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Goal-based angular adaptivity applied to the spherical harmonics discretisation of the neutral particle transport equation

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ABSTRACT

A variable order spherical harmonics scheme has been described and employed for the solution of the neutral particle transport equation. The scheme is specifically described with application within the inner-element sub-grid scale finite element spatial discretisation. The angular resolution is variable across both the spatial and energy dimensions. That is, the order of the spherical harmonic expansion may differ at each node of the mesh for each energy group. The variable order scheme has been used to develop adaptive methods for the angular resolution of the particle transport phase-space. Two types of adaptive method have been developed and applied to examples. The first is regular adaptivity, in which the error in the solution over the entire domain is minimised. The second is goal-based adaptivity, in which the error in a specified functional is minimised. The methods were applied to fixed source and eigenvalue examples. Both methods demonstrate an improved accuracy for a given number of degrees of freedom in the angular discretisation.

1. Introduction

The Boltzmann transport equation governs the transport of fundamental particles. The equation is solved to obtain the average statistical distribution of a given particle type within a certain model. This distribution is dependent on space, direction of travel and energy. Knowledge of this distribution is required in disciplines such as atmospheric physics, medical imaging, and the primary focus of this work, nuclear engineering. The deterministic solution of the transport equation is possible through a variety of numerical methods; however, the computational cost of such a solution can grow rapidly if high accuracy is desired. This arises primarily due to the directional/angular dependence of the particle distribution. The typical approach to solve the transport equation is to apply a uniform angular resolution over the space and energy dimensions. However, this requires that the whole space-energy domain use the same angular resolution required to resolve the most directional part of a distribution. This is inefficient because in many problems the angular distribution may be isotropic in certain regions whilst highly anisotropic in others. A specific example is that of a thermal nuclear reactor, high energy neutrons within fuel pins have an isotropic distribution due to the nature of fission, however, the angular distribution becomes more directional in the clad and moderator region outside the fuel pin. The low energy neutrons will in general demonstrate the opposite, they will be isotropic in the moderator but show more directional feature near control rods and fuel pins. Therefore, the required angular resolution for a given accuracy is highly dependent upon the model geometry and material properties. This paper presents an adaptive method designed to optimise the angular resolution to obtain the greatest accuracy for the lowest computational expense.

An adaptive method may be defined as an automated process which modifies discretisations in numerical calculations in order to optimise computational usage. There are two main categories of adaptivity, regular and goal-based. Regular adaptivity reduces the error in the solution over the entire domain. Goal-based adaptivity reduces the error in a user-defined functional of the solution. Goal-based adaptivity in general will produce a more efficient and accurate discretisation for a given quantity than regular. The use of adaptive methods in spatial dimensions for finite elements and similar discretisations is well researched due to its utilisation in a large number of fields. Spatial adaptivity has been applied to

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the Boltzmann transport equation in various forms and shown to produce beneficial results (Duo et al., 2009; Mirza et al., 2007; Wang et al., 2009; Wang and Ragusa, 2011; Zhang and Lewis, 2002; Lathouwers, 2011b; Lathouwers, 2011a; Turcksin et al., 2010). Despite the large computational cost related to the angular component of the transport solution there has not been significant study into adaptivity within the angular dimension.

There are two well known and commonly used discretisations for the angular dimension of the particle distribution; the spherical harmonics (P_N) method and the discrete ordinates (S_N) method. There has been recent investigation into using wavelets as angular basis functions but this is less commonly used (Buchan et al., 2008a; Buchan et al., 2005; Cao et al., 2008; Yang et al., 2010; Zheng et al., 2009; Zheng et al., 2012). The literature shows that research has been undertaken in optimising each of these methods. The first known attempt to improve the efficiency of a transport calculation through adjusting the angular discretisation was by Ackroyd and Wilson (1988). In this work they use the even-parity (second-order) P_N method in 1D with variable resolution over the spatial domain. The resolution was set by intuitively using a priori knowledge of the material properties and the predicted solution. This is not an adaptive process but it demonstrates the same principles whereby the automated process is replaced by user intuition. This idea was extended by Mohan et al. to first-order transport in 3D (Mohan et al., 2011). This demonstrated the variable resolution P_N method over space within a spherical geometry. The results showed that solutions with comparable accuracy could be obtained for fewer degrees of freedom and smaller run times.

The first implementation of adaptivity within the angular dimension was completed by Watson (2005). In his work he developed an angular scheme that used a discrete ordinate discretisation in the polar angle and a wavelet expansion in the azimuthal angle. He demonstrated an adaptive algorithm using a thresholding technique for the coefficients of the wavelet basis functions. This method showed promise because it delivered a smaller error for a reduced number of unknowns and computation time. Research in adaptivity with wavelets was expanded by Buchan et al. which used a two-dimensional wavelet expansion over the surface of the sphere for both the polar and azimuthal angles (Buchan et al., 2008b). This work uses higher order wavelet functions and applies a similar thresholding type of adaptive algorithm. It was found that the number of unknowns could be reduced by an order of magnitude and retain the same accuracy for two-dimensional models.

