverse leakage approximation is also used in the NEM-M2B2 equations to model the Transverse Leakage (TL) term inside a node.

One of the main contributions of this paper is related to adjoint-based perturbation analysis. It is important and has been used in many scientific areas that deal with optimization, engineering design, and sensitivity analysis. According to Marchuk (1995), adjoint operators were originally defined by Lagrange in the 1770s. The adjoint concept was however not being applied much until the development of quantum mechanics (Marchuk, 1995), where it became crucial for the mathematical formulation of the perturbation theory used in that field. Adjoint concepts are also used in theory of climate and its changes, as well in mathematically modelling immunology and infectious disease dynamics as explored in Marchuk (1995). Scientific studies pursued in the context of present-day rising concerns, such as global climate change

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