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Original Article

Development of Galerkin Finite Element Method Three-dimensional Computational Code for the Multigroup Neutron Diffusion Equation with Unstructured Tetrahedron **Elements**

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A B S T R A C T

In the present paper, development of the three-dimensional (3D) computational code based on Galerkin finite element method (GFEM) for solving the multigroup forward/adjoint diffusion equation in both rectangular and hexagonal geometries is reported. Linear approximation of shape functions in the GFEM with unstructured tetrahedron elements is used in the calculation. Both criticality and fixed source calculations may be performed using the developed GFEM-3D computational code. An acceptable level of accuracy at a low computational cost is the main advantage of applying the unstructured tetrahedron elements. The unstructured tetrahedron elements generated with Gambit software are used in the GFEM-3D computational code through a developed interface. The forward/adjoint multiplication factor, forward/adjoint flux distribution, and power distribution in the reactor core are calculated using the power iteration method. Criticality calculations are benchmarked against the valid solution of the neutron diffusion equation for International Atomic Energy Agency (IAEA)-3D and Water-Water Energetic Reactor (VVER)-1000 reactor cores. In addition, validation of the calculations against the P_1 approximation of the transport theory is investigated in relation to the liquid metal fast breeder reactor benchmark problem. The neutron fixed source calculations are benchmarked through a comparison with the results obtained from similar computational codes. Finally, an analysis of the sensitivity of calculations to the number of elements is performed.

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1. Introduction

Numerical methods have played a vital role in science and engineering in terms of solving and analyzing problems. Solutions to engineering problems can more easily be achieved with the help of computers. The importance of numerical methods in an analysis is due to several factors. First, most natural phenomena can best be described by differential equations with varying boundary conditions the solutions of which cannot be obtained by analytical means, except in very simple cases. Significant improvements have been made in various numerical techniques such that problems can be solved at a low cost and within a short span of time. Due to the absence of automatic computation, progress in the development of numerical methods was quite slow before the 1940s. With the arrival of high-speed computers, engineers and scientists succeeded in exploiting numerical methods. During the mid-1950s, the finite element method grew out of a number of intuitive procedures and associated mathematical techniques. Prior to its conception, the finite difference method held a dominant position in the numerical solution of continuum problems [\[1,2\].](#page--1-0) Today, both of these methods are equally important and have their own advantages and disadvantages. However, certain problems are more amenable to the finite element method than to the finite difference method. Other numerical methods, such as nodal $[3-5]$ $[3-5]$ $[3-5]$ and finite volume $[6,7]$, may also be used to solve neutron diffusion equations.

The finite element method is a computational technique for obtaining approximate solutions to the partial differential equations that arise in scientific and engineering applications. It is a general technique for constructing approximate solutions to the boundary value problems. The methods involve dividing the domains of a solution into a finite number of elements. Variational schemes employing a weighted residual approach or an extremum principle-based approach are used to construct an approximate solution over the collection of finite elements. Owing to the generality and richness of the ideas underlying the method, it has been used with remarkable success in solving a wide range of problems in virtually all areas of engineering and sciences. In contrast to the older finite difference methods that are usually based on differential formulations, the finite element method is based on integral formulations. In the finite element method, the solution is approximated by local piecewise polynomial trial functions within an element. Expansion coefficients are then determined by applying either weighted residual or variational approaches. Finite elements have been utilized in different ways to solve neutron diffusion equations. In some formulations a weighted residual approach is adopted, while in others variational approaches are considered, with a combination of the applications of the finite elements to one or more of the independent variables. In the weighted residual approach, the integral form of the original integrodifferential equation is considered and expanded in a set of finite element basis functions. The integral form is obtained by multiplying the original equation by an arbitrary weighting function. If the arbitrary weighting functions are the finite element basis functions, then the approach is called the Galerkin technique [\[8\].](#page--1-0)

The neutron diffusion theory is the most widely used method in the analysis of criticality of nuclear reactors. Consideration of criticality is generally referred to as an eigenvalue problem for the multigroup neutron diffusion equation for which the solution provides the eigenvalue effective multiplication factor, neutron flux distribution, and power profiles in reactor cores. An adequate calculation may be obtained from the solution of a three-dimensional (3D) neutron diffusion equation using the aforementioned numerical methods. The finite element method has always been a fundamental numerical technique in reactor core calculations. It has continuously been improved over decades, starting from primal implementation in neutron diffusion equations up to modern implementations with Raviart-Thomas, hybrid, hadaptivity, and response matrix bases $[9-11]$ $[9-11]$.

In general, in most applications, the finite element method is preferred to its principal alternative, the finite difference method, due to its flexibility in the treatment of curved or irregular geometries and the high rates of convergence attainable by the use of high-order elements. Several researchers have tried to develop convenient methods for solving 3D multigroup neutron diffusion equations using finite element methods in 3D geometries. For example, Wang and collogues [\[11\]](#page--1-0) presented 3D h-adaptivity for multigroup neutron diffusion equations. The solution of partial differential equations obtained using adaptive mesh refinement gives significantly higher accuracy at a reduced numerical cost. In another paper, Hébert ^{[\[9\]](#page--1-0)} presented how the Raviart-Thomas-Schneider finite element method was implemented for solving the diffusion equation in hexagonal 3D geometry. The Raviart-Thomas-Schneider method was based on a dual variational formulation defined over lozenges with a Piola transformation of the polynomial basis. An efficient Alternating Direction Implicit (ADI) numerical technique was set up to solve the resulting matrix system.

In the present study, the Galerkin finite element method (GFEM) [\[12\],](#page--1-0) a weighted residual method, is used to solve the multigroup neutron diffusion equation in any arbitrary 3D geometries such as rectangular and hexagonal reactor cores. The unstructured tetrahedron elements generated by Gambit are used to discretize the equations. Indeed, a key advantage of the unstructured tetrahedron elements is their superiority in mapping the curved boundaries or material interfaces in 3D geometries. In addition, the running time of computation code and the accuracy of the calculation may be optimized using proper unstructured tetrahedron elements. For several reasons, such as precision and simplicity, the Galerkin method has been used widely in the development of computer codes for solving diffusion or transport equations in different geometries [\[12,13\].](#page--1-0) The main advantage of the GFEM is that the definition of boundary conditions in this method is easier than that in the other methods [\[14\].](#page--1-0) The mentioned reasons convinced us to use the GFEM for solving the multigroup forward/adjoint neutron diffusion equation in 3D geometries.

An outline of the remainder of this contribution is as follows: In Section [2,](#page--1-0) we briefly introduce the numerical solution of the multigroup neutron diffusion equation in 3D geometries used to solve the forward/adjoint neutron diffusion equation. Section [3](#page--1-0) presents the main specification of the IAEA-3D [\[15\]](#page--1-0), VVER-1000 [\[16\]](#page--1-0), and liquid metal fast breeder reactor (LMFBR) [\[17\]](#page--1-0) benchmark problems. Numerical results and an analysis of the sensitivity of calculations to the

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