There are two known implementations of adaptivity using spherical harmonics, the first was completed by Park (2006, 2009). The focus of his work was a coupled space-angle adaptive process which used the P_N method within a finite element discretisation. Park developed an implicit angular error estimator for the second order even-parity transport equation and used it to adapt the resolution of the spherical harmonics over the spatial domain. He demonstrated the use of both regular and goal-based adaptivity for the angular discretisation. The results showed significant decrease in the number of unknowns for a given accuracy and a decrease in run time for most problems. The second implementation of adaptive spherical harmonics was by Rupp et al. (2011) in solving the Boltzmann transport equation with application to semiconductors. A variable order spherical harmonics resolution was applied over the space and energy domain whilst solving the first order transport equation. The error measure in this work uses an analytical property of the spherical harmonics expansion which relates the rate of decay of the expansion coefficients to the smoothness of the function. This work reported a decrease in the computational cost for a given accuracy by just under an order of magnitude.

Adaptivity within the discrete ordinates discretisation was initially investigated by Stone (2007). This work used adaptive quadrature sets for the discrete ordinates discretisation. The difference between an interpolated value and a value calculated through sweeping was used as the error measure. If the error was larger than a user-set tolerance then additional quadrature points were added to the discretisation. The method was shown to reduce the ray effects phenomenon for far fewer degrees of freedom than a uniform resolution over space. Jarrell built upon this method by employing the same error measure to adapt using a new type of quadrature set derived from linear discontinuous basis functions on the surface of a sphere (Jarrell, 2010). He found that his method obtained an excellent order of convergence but it was difficult to predict the accuracy for highly directional distributions.

This paper extends upon the work completed by Park and Rupp using spherical harmonics within an adaptive algorithm. The two main differences in this work are: (i) the first order transport equation is solved using a different spatial discretisation, and (ii) the error estimators used in the adaptive process are different. This article begins by describing the discretisations used for the first order transport equation in Section 2. The regular and goal-based error measures are described in Sections 3 and 4. An overview of the procedure used for adapting the angular discretisation is outlined in Section 5. Section 6 provides a simple example to demonstrate a problem encountered during the work. The adaptive algorithm has been applied to several examples and the results are displayed in Section 7. Finally, the conclusions of the research are provided in Section 8.

2. Transport equation

2.1. Multigroup energy discretisation

The multigroup approximation of the fixed source transport equation results in the following set of equations:

$$\mathbf{\Omega}\cdot\nabla\psi_g(\mathbf{r},\mathbf{\Omega})+\Sigma_{t,g}(\mathbf{r})\psi_g(\mathbf{r},\mathbf{\Omega})= \tag{1}$$

$$\int_{\mathbf{\Omega}'}\sum_{g'=1}^{G}\Sigma_{s,g'\to g}(\mathbf{r},\mathbf{\Omega}'\to\mathbf{\Omega})\psi_{g'}(\mathbf{r},\mathbf{\Omega}')\mathrm{d}\mathbf{\Omega}'+S_{e,g}(\mathbf{r},\mathbf{\Omega}) \quad \text{for} \quad g\in\{1,2,\ldots,G\}, \tag{2}$$

where there are G energy groups and the subscript g denotes the given quantities for each energy group. The multigroup equations for an eigenvalue problem are

$$\mathbf{\Omega}\cdot\nabla\psi_g(\mathbf{r},\mathbf{\Omega})+\Sigma_{t,g}(\mathbf{r})\psi_g(\mathbf{r},\mathbf{\Omega})=\int_{\mathbf{\Omega}'}\sum_{g'=1}^{G}\Sigma_{s,g'\to g}(\mathbf{r},\mathbf{\Omega}'\to\mathbf{\Omega})\psi_{g'}(\mathbf{r},\mathbf{\Omega}')\mathrm{d}\mathbf{\Omega}'+\lambda\frac{\chi_g}{4\pi}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}(\mathbf{r})\int_{\mathbf{\Omega}'}\psi_{g'}(\mathbf{r},\mathbf{\Omega}')\mathrm{d}\mathbf{\Omega}' \quad \text{for} \quad g\in\{1,2,\ldots,G\}. \tag{3}$$

The group angular flux distribution, $\psi_g(\mathbf{r},\mathbf{\Omega})$, is dependent on space, $\mathbf{r}$, and direction of particle travel, $\mathbf{\Omega}$. The group macroscopic cross-sections are represented by $\Sigma_{t,g}$, $\Sigma_{s,g'\to g}$ and $\Sigma_{f,g}$ for the total, scatter and fission reactions respectively. In the fixed source equation, the source term, S_e, is an extraneous particle source. The fission spectrum and average number of neutrons produced per fission are represented by χ_g and ν respectively. The eigenvalue of the equation is represented by λ.

The multigroup equations are coupled through the scatter and fission terms. The equation for each energy group can be considered as a mono-energetic equation with an additional source from the scatter and fission terms. The following sections will consider a single group equation for simplicity and thus the subscript g will be neglected but should be assumed implicit.