Journal of Computational Physics 281 (2015) 1032–1062

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Goal-based angular adaptivity applied to a wavelet-based discretisation of the neutral particle transport equation

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ARTICLE INFO

Article history:
Received 16 July 2014
Received in revised form 27 October 2014
Accepted 31 October 2014
Available online 6 November 2014

Keywords:
Radiation transport
Adaptivity
Goal-based adaptivity
A posteriori error analysis
Wavelets

ABSTRACT

A method for applying goal-based adaptive methods to the angular resolution of the neutral particle transport equation is presented. The methods are applied to an octahedral wavelet discretisation of the spherical angular domain which allows for anisotropic resolution. The angular resolution is adapted across both the spatial and energy dimensions. The spatial domain is discretised using an inner-element sub-grid scale finite element method. The goal-based adaptive methods optimise the angular discretisation to minimise the error in a specific functional of the solution. The goal-based error estimators require the solution of an adjoint system to determine the importance to the specified functional. The error estimators and the novel methods to calculate them are described. Several examples are presented to demonstrate the effectiveness of the methods. It is shown that the methods can significantly reduce the number of unknowns and computational time required to obtain a given error. The novelty of the work is the use of goal-based adaptive methods to obtain anisotropic resolution in the angular domain for solving the transport equation.

1. Introduction

The neutral particle transport equation describes the mean distribution of particles within a given system. This distribution of particles is important in a range of fields such as nuclear engineering, atmospheric physics and medical imaging. When dealing with particle transport this distribution is typically referred to as the angular flux. The angular flux exists in a seven dimensional phase-space which is composed of location, direction of travel, energy and time variables. Analytical solutions of the transport equation are only possible in a small number of simplified systems. The solution for practical applications requires the use of numerical methods. In complex systems, a high resolution of the phase-space is required to obtain the angular flux with an acceptable accuracy. Solving the equation with a high-resolution of the phase-space leads to significant computational cost. One method of minimising this computational cost is optimising the resolution of the phase-space to obtain the most accurate solution. This paper presents an automated method for optimising the resolution of the angular dimensions representing the particle direction within the phase-space.

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http://dx.doi.org/10.1016/j.jcp.2014.10.063
0021-9991/

There are two well known discretisation techniques for the angular dimensions of the phase-space: the spherical harmonics (P_N) method and the discrete ordinates (S_N) method. The P_N method uses an expansion of continuous functions on the surface of the sphere to approximate the angular dependence of the solution. The S_N method solves the transport equation for a discrete set of directions. The P_N method is beneficial for capturing solutions with a smooth angular dependence, however it cannot capture discontinuities in the angular domain. The S_N method can capture such discontinuities but is susceptible to a phenomenon known as ray effects. This is where the solution incurs error because the characteristic number of directions for particle transport is restricted to a discrete set. The effect is most evident in transparent media in which transport effects dominate. The S_N method is commonly employed in commercial codes because it may be implemented in a very efficient manner.

In the last decade or so there has been research into discretisations representing the angular dimensions of the phase-space using a wavelet basis. One of the earliest applications was a two-dimensional wavelet expansion of the angular dimensions performed by Guven [13]. This application was in the field of radiative transfer which is governed by an equation of the same form as the neutral particle transport equation. This work used a two-dimensional Daubechies wavelet expansion to represent the two angular variables of the phase-space. An example demonstrated that the wavelet expansion did not exhibit ray effects when compared with a discrete ordinate solution using a similar number of angular degrees of freedom. In other work, Watson took a different approach and used a wavelet basis for the azimuthal angle but used a discrete ordinate representation for the polar angle [27]. The simpler Haar wavelet family was used as the wavelet basis for the azimuthal variable. This work was related to adaptivity and will be discussed in the next paragraph. Research into the two-dimensional wavelet expansion was extended by Buchan et al. [5]. In this work, a wavelet basis is constructed on the surface of an octahedron and a linear mapping is used to project this onto the surface of the sphere. First and second order bases were trialled on the surface of the octahedron and each octant of the octahedron was discontinuous. It was found that the octahedral wavelets provided solutions of comparable accuracy to the standard P_N and S_N methods. It was noted that the quadratic basis provided little benefit over the linear basis. Buchan further investigated this idea and constructed two other wavelet bases by construction on the surface of a hexahedron [4,6]. Again, the solutions were of comparable accuracy to the standard angular discretisations. Each wavelet basis presented by Buchan demonstrated that ray effects were present in the solutions but they are less severe than those seen with discrete ordinates. The one-dimensional wavelet expansion in conjunction with discrete ordinates was furthered by Cao et al. [9]. They presented a two-dimensional wavelet expansion formed by a tensor product of a one-dimensional basis but noted that the number of unknowns would be large. It was also reasoned that the solution in most 2D problems has a smooth variation in the polar angle therefore less resolution is required in this variable. They used a Daubechies wavelet basis in the azimuthal angular variable. The wavelet basis performed well and it was demonstrated to capture the complex azimuthal dependence present in an infinite pin cell calculation first acknowledged by Adams [1]. However, there was an issue with the discretisation that caused anomalies in the azimuthal dependence of the solution. These anomalies were edge effects attributed to the forcing of continuity between angular subdomains. Zheng followed this and published an improved version of the discretisation which eliminated the edge effects and improved the efficiency by increasing the sparsity of the matrices [28]. This work extended the method to 3D problems and included anisotropic scatter. It was found the Daubechies wavelet basis is also susceptible to ray effects.

Other than the work by Watson, each of the discretisations mentioned have employed a uniform resolution of the angular domain using the wavelet basis. This is not necessarily always the most efficient means to obtain a solution. In many situations, problems which require high angular resolution will only require resolution in specific directions at certain points in space. One could attempt to set the angular resolution manually using intuition and *a priori* knowledge of the solution, however this is unlikely to return the most accurate or optimum solution. Another solution is to automate this process by using *a posteriori* error measures; these are errors that are calculated after obtaining the solution to the system. The automated process of optimising the resolution/discretisation of a variable is referred to as an adaptive method or adaptivity. Adaptive methods applied to the spatial discretisation of the transport equation have been widely researched [17,16,2,10,22,26]. There has been less research into adaptive methods applied to the angular dimensions of the transport equation. Adaptivity applied to the P_N method has been investigated in various forms by Park et al., Rupp et al. and Goffin et al. [20,23,11]. In addition, research into adaptive methods for the S_N method has been carried out separately by Stone and Jarrell [25,14]. Kópházi and Lathouwers developed a novel finite element type angular discretisation that is suitable for adaptive angular resolution [15]. This method has the benefit that it may be solved efficiently in a similar manner as the usual S_N method. It was demonstrated the method had second order convergence with respect to the angular error using uniform angular resolution, however, further work is required to demonstrate the application of the angular method in an adaptive procedure.

A wavelet discretisation is ideal for use with an adaptive method because the basis is hierarchical and the functions have local support. This allows local refinement of resolution with relative ease. Watson was the first to investigate an adaptive scheme using wavelets for the transport equation. As mentioned previously, Watson's scheme uses an S_N representation for the polar angle and a wavelet basis for the azimuthal dependence. The main reason Watson was testing the wavelet basis for the azimuthal dependence was for the purpose of adaptivity. It was shown that the solutions obtained using adaptivity could produce accurate results whilst reducing the computational cost in terms of unknowns and calculation time. Adaptivity with a two-dimensional wavelet basis was explored by Buchan et al. using the octahedral wavelet basis [6]. This work found that the number of unknowns could be reduced by nearly an order of magnitude and retain a similar accuracy for some examples.