Journal of Computational Physics 335 (2017) 352–386

Contents lists available at ScienceDirect

Journal of Computational Physics

www.elsevier.com/locate/jcp

Energy dependent mesh adaptivity of discontinuous isogeometric discrete ordinate methods with dual weighted residual error estimators

A.R. Owens *, J. Kópházi, J.A. Welch, M.D. Eaton

Nuclear Engineering Group, Department of Mechanical Engineering, City and Guilds Building, Imperial College London, Exhibition Road, South Kensington, London, SW7 2AZ, United Kingdom

ARTICLE INFO

Article history:
Received 24 August 2016
Received in revised form 6 December 2016
Accepted 18 January 2017
Available online 24 January 2017

Keywords:
Isogeometric analysis
Discrete ordinates
Dual weighted residual
Group-dependent mesh
Adaptive
Discontinuous Galerkin

ABSTRACT

In this paper a hanging-node, discontinuous Galerkin, isogeometric discretisation of the multigroup, discrete ordinates (S_N) equations is presented in which each energy group has its own mesh. The equations are discretised using Non-Uniform Rational B-Splines (NURBS), which allows the coarsest mesh to exactly represent the geometry for a wide range of engineering problems of interest; this would not be the case using straight-sided finite elements. Information is transferred between meshes via the construction of a supermesh. This is a non-trivial task for two arbitrary meshes, but is significantly simplified here by deriving every mesh from a common coarsest initial mesh. In order to take full advantage of this flexible discretisation, goal-based error estimators are derived for the multigroup, discrete ordinates equations with both fixed (extraneous) and fission sources, and these estimators are used to drive an adaptive mesh refinement (AMR) procedure. The method is applied to a variety of test cases for both fixed and fission source problems. The error estimators are found to be extremely accurate for linear NURBS discretisations, with degraded performance for quadratic discretisations owing to a reduction in relative accuracy of the "exact" adjoint solution required to calculate the estimators. Nevertheless, the method seems to produce optimal meshes in the AMR process for both linear and quadratic discretisations, and is $\approx \times 100$ more accurate than uniform refinement for the same amount of computational effort for a 67 group deep penetration shielding problem.

1. Introduction

Even with today's computational algorithms and high performance computing architectures, the numerical solution of the neutron transport equation over heterogeneous whole-core reactor physics and shielding geometries remains a significant challenge. A large part of this challenge stems from the seven dimensional nature of the solution space, with resolution required in energy, direction, space and time in transient problems. Traditional reactor physics techniques involve initially solving the neutron transport equation over assembly-sized domains with periodic boundary conditions [1,2]. The heterogeneous cross-section data within the fuel assembly is then homogenised, and the resulting whole-core system is solved using the neutron diffusion equation with nodal spatial discretisation techniques [3].

* Corresponding author.
E-mail address: a.owens12@imperial.ac.uk (A.R. Owens).

http://dx.doi.org/10.1016/j.jcp.2017.01.035

If a more detailed description of the geometry is required, discontinuous Galerkin finite element methods (DGFEM) with a discrete ordinate angular discretisation can be applied. It was originally developed for the first-order form of the discrete ordinates equations [4–6], but has since been applied to a wide range of fields such as radiative heat transfer [7], the compressible Navier–Stokes equations [8] and the Euler equations of gas dynamics [9]. Complex geometries can be subdivided into geometric primitives such as triangles, quadrilaterals, tetrahedra and hexahedra by the use of a mesh generator [10]. This mesh generator converts the NURBS geometry output by the computer aided design (CAD) program into surface and volumetric mesh elements, over which the discrete ordinates equations can then be solved with a DGFEM spatial discretisation. However, most elements employed have straight or planar sides [10], and so cannot exactly represent the underlying NURBS geometry. It is crucial that the polygonal geometry representation preserves the fissile mass of the system in reactor physics applications, otherwise large errors can be introduced into the criticality solution [11,12].

