

# Discontinuous finite element formulations for neutron transport in spherical geometry



Mehmet Mercimek\*, H. Atilla Özgener

Energy Institute, Istanbul Technical University, Ayazağa Campus, 34469 Maslak, Istanbul, Turkey

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## ABSTRACT

We have developed the linear and quadratic Galerkin discontinuous finite element methods for the solution of both time-independent and time-dependent spherical geometry neutron transport problems. Discrete ordinates method is used for the angular discretization while the implicit method is utilized for temporal discretization in time-dependent problems. In order to assess the relative performance of the newly developed linear and quadratic discontinuous finite element spatial differencing methods relative to the previously developed linear discontinuous finite element and diamond difference discretizations, a computer code is developed and numerical solutions of the neutron transport equation for some benchmark problems are obtained. These numerical applications reveal that the newly developed quadratic discontinuous finite element method produces the most accurate results while the newly developed linear discontinuous finite element method follows as the second best discontinuous finite element method.

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## 1. Introduction

The discontinuous finite element method (DFEM) is among the most flexible numerical methods in discrete ordinates ( $S_N$ ) formulations of neutral particle transport. The method was first introduced for the solution of the time-independent neutron transport equation (Reed and Hill, 1973). The developments in general DFEM have been recently reviewed (Cockburn et al., 2000; Cockburn, 2001). DFEM uses piecewise polynomial spaces similar to the (continuous) finite element method (FEM) but with relaxed continuity conditions at interelement boundaries. Trial functions can be chosen so that the field variable, its derivative or both are discontinuous across interelement boundaries. The method includes as its subsets both the FEM and finite difference methods (FDM). It has been reported that DFEM has the advantages of both the FDM and FEM (Li, 2006).

Several computer programs have been developed for neutron transport using the linear discontinuous finite element method (LDFEM) (Reed et al., 1973, 1977; Seed et al., 1977, 1978; Wareing et al., 1996). ONETRAN and TIMEX are examples of these codes for the solution of time-independent and time-dependent transport, respectively (Hill, 1975, 1977; Hill et al., 1976). Recently, the LDFEM formulation, similar to the formulation used in TIMEX, has been employed in spherical geometry (Hong et al., 2010). In another study, piecewise LDFEM is applied to the two-dimensional

cylindrical geometry and accurate results are reported (Bailey et al., 2009).

Higher-order DFEM has been extensively investigated in other disciplines (Hesthaven and Warburton, 2008). But, in neutron transport, limited research has been carried out using elements of higher degree. For example, a higher order DFEM has been developed for the time-independent transport equation by using hierarchical basis functions (Wang, 2009). In another study, higher order DFEM was used in both angular and spatial differencing for the solution of time-independent, pure absorber problems, in spherical geometry (Machorro, 2007). A comparison of linear and quadratic DFEM for triangular lattice discrete ordinates calculations was also presented (Chang and Warsa, 2007).

The first objective of this study is to reformulate and implement LDFEM for time-independent and time-dependent neutron transport problems in spherical geometry. The time dependent formulation will be based on the prompt neutron transport equation and the delayed neutron effects will not be treated. Our LDFEM formulation will be henceforth called as LD2 while the spherical geometry LDFEM formulation of TIMEX will be called as LD1 (Hill, 1975, 1977; Hill et al., 1976; Hong et al., 2010).

The second objective of this study is to develop a higher-order DFEM formulation for the solution of neutron transport problems in spherical geometry both for the time-independent and time dependent variety. As a higher-order DFEM, we employ the quadratic discontinuous finite element method (QDFEM).

In this paper, we will first present the derivations of linear systems of equations for LD1, LD2 and QDFEM for the solution of time-independent and time-dependent prompt neutron transport

\* Corresponding author. Tel.: +90 538 641 90 36.

E-mail addresses: [mercimek@itu.edu.tr](mailto:mercimek@itu.edu.tr) (M. Mercimek), [ozgenera@itu.edu.tr](mailto:ozgenera@itu.edu.tr) (H. Atilla Özgener).

equation in spherical geometry. We will use the classical Galerkin method in which the weight functions are taken to be the same as the shape functions which are Lagrange type polynomials with compact support in LD2 and QDFEM. We have developed a discrete ordinates computer code, SPDOT, in which the spatial discretization can be carried out using diamond difference (DD), LDFEM (LD2) or QDFEM approaches. Also, we have developed another version of the SPDOT for LD1 calculations of this study. Since DD formulation is given elsewhere (Lewis and Miller, 1984), it would not be repeated here.

Implicit method is used for the temporal differencing in time-dependent problems. Both codes are run for several time-independent and time-dependent benchmark problems to assess the performance of various spatial discretization methods in the solutions of neutron transport problems by the discrete ordinates method.

The remainder of this paper is organized as follows. In Section 2, LDFEM and QDFEM formulations are described. Section 2.1 describes the discrete ordinate spherical geometry transport equation and the weighted residual forms of this equation for spatial discretization methods LD1, LD2 and QDFEM. LD2 and QDFEM approximations are given in Section 2.2 while LD1 approximation is given in Section 2.3. Finite element formulations of LDFEM and QDFEM are given in Sections 2.4 and 2.5 respectively. In Section 2.6, time differencing scheme is applied to the derived equations in previous sections. Section 2.7 describes the boundary condition applied at the centre of the sphere. In Section 3, numerical results of DD, LDFEM and QDFEM are compared. Section 3.1 is devoted to time-independent criticality problems while Section 3.2 is for the analysis of time-dependent behavior of the methods. In the final section, some concluding remarks are given.

