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An arbitrary geometry finite element method for the adjoint neutron transport equation

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ABSTRACT

In this paper a variational formulation for the adjoint even parity neutron transport equation (NTE) based on the generalized least squares method is adopted. The so-called P_N method or expansion via Spherical Harmonics Polynomials (SHPs) is then summoned to treat the angular dependency of the equation while Finite Element Method (FEM) is invoked for the spatial domain. Based on our matrix form approach, it is shown that the scalar adjoint flux, $\phi^{\dagger}(\mathrm{r})$, can be determined through an efficient approach solely or in parallel with the scalar forward flux, $\phi(\mathbf{r})$. Eigenvalue problems as well as detector readings are of most useful applications of the adjoint calculation which are also discussed in this survey. To verify the equations we upgraded our Even parity Neutron TRANSport code, ENTRANS, with an adjoint solver which is capable of handling one-, two- and three-dimensional problems of arbitrary geometry. Ability to cover any order of multigroup scattering anisotropy (with or without up-scattering) as well as higher order elements is also embedded in the ENTRANS. Finally, several test cases are examined against reference results to illustrate the accuracy and efficiency of the proposed approach.

1. Introduction

Adjoint or *dual* space alongside the *regular* or *direct* space brings a variety of interesting physical and mathematical concepts which expands our insight over a purely physical phenomenon. It also serves as a quite efficient mathematical tool empowering numerical experts and simulating societies to perform numerical analysis via a low cost approach. Increasing application of adjoint equations beside direct calculations has made Marchuk (1995) exaggeratedly believe in adjoint statement of the problems as "*part of our life*". Today, adjoint approach has proved its usefulness in many branches of science including inverse engineering, optimization, sensitivity analysis, meteorology, earth science, natural resource explorations, mechanical design etc. Rigorous and precise studies on adjoint operator and space can be found in many mathematical physics literature including (Arfken and Weber, 2005; Cacuci and Ionescu-Bujor, 2010; Marchuk, 1995, 2006).

In reactor theory however, adjoint function plays an important role in neutronic design of a reactor since it carries a valuable quantity called *neutron importance.* In a source-detector problem approximately all reactor scientist including (Bell and Glasstone, 1970; Lewins, 1965; Lewis and Miller, 1984) have interpreted the adjoint flux, $\psi^{\dagger}(\mathbf{r}, E, \mathbf{\Omega})$ as the expected response of a detector at $(\mathbf{r}, E, \mathbf{\Omega})$. However, various but equivalent statements has been proposed for the definition of neutron importance in a reactor. Based on Lewins (1960) statement the adjoint equation was first introduced to the reactor field by Wigner (1945) through a perturbation analysis, but it was Soodak (1948) who first interpreted the widely accepted term "importance" as the "*ultimate progeny of one neutron*". While Hurwitz (1948) normalized the adjoint function in a way and called it the *iterated fission probability*, Wachspress (1964) interpreted it as the relative probability of one neutron goes fission. Irving (1971) turned the $\psi^{\dagger}(\mathbf{r}, E, \mathbf{\Omega})$ as the "*value of a particle leaving a collision*", meanwhile Zweifel (1973) related the importance of a neutron to the amount of power level variation due to that neutron, so that insertion of a neutron in a position with high (low) value adjoint flux causes more (less) increase in power level hence different importance. Bell and Glasstone (1970) believe that in an exactly critical reactor $\psi_0^{\dagger}(\mathbf{r}, E, \mathbf{\Omega})$ can be interpreted as "*the importance of a neutron at* $(\mathbf{r}, E, \mathbf{\Omega})$ *for establishing the fundamental mode*". The accurate and generalized definition of adjoint flux and importance of a neutron in a time-dependent sense however, proposed by Lewins (1960) who related the importance of one neutron to its contribution to an arbitrary detectable process at a final time t_f in the sense of a Gibbsian ensemble. This definition is based upon an axiom which states that the importance of one

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neutron or precursor at time t, before t_f, is equal to the total importance of its probable progeny at any later time before t_f (Lewins, 1960). Therefore, many of authors take this definition as the reference and express the adjoint flux, $\psi_0^\dagger(\mathbf{r},E,\mathbf{\Omega})$, in a critical reactor as the asymptotic increase in the number on neutrons due to injection of one neutron at $(\mathbf{r},E,\mathbf{\Omega})$ (Akcasu et al., 1971; Henry, 1980; Stacey, 2007).