An extension of the finite element method (FEM), isogeometric analysis (IGA), was recently introduced in order to overcome some of these deficiencies [13]. As in FEM, prescribed shape and test functions are used to discretise the weak form of the underlying partial differential equation (PDE). In order to preserve the CAD geometry, the same NURBS used to mathematically describe the geometry are used to discretise the weak form of the PDE. In this manner, the exact geometry output by the CAD program is preserved at the coarsest level of refinement, as well as when the mesh is further refined. A further advantage of IGA is that the parameterisation of the physical space does not change under mesh refinement, simplifying the implementation of the group dependent mesh (GDM) methods presented here.

The first applications of IGA were in Bubnov–Galerkin discretisations of solid mechanics problems and streamline-upwind Petrov–Galerkin discretisations of advection-diffusion equations [13]. In reactor physics, Hall et al. [14] solved the one group diffusion equation over a pincell geometry using a Bubnov–Galerkin NURBS discretisation, which was extended by Welch et al. [15] to multigroup problems over heterogeneous quarter-core style geometries.

Discontinuous IGA methods were first applied to elliptic systems [16,17]. For hyperbolic systems, two discontinuous IGA discretisations have recently been developed. The Blended Isogeometric Discontinuous Galerkin method [18] meshed the geometry using rational Bernstein–Bézier triangles. The solution fields were then approximated using standard polynomial basis functions and the method applied to Maxwell's equations of electromagnetics and the acoustic wave equations.

In [19], discontinuous IGA was applied to the first-order form of the discrete ordinates equations with conforming meshes (i.e. no hanging-nodes). This was extended in [20] to an adaptive, hanging-node formulation for one group problems where the adaptivity was driven by heuristic error indicators. This work is a further extension of that in [20], in which each energy group now has its own associated mesh. This can be advantageous, as in many practical problems the solutions in different energy groups exhibit very different behaviour, and so require mesh resolution in different parts of the geometry [21,22]. This technique was employed by Ragusa and coworkers [21,22] for the multigroup neutron diffusion equation with Cartesian grid geometries, and by Goffin et al. [23] for the first-order form of the neutron transport equation with a spherical harmonics angular discretisation. In [23], the meshes in each group were formed independently of each other, and so the calculation of a "supermesh" to transfer information between groups is a non-trivial task [24]. In contrast, the method presented in [21,22] relies on every mesh being derived from a common coarsest description. This significantly simplifies the generation of the supermesh, but naturally limits a scheme to geometries that can be represented exactly by the elements employed. In [20] it was shown that using an inexact DGFEM geometry to represent circular fuel pins was impractical for use with AMR, as eventually the geometric error dominated the spatial discretisation error. However this is not a limitation faced by NURBS-based IGA, and so the approach of Ragusa et al. of deriving every mesh from a common coarsest description is followed here, with that coarsest description being precisely the geometry of the problem.

In order to take full advantage of the GDM IGA discretisation, goal-based adaptivity based on dual weighted residual (DWR) error estimators will be used here to drive the AMR. The general framework for these error estimators was originally presented by Rannacher and coworkers [25–29]. The specific form of the error estimators for the first order form of the one group discrete ordinates equations with linear DGFEM spatial discretisation were derived by Lathouwers for both fixed source [30] and eigenvalue [31] problems. These estimators are extended here to multigroup problems of both fixed source and eigenvalue varieties and using discontinuous NURBS of arbitrary order for the spatial discretisation. This allows the meshes in each group to be refined towards a specific goal functional of the flux, as well as providing an estimate of the remaining error in the functional due to the spatial discretisation, a useful property in a "best estimate plus uncertainty" design process.

The remainder of the paper is organised as follows. Section 2 gives a brief overview of isogeometric analysis and the basis functions employed. Section 3 derives the spatially discretised version of the weak form of the equations, with a special focus on supermesh calculation and the transfer of information between meshes. In Section 4 the multigroup DWR error estimators are derived for both fixed source and eigenvalue problems, and the adaptive procedure followed here is explained. Section 5 contains numerical results of the error estimators and GDM methodology applied to a variety of verification test cases.

2. Isogeometric analysis

Isogeometric analysis aims to unify the geometric description of physical problems used by CAD programs with that employed in the computational analysis, by using the NURBS prevalent in the CAD community to discretise the governing equations [13]. The design and analysis cycle time can be dominated by procedures associated with mesh generation, par-