## 2. Discontinuous finite element formulation

First, we describe the linear and quadratic discontinuous finite element methods for the spatial discretization of the time-independent within group neutron transport equation in spherical geometry using the discrete ordinates form. Details of the sweep of the space-angle mesh in the spherical geometry discrete ordinates neutron transport are given elsewhere (Lewis and Miller, 1984).

### 2.1. The discrete ordinates spherical geometry transport equation and the weighted residual forms

The spherical geometry time-independent within group neutron transport equation in conservation form is written as:

$$\mu \frac{\partial(r^2\psi)}{\partial r} + r \frac{\partial[(1-\mu^2)\psi]}{\partial \mu} + r^2\sigma(r)\psi(r, \mu) = r^2q(r, \mu) \quad (1)$$

We omit group indices for the sake of clarity. In Eq. (1), angular variable  $\mu$  denotes the radial component of particle direction, spatial variable  $r$  is the distance from the origin,  $\psi$  is the angular neutron flux,  $\sigma$  is the macroscopic total cross section and  $q$  is the emission density which includes the inhomogeneous (or fixed) source, scattering source and fission contribution to the group source.

In order to develop the discrete ordinates equations, the angular domain  $\mu \in [-1, +1]$  is discretized into  $M$  ( $m = 1, 2, \dots, M$ ) quadrature points  $\mu_m$  with weights  $w_m$ . We introduce the spherical geometry discrete ordinates form of transport equation by introducing the angular differencing coefficients,  $\alpha_{m+1/2}$  and  $\alpha_{m-1/2}$  (Lewis and Miller, 1984) into Eq. (1):

$$\begin{aligned} \mu_m \frac{\partial(r^2\psi_m)}{\partial r} + \frac{2r}{w_m} [\alpha_{m+1/2}\psi_{m+1/2}(r) - \alpha_{m-1/2}\psi_{m-1/2}(r)] + r^2\sigma(r)\psi_m(r) \\ = r^2q_m(r) \end{aligned} \quad (2)$$

Diamond differencing (DD) in angle is used to relate the edge ( $\psi_{m+1/2}(r)$ ,  $\psi_{m-1/2}(r)$ ), and cell-centered ( $\psi_m(r)$ ) angular fluxes:

$$\psi_{m+1/2}(r) \cong 2\psi_m(r) - \psi_{m-1/2}(r) \quad (3)$$

In order to make the derivation easier, the local spatial variable  $\xi \in [-1, +1]$ , is introduced as:

$$r(\xi) = \bar{r}_i + \frac{\Delta r_i}{2}\xi \quad (4)$$

where  $\bar{r}_i = (r_{i-1/2} + r_{i+1/2})/2$  and  $\Delta r_i = r_{i+1/2} - r_{i-1/2}$  represent the midpoint and interval size of the  $i$ th mesh interval which is assumed to be homogeneous. Fig. 1 illustrates the arrangement of angular flux node points in  $(i, m)$ th cell of the spherical domain.

Using Eqs. (3) and (4), Eq. (2) is written with respect to local variable as:

$$\begin{aligned} \frac{2\mu_m}{\Delta r_i} \frac{d}{d\xi} [r^2(\xi)\psi_m(\xi)] + \frac{2r(\xi)}{w_m} [2\alpha_{m+1/2}\psi_m(\xi) - (\alpha_{m+1/2} + \alpha_{m-1/2})\psi_{m-1/2}(\xi)] \\ + \sigma_i r^2(\xi)\psi_m(\xi) = r^2(\xi)q_m(\xi), \quad -1 \leq \xi \leq 1 \end{aligned} \quad (5)$$

#### 2.1.1. Weighted residual form for the LD2 and QDFEM formulations

LD2 and QDFEM formulations are based directly on Eq. (5). Since  $\psi_m(\xi)$  and  $\psi_{m-1/2}(\xi)$  are approximate solutions then they cannot be expected to satisfy Eq. (5) at all points in the mesh interval. We require that these approximate solutions satisfy Eq. (5) only in an integral sense by integrating Eq. (5) after multiplication with a weight function,  $w(\xi)$ , and arrive at the weighted residual (Galerkin) form:

$$\begin{aligned} \frac{2\mu_m}{\Delta r_i} \int_{-1}^1 w(\xi) \frac{d}{d\xi} [r^2(\xi)\psi_m(\xi)] d\xi \\ + \frac{2}{w_m} \left[ 2\alpha_{m+1/2} \int_{-1}^1 w(\xi)r(\xi)\psi_m(\xi)d\xi - \alpha_m \int_{-1}^1 w(\xi)r(\xi)\psi_{m-1/2}(\xi)d\xi \right] \\ + \sigma_i \int_{-1}^1 w(\xi)r^2(\xi)\psi_m(\xi)d\xi \\ = \int_{-1}^1 w(\xi)r^2(\xi)q_m(\xi)d\xi \end{aligned} \quad (6)$$

where

$$\alpha_m = \alpha_{m+1/2} + \alpha_{m-1/2} \quad (7)$$

Applying integration by parts to the first term on the left hand side of Eq. (6), we obtain:

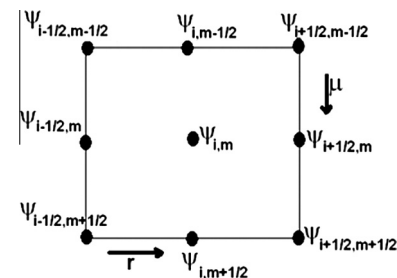


Fig. 1. A unit cell for DFEM formulations.

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