Since recognition, adjoint calculation has been successfully exploited in different fields of reactor analysis e.g. perturbation theory, variational methods, shielding design as well as neutron kinetic theory (Prinja and Larsen, 2010). Also, adjoint sensitivity analysis procedure (ASAP) has proved superiority and robustness over its forward counterpart (FSAP) in many applications (Cacuci, 2005; Cacuci et al., 2005). In addition to noise analysis (Malmir and Vosoughi, 2015; Malmir et al., 2010; Van Dam, 1977) adjoint approach has also been utilized in damage assessment as well as calculation of some integral properties regarding NTE with no significant spread (Ronen, 1976; Williams, 1978, 1979). Moreover, adjoint- or dual-based adaptive mesh refinement (AMR) has newly attracted massive interests of numerical experts due to its excellent ability to optimally refine the spatial domain upon a goal-oriented approach, hence noticeable saving in the number of unknowns. This approach has penetrated the numerical solution of diffusion and transport equations as well with hopeful results (Baker et al., 2013; Lathouwers, 2011a,b; Merton et al., 2014). Adjoint solution coupled with the forward results has also incorporated in achieving a deep physical insight in shielding design and material performance analysis via the outstanding *theory of "contributon" transport* or equivalently *spatial channel theory* which never would realized with regular or dual approach solely (Painter et al., 1980; Seydaliev and Henderson, 2008; Williams, 1991, 1994; Williams and Engle, 1977). Monte Carlo field, on the other hand, has widely been empowered by the adjoint calculations which are excluded from this investigation due to focusing on deterministic approach only.

Despite extensive coverage of adjoint problem in many reactor textbooks, discussions are usually limited to the diffusion equation or utmost first order NTE with usually a S_N technique for its angular treatment. While normally the amount of published works on the adjoint NTE is not comparable with those focused on the forward NTE, the situation gets much worse for the subject of even parity adjoint NTE. Paucity of papers evidences that second order or even parity adjoint NTE has not been widely studied up to know. The only related variational formulation of even parity adjoint NTE can be found in (Ackroyd et al., 1980) followed by De Oliveira (1986) without much discussion. Although both references are valuable and original, the former leaves the case with no attempt to open the issue exclusively and while in the latter it is claimed that the developed code (EVENT) is able to solve even parity adjoint NTE, no evidence is provided for and no signal is received through its subsequent developments e.g. (De Oliveira, 1987; de Oliveira and Goddard, 1997). Later however, adjoint analysis was employed as a part of *a posteriori* error estimator in development of adaptive code EVENT (Park and de Oliveira, 2009). In a separate work, while Issa et al. (1986) mention to the even parity NTE embedded in code FELTRAN, only a 1D fixed source problem is investigated as an adjoint benchmark and no explicit formulation is presented for adjoint problem.

Using the even parity approach considerably reduces the amount of numerical cost (Ackroyd, 1997; Lewis, 2010); Besides, it can also be utilized to carry out the adjoint flux over a nuclear system either for an eigenvalue search problem or a source-detector case. In addition, variational principles formulation enjoy from the appealing feature of providing hi-accuracy results on the basis of nearly rough trial functions (Zweifel, 1973), forming a suitable launch for solution of NTE. Therefore, a variational principle for the adjoint even parity NTE may become a collection of motivations for those interested in optimal solution techniques; an idea to be probed in this paper.

