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Adjoint eigenvalue correction for elliptic and hyperbolic neutron transport problems

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ABSTRACT

An adjoint-based *a posteriori* error measure is developed and applied to the K_{eff} eigenvalue in particle transport problems using the diffusion approximation and full transport solutions. This demonstrates application of an eigenvalue error recovery scheme that can be applied to both elliptic and hyperbolic operators. The K_{eff} eigenvalue is first obtained via a conventional inverse power iteration on the fission source, from the forward system of equations using a simple linear finite element type. The solution procedure is then repeated using the adjoint equations. The eigenvector solution to the adjoint system is enriched in a post-processor step, and convolved with the residual of the forward equations. This produces a computable approximation to the error in the eigenvalue. This approximation to the error is then subtracted from the eigenvalue producing a better estimate. It is shown how this approach can accelerate the mesh convergence of the eigenvalue in both smooth, diffusive problems using an elliptic operator and also in non-smooth transport problems in which the operator is of hyperbolic form. In the elliptic case, the diffusion equation is discretised with continuous finite elements. In the hyperbolic case, the Boltzmann Transport Equation is discretised with discontinuous Galerkin weighted finite elements. The approach to recovering the error in the K_{eff} eigenvalue is common to both cases.

1. Introduction

An *a posteriori* scheme for improving the accuracy and reducing the error in eigenvalue calculations is presented, for neutron diffusion and transport applications (Lewis and Miller, 1993). Using a first order Taylor series expansion of both the eigenvalue solution and the residual of the governing equation, an approximation to the error in the eigenvalue is derived. This is done using a convolution of the equation residual and adjoint solution, which is calculated in-line with the primal solution. A defect iteration on the solution is then performed in which the approximation to the error is used to apply a correction to the eigenvalue. The method is shown to dramatically improve convergence of the eigenvalue. The equation for the eigenvalue is shown to simplify when certain normalisations are applied to the eigenvector. Two such normalisations are considered; the first of these is a fission-source type of normalisation and the second is an eigenvector normalisation. Results are demonstrated on a number of demanding neutron diffusion and neutron transport problems. The diffusion problems are discretised using continuous Galerkin weighted finite elements. The neutron transport problems are discretised using discontinuous Galerkin (DG) weighted finite elements. This shows the correction scheme may be applied to both elliptic and hyperbolic problems and within different discretisation frameworks. This is not limited to spatial corrections and may be used throughout the phase space of the discrete equation. The *a posteriori* approach to error estimation not only improves the fidelity of a calculation, it can assess the reliability of numerical schemes (Houston et al., 2000, 2007a, 2007b; Georgoulis et al., 2011) and can be used to guide mesh adaption algorithms (Cliffe et al., 2010a, 2010b, 2011; Zhu et al., 2011) or to automate mesh generation (Georgoulis et al., 2009). This has been demonstrated for both bulk functionals (Baker, 2011) and eigenvalue problems (Lathowers, 2011). The current work uses an *a posteriori* approach to recovering errors in the K_{eff} eigenvalue.

Eigenvalue problems arise in many areas of science, mathematics and engineering. They characterise a diverse range of systems that are of interest such as glacier movements in geology, to lift and drag past obstructions to flow in aircraft and ship design. In mathematics they describe the orthogonal properties of a matrix

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and in reactor physics the distribution of neutrons in a lattice, allowing criticality of a loaded core to be assessed. Accurate determination of the largest (or principal) eigenvalue is clearly important in a wide range of applications. The need to improve it as an approximation is apparent in many areas of science and mathematics, as discussed in Merton (2011). This is because computational procedures for obtaining the eigenvalue are typically very intensive numerically, notably so in criticality problems where a large number of non-linear iterations are required to accurately characterise the system. Coarsened computational meshes make calculations of the eigenvalue numerically feasible, however they are unable to capture or contain enough information about the problem to achieve solutions of acceptable accuracy. Finer meshes that offer reasonable accuracy are in many cases unfeasible where highly iterative solution schemes are employed, such as source iteration schemes used to obtain eigenvalues in neutron transport applications. This has motivated the development of methods that improve the numerical solution on meshes that would otherwise not offer sufficient accuracy. An example of this type of approach is the *a posteriori* error measure (Elman et al., 2008), in which the solution itself is used in some way to obtain a defect estimate (Ainsworth and Oden, 1997). Another popular approach is to use the adjoint problem to obtain an approximation to the error, and subsequently remove this approximation from the solution obtaining improved functional estimates (Venditti and Darfomal, 2000; Pierce and Giles, 2004; Giles et al., 2004). Alternatively, one might use it as a metric to guide a grid adaption step. This has been shown to be successful in Venditti and Darfomal (2002, 2003). However, the error across the whole phase space of the discrete equation needs to be understood when any type of adaption is applied to the grid, as it is not always clear in which order variables should be refined (or de-refined). Adjoint solutions are useful for deriving errors because they provide information on the first-order sensitivities of a functional (or eigenvalue) to the forward solution of a partial differential equation. The sensitivity information provided depends on how the source term of the adjoint equation is defined; for example, if one seeks to obtain eigenvalue sensitivity to the forward solution, then the eigenvalue must be differentiated with respect to the eigenvector. The adjoint solution will then describe how a small perturbation in the forward solution effects the eigenvalue. Since the computational solution may be regarded as a perturbation from the true solution to the underlying problem, one can use the adjoint equation to derive improvements to the eigenvalue. The approach developed in the present work is an adjoint-based *a posteriori* scheme that derives an approximation to the error in the eigenvalue. This is a similar strategy to that developed for bulk functionals in Giles et al. (2004) and to that developed for anisotropic grid optimisation in viscous flow (Venditti and Darfomal, 2000).

