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Goal-based h-adaptivity of the 1-D diamond difference discrete ordinate method

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ABSTRACT

The quantity of interest (QoI) associated with a solution of a partial differential equation (PDE) is not, in general, the solution itself, but a functional of the solution. Dual weighted residual (DWR) error estimators are one way of providing an estimate of the error in the QoI resulting from the discretisation of the PDE.

This paper aims to provide an estimate of the error in the QoI due to the spatial discretisation, where the discretisation scheme being used is the diamond difference (DD) method in space and discrete ordinate (S_N) method in angle. The QoI are reaction rates in detectors and the value of the eigenvalue (K_{eff}) for 1-D fixed source and eigenvalue (K_{eff} criticality) neutron transport problems respectively. Local values of the DWR over individual cells are used as error indicators for goal-based mesh refinement, which aims to give an optimal mesh for a given QoI.

1. Introduction

Goal-based dual weighted residual (DWR) methods have already been applied to the field of neutron transport for solvers that discretise in space using the finite element method, a method for which the development of DWR error estimates is very mature. Despite the increased use of finite element codes in the industry, many full scale production codes use the diamond difference (DD) method for solving the discrete ordinate (S_N) angular discretisation of the neutron transport equation. Examples include the PARTISN code developed at LANL [1], the Denovo S_N module in the SCALE code (developed at ORNL) [2] and the DOMINO solver that is a part of EDF's COCAGNE code [3]. Reliable error estimates are desirable to ensure that the error in a calculated quantity of interest (QoI) due to spatial discretisation is within a prescribed tolerance. The derivation and application of rigorously derived goal-based DWR error estimators has not yet been applied to the diamond difference method.

In addition to this, full core pressurised water reactor (PWR) eigenvalue (K_{eff}) problems often require the solution of a large number of degrees of freedom (number of unknowns) due to the discretisation of a seven dimensional phase space. $\mathcal{O}(10^{12})$ DoF were used recently in the DOMINO solver [3]. Being able to reduce this number by only refining the spatial mesh where needed, for a specific QoI, would also be useful in producing computationally efficient solutions. Using

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goal-based DWR error indicators to guide adaptive mesh refinement (AMR) would be essential in this case since it has been shown that AMR using error indicators that aim to reduce the global error in the forward solution can, in certain circumstances, fail to yield an accurate answer to the QoI compared to uniform refinement (see [4, p. 783], [5, p. 306], [6, p. 3]).

The focus of this paper is the development, implementation and application of goal-based DWR error estimates and AMR to the 1-D DD spatial discretisation of the S_N discretised neutron transport equation. This is a necessary step before extending these methods to multidimensional problems. The estimators are derived for fixed source and eigenvalue (K_{eff} criticality) problems and the QoI can be linear or non-linear (detector response and the value of K_{eff} respectively).

Many researchers in reactor physics have implemented goal-based error estimation and mesh refinement techniques to finite element (FE) approximations of the neutron transport equations. Wang and Ragusa in particular have investigated goal-based error estimators and indicators for the spatial error in the diffusion approximation [7], simplified P_N (SP_N) equations (along with Turcksin and Bangerth) [5] and the S_N approximation of the neutron transport equation [4], where the spatial dimension was discretised using either continuous (for diffusion and SP_N) or discontinuous (for S_N transport) FEs.

Lathouwers applied the DWR goal-based scheme described in a text book by Bangerth and Rannacher [8] to drive h-adaptation in the discontinuous FE spatial discretisation of the discrete ordinate (S_N) angularly discretised transport equation (DG-FEM-S_N). Both detector functions [9] and eigenvalues [10] were investigated as QoI. The difference between Lathouwers's work and Wang and Ragusa's work for S_N transport is that Lathouwers calculates the DWR for each angle and integrates via quadrature, whereas Wang and Ragusa take the norm of the difference between the approximate solution and a reference solution (the solution obtained on a refined/higher order mesh) of either the scalar flux or current, then weight this by the norm of the same error estimate for the adjoint solution [4].

Goffin et al. [11] also applied a DWR h-adaptive mesh refinement scheme to the transport equations with the eigenvalue being the QoI. In this case the angular discretisation used was the spherical harmonics (P_N) discretisation with a sub-grid scale finite element spatial discretisation. This work was later extended to provide both regular and goal-based angular adaptivity, by allowing the order of the spherical harmonic (P_N) expansion to be different at each node of the mesh for each energy group [12].

An error indicator for spatial refinement of the Arbitrarily High Order Transport Method of the Nodal type (AHOT-N) was derived by Duo et al. [13], with the aim of reducing the global L^2 error norm. Although duality arguments are used in the derivation of the error estimator, a dual solution is not required for its evaluation, since the error in the adjoint solution is replaced by bounds to that term in terms of the forward solution. Similar arguments were used by Park et al. for spatial and angular adaptivity of the of the FE-P_N discretisation of the even parity equations [14]. It is noted that, in both of these cases, the goal quantity is limited to be the L^2 error, hence the mesh which results may not be optimal for other quantities of interest.

Researchers outside of the neutronics field have investigated how to apply goal-based error estimators to methods other than FEs [15]. Giles and Pierce lay out the theory for general discretisation schemes noting that the function given by a FE solution could be used, or a function could be fit through nodal values of other discretisation schemes [16,17]. Chen et al. take a similar approach to presenting a general functional analytic framework for the DWR (goal-based) *a posteriori* error estimation for general discretisation methods, but handle the hyperbolic case more rigorously [18].

Venditti and Darmofal obtain a discrete adjoint equation from the discretised forward equations rather than discretising the continuous adjoint equations [19]. Kuzmin et al. also employed the technique of obtaining a DWR method from an arbitrary numerical scheme by deriving a finite element interpolant of the resulting values [20,21]. Some attempts have been made to reformulate difference schemes as variational problems so that a variation on the DWR scheme used in FE can be employed. Collins et al. applied this idea to the Lax–Wendroff finite difference scheme [22].

This paper extends the work of Chen et al. [18] to the system of coupled S_N equations that are then discretised by the DD method. Chen et al. mention that finite volume (FV) schemes do not require the adjoint solution to be approximated in a space that is larger than the forward solution since FV schemes "do not naturally fit into variational forms" [18, p. 70]. We show that in the 1D-DD scheme, Galerkin orthogonality applies to the test functions, which are in a different space than the approximate forward solution. It is for this reason that Galerkin orthogonality does not apply to the adjoint solution calculated on the same mesh as the forward equation (see section 4.4). We also show that, for the DD scheme, the discretised adjoint equations must be derived from the continuous adjoint equations, not obtained by transposing the discretised forward equations as in the work of Venditti et al. [19].

All goal-based DWR schemes require the solution of both a forward and an adjoint equation. When error estimation is coupled with mesh refinement, the computational overhead of calculating the adjoint solution is often more than made up for by the saving made by the reduction in the number of DoF in the system. In all Bubnov–Galerkin FE cases the adjoint solution must be calculated on a mesh that is more refined than the forward equation due to Galerkin orthogonality [8–10]. Some variants of the goal-based method involve calculating the solution on two separate meshes for both the forward and adjoint equations [4]. This paper shows that for the DD equations, only one forward and one adjoint solution is required, and that in almost all cases analysed here, calculating an adjoint solution on the same mesh as the forward is sufficient to give a good error indicator for refinement. In most cases, the accuracy of the overall error estimation is also sufficient in this case.