In our previous papers (Abbassi et al., 2011; Yousefi et al., 2017, Unpublished Results) we comprehensively discussed the application of SHPs coupled with FEM for solution of second order NTE based on our matrix approach. Furthermore, the code ENTRANS was introduced with capability to solve multi-group even parity NTE in an arbitrary multi-dimensional geometry boosted with high order finite elements as well as any order anisotropic scattering support. Recently, we upgraded ENTRANS with an alternative solver to obtain the adjoint flux for the same problems solely or in parallel with the forward flux. Consequently, eigenvalue search problems as well as user defined adjoint sources can now be treated by the ENTRANS.

The rest of this paper is organized as follows. In Section 2 we review some theoretical aspects of adjoint NTE as well as different trends in deriving final adjoint formulation. Variational principle of adjoint even parity neutron transport is discussed in Section 3 while the numerical approximations adopted for maximizing the principle is investigated in Section 4. An applicable procedure for solution of multigroup adjoint even parity NTE is proposed in Section 5 while Section 6 is allotted for the numerical examples performed via our upgraded code (ENTRANS) over eigenvalue and fixed source problems. We eventually finalize this article with a conclusion in Section 7.

2. Preliminaries

The steady-state energy dependent NTE can be cast as (Lewis and Miller, 1984)

$$\begin{aligned}&\mathbf{\Omega}.\nabla\psi(\mathbf{r},E,\mathbf{\Omega})+\sigma_t(\mathbf{r},E)\psi(\mathbf{r},E,\mathbf{\Omega})-\int_0^{E_{max}}\int_{4\pi}\sigma_s(\mathbf{r},E'\\&\to E,\mathbf{\Omega}.\mathbf{\Omega}')\psi(\mathbf{r},E',\mathbf{\Omega}')d\Omega'dE'\\&=\frac{1}{k_{\text{eff}}}\frac{\chi(E)}{4\pi}\int_0^{E_{max}}\upsilon\sigma_f(\mathbf{r},E\prime)\psi(\mathbf{r},E')dE'+Q(\mathbf{r},E,\mathbf{\Omega}).\end{aligned}\tag{1}$$

where $Q(\mathbf{r},E,\mathbf{\Omega})$ is the external particle source density (in fixed source problems) and k_{eff} is the effective multiplication factor of neutrons (in eigenvalue search problems). Using the famous Lagrange identity (Marchuk, 1995),

$$\langle\psi^\dagger,\hat{\mathcal{O}}\psi\rangle=\langle\hat{\mathcal{O}}^\dagger\psi^\dagger,\psi\rangle\tag{2}$$

one can derive the steady-state energy dependent adjoint NTE as (Bell and Glasstone, 1970; Lewis and Miller, 1984)

$$\begin{aligned}&-\mathbf{\Omega}.\nabla\psi^\dagger(\mathbf{r},E,\mathbf{\Omega})+\sigma_t(\mathbf{r},E)\psi^\dagger(\mathbf{r},E,\mathbf{\Omega})-\int_0^{E_{max}}\int_{4\pi}\sigma_s(\mathbf{r},E\\&\to E',\mathbf{\Omega}.\mathbf{\Omega}')\psi^\dagger(\mathbf{r},E',\mathbf{\Omega}')d\Omega'dE'\\&=\frac{1}{k^\dagger_{\text{eff}}}\upsilon\sigma_f(\mathbf{r},E)\int_0^{E_{max}}\chi(E')\psi^\dagger(\mathbf{r},E')dE'+Q^\dagger(\mathbf{r},E,\mathbf{\Omega}).\end{aligned}\tag{3}$$

Recalling the fact that in eigenvalue search problems $k^\dagger_{\text{eff}}=k_{\text{eff}}$, for the above equation it is set:

(a) $\psi^\dagger(\mathbf{r},E,\mathbf{\Omega})$, the energy dependent angular adjoint flux "function" (not a density or distribution generally);
(b) $Q^\dagger(\mathbf{r},E,\mathbf{\Omega})$, an arbitrary external adjoint (importance) source function; and finally,
(c) $\psi^\dagger(\mathbf{r},E)$, the angular averaged energy dependent adjoint function at $(\mathbf{r},E)$ defined by (Van Dam, 1977)