2. Eigenvalue problem

The present work derives a correction to the eigenvalue problem arising in transport and diffusion problems. The correction is based on the forward and adjoint system of equations. This section introduces the transport equation, the diffusion equation and the space-angle discretisation used in the present work. The eigenvalue and its derivative are then defined.

2.1. Space-angle discretisation

The first-order time-independent transport equation, in a domain that contains a fission source and no external or imposed source, may be written in two-dimensional Cartesian geometry as:

$$\mathbf{\Omega}\cdot\nabla\psi(\mathbf{r},\mathbf{\Omega},E)+\sigma_t(\mathbf{r})\psi(\mathbf{r},\mathbf{\Omega},E)\;=\;\lambda\chi(E)\int_{\mathbf{\Omega}'}\int_{E'}\Big(\nu(E')\sigma_f(\mathbf{r},E')\psi(\mathbf{r},\mathbf{\Omega}',E')\Big)dE'd\mathbf{\Omega}'+\int_{E'}\int_{\mathbf{\Omega}'}\left(\sigma_s(\mathbf{r},\mathbf{\Omega}'\rightarrow\mathbf{\Omega},E'\rightarrow E)\psi(\mathbf{r},\mathbf{\Omega}',E')\right)d\mathbf{\Omega}'dE',\qquad(1)$$

in which $\mathbf{\Omega}=(\mathbf{\Omega}_x,\mathbf{\Omega}_y)^T$ is the direction of particle travel expressed in terms of the Cartesian components $\mathbf{\Omega}_x$,$\mathbf{\Omega}_y$, $\psi(\mathbf{r},\mathbf{\Omega},E)$ is the angular flux at position $\mathbf{r}$, angle $\mathbf{\Omega}$ and energy E. λ is the leading eigenvalue that characterises the criticality of the system. The fission spectrum is given by $\chi(E)$ which describes the probability that a fission neutron will have an energy within dE about E, and the mean number of neutron per fission is given by $\nu(E)$. The quantity $\sigma_f(\mathbf{r},E)$ is the fission cross-section at position $\mathbf{r}$ for a neutron with energy E. This is assumed to be (on average) isotropic. It therefore lacks dimension in angle. $\sigma_t(\mathbf{r},E)$ is the total cross-section at position $\mathbf{r}$ for energy E. $\sigma_s(\mathbf{r},\mathbf{\Omega}'\rightarrow\mathbf{\Omega},E'\rightarrow E)$ is the scattering cross-section at position $\mathbf{r}$ describing the contribution to energy E and angle $\mathbf{\Omega}$ from energy E' and angle $\mathbf{\Omega}'$. In the present work, energy dependence is omitted from consideration to be left as a future topic. Therefore, in each test problem used in the present paper, neutrons are assumed to travel at a constant energy. Eq. (1) may then be written in an angular discrete form, in terms of the $\mathscr{M}$ angular moments of the solution:

$$\mathbf{a}\cdot\nabla\Psi(\mathbf{r})+\mathbf{H}(\mathbf{r})\Psi(\mathbf{r})-\lambda\mathbf{C}(\mathbf{r})\Psi(\mathbf{r})\;=\;0,\qquad(2)$$

in which $\mathbf{a}=(\mathbf{a}_x,\mathbf{a}_y)^T$ is an $\mathscr{M}\times\mathscr{M}$ matrix containing the spatially invariant Jacobian of the direction of particle travel $\mathbf{\Omega}$. The derivation of $\mathbf{a}$ is described elsewhere, for different choices of angular approximation (Lewis and Miller, 1993; Miller et al., 1973; Wareing et al., 2001; Merton, 2011). The number of moments $\mathscr{M}$ is simply the number of angular unknowns in the angular discrete equation. $\mathscr{M}$ depends on the choice of basis function in direction of particle travel, and on the order of approximation made. For example, for discrete ordinates there are $n(n+2)$ unknowns on the sphere where n is the S_n order. Typically in two dimensional problems, one hemisphere is solved and therefore one would use $\mathscr{M}=n(n+2)/2$. In the case of spherical harmonics, there are $(n+1)^2$ moments on the sphere, where n is the order of the P_n expansion. In two dimensions, one solves a subset of these in which there are $(n+1)(n+2)/2$ moments. Thus $\mathscr{M}=\frac{(n+1)(n+2)}{2}$ for typical two-dimensional P_n problems. $\mathbf{H}(\mathbf{r})$ is an $\mathscr{M}\times\mathscr{M}$ matrix containing the angular moments of the scattering-removal data, at position $\mathbf{r}$. The $\mathscr{M}\times\mathscr{M}$ matrix $\mathbf{C}(\mathbf{r})$ contains the fission data, multiplied by the angular weights, at position $\mathbf{r}$. This generates an isotropic source term. The quantity $\mathbf{\Psi}(\mathbf{r})$ is a vector of length $\mathscr{M}$ containing the angular moments of the solution at position $\mathbf{r}$. The vector $\mathbf{r}$ is the space that remains to be discretised. For example, $\mathbf{r}=(x,y)^T$ in which x,y are the Cartesian coordinates in the spatial continuum. The vector $\mathbf{0}$ is of length $\mathscr{M}$ and contains zeroes. The residual $\mathscr{R}=\mathscr{R}(\Psi)$ is therefore a vector of length $\mathscr{M}$ at position $\mathbf{r}$ and may be written: