

AN ADJOINT-BASED SCHEME FOR EIGENVALUE ERROR IMPROVEMENT

S. R. Merton and R. P. Smedley-Stevenson

AWE plc

Aldermaston, Reading, Berkshire RG7 4PR, United Kingdom
Simon.Merton@awe.co.uk; Richard.Smedley-Stevenson@awe.co.uk

C. C. Pain, A. H. El-Sheikh and A. G. Buchan

Department of Earth Science and Engineering

Imperial College London

South Kensington Campus, London SW7 2AZ, United Kingdom
c.pain@imperial.ac.uk; a.el-sheikh@imperial.ac.uk; andrew.buchan@imperial.ac.uk

ABSTRACT

A scheme for improving the accuracy and reducing the error in eigenvalue calculations is presented. 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 correction 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 elliptic problems using continuous Galerkin weighted finite elements. Moreover, the correction scheme may also be applied to hyperbolic problems and arbitrary discretisation. This is not limited to spatial corrections and may be used throughout the phase space of the discrete equation. The applied correction not only improves fidelity of the calculation, it allows assessment of the reliability of numerical schemes to be made and could be used to guide mesh adaption algorithms or to automate mesh generation schemes.

Key Words: Eigenvalue, Eigenvector, Adjoint, Galerkin.

1. INTRODUCTION

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 and in reactor physics the distribution of neutrons in a lattice, allowing criticality to be assessed. Accurate determination of the system eigenvalue is clearly important in a wide range of applications. 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, in which the solution itself is used in some way in order to obtain a defect estimate [6]. 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 [3–5]. Alternatively, one might use it as a metric to guide a grid adaption step. This has been shown to be successful in [1, 2]. 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 which order variables should be refined (or derefined).

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 paper 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 [5] and to that developed for anisotropic grid optimisation in viscous flow [3]. Focusing on this approach, the current paper is arranged as follows: In section 2., the approach to functional and eigenvalue correction in particle transport problems is considered. The eigenvalue itself is used to define an approximation to the error based on forward and locally refined adjoint solutions to the discrete equation. Two normalisations of the eigenvector are considered that simplify the residual. One of these normalisations is based on the fission source and the second is based on the eigenvector. In section 3., the correction procedure is introduced. This involves expanding the eigenvalue and residual in a first order Taylor series, and an approximation to the error in the eigenvalue is derived. In section 4., results are demonstrated on a series of demanding elliptic problems, that relate the correction procedure to particle diffusion applications. Conclusions are drawn in section 5. with recommendations for further work.

2. EIGENVALUE CORRECTION SCHEMES

An approach to eigenvalue correction in particle transport diffusion simulations is considered. The aim is to use the eigenvalue directly in order to derive a defect correction based on the adjoint and a locally refined primal solution. It is also possible to use this correction to automate mesh adaptivity.

2.1 Definition of the Eigenvalue

This paper describes one possible technique for eigenvalue correction based on the definition of a functional $F(\Psi)$ of the eigenvector Ψ . In the case of an eigenvalue one can write the residual of the governing equation as

$$\mathcal{R}(\Psi_i) = (\mathbf{A} - \lambda_i \mathbf{B})\Psi_i = \mathbf{0} \quad (1)$$

where λ_i and Ψ_i are the i th generalised eigenvalue and eigenvector respectively, of the matrix \mathbf{A} with respect to the matrix \mathbf{B} . Both \mathbf{A} and \mathbf{B} are square matrices of size $\mathcal{N} \times \mathcal{N}$ and $\mathbf{0}$ is a vector of length \mathcal{N} containing zeroes, where \mathcal{N} is the number of unknowns in the problem. This expression can be simplified by normalising the eigenvectors, which is a traditional approach when solving eigensystems. The type of normalisation used for this depends on the physical system. For eigenvector normalisation (EN), one can write

$$C_{EN}(\Psi_i) = \Psi_i^T \mathbf{B} \Psi_i = 1 \quad (2)$$

in which C_{EN} is referred to as the Eigenvector Constraint. Substituting this constraint into Eqn. 1 one may write the functional as

$$F_{EN}(\Psi_i) = \lambda_i = \Psi_i^T \mathbf{A} \Psi_i \quad (3)$$

However, the associated functional has a saddle point at each of the eigenvalues i.e. the functional has zero first derivatives for a symmetric (self adjoint) operator. One may demonstrate this by choosing two mutually independent vectors Ψ_1 and Ψ_2 . A third vector $\Psi_3 = \Psi_3(\Psi_1, \Psi_2)$ is then obtained that satisfies the constraint Eqn. 2. Eigenvalues are then generated by substituting Ψ_3 into Eqn. 3. The result is illustrated in Fig. 1 to demonstrate the saddle point.

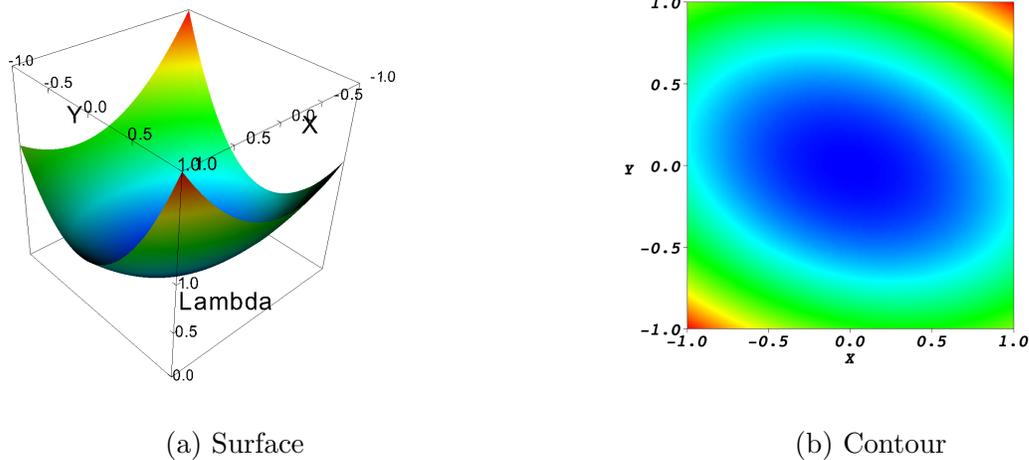


Figure 1: Eigenvalue normalisation gives rise to a saddle point.

Consequently, in this case there is no information on the first order sensitivity of eigenvalues to the components of the eigenvector and one must include quadratic terms in order to apply a defect correction to this functional. Approaches to this are not pursued in the present work. Matrices containing high order derivatives of the eigenvalue would need to be computed in order to implement a quadratic correction, and this is believed to be computationally unfeasible. Use of eigenvector normalisations are therefore not recommended with the present scheme.

In order to derive a non-zero linear correction, an alternative form for the normalisation of the eigenvectors is considered, based on the fission source accumulated over the problem. This normalisation is used instead of that defined in Eqn. 2, and is defined as

$$C_{\text{FS}}(\Psi_i) = \mathbf{b}^T \mathbf{B} \Psi_i = 1 \quad (4)$$

in which C_{FS} is referred to as the Fission Source Constraint, and $\mathbf{b} = [1, 1, \dots, 1]$ is the unit vector of length \mathcal{N} which performs the integration over the problem domain. The functional associated with the fission source normalisation is thus

$$F_{\text{FS}}(\Psi_i) = \lambda_i = \mathbf{b}^T \mathbf{A} \Psi_i \quad (5)$$

For clarity the subscript i is dropped in the remainder of the paper. The eigenvalue resulting from this normalisation is shown in Fig. 2. In this case, the first-order derivatives of λ are non-zero, and all higher order derivatives are zero, as seen from Fig. 2 which shows there is no curvature when this normalisation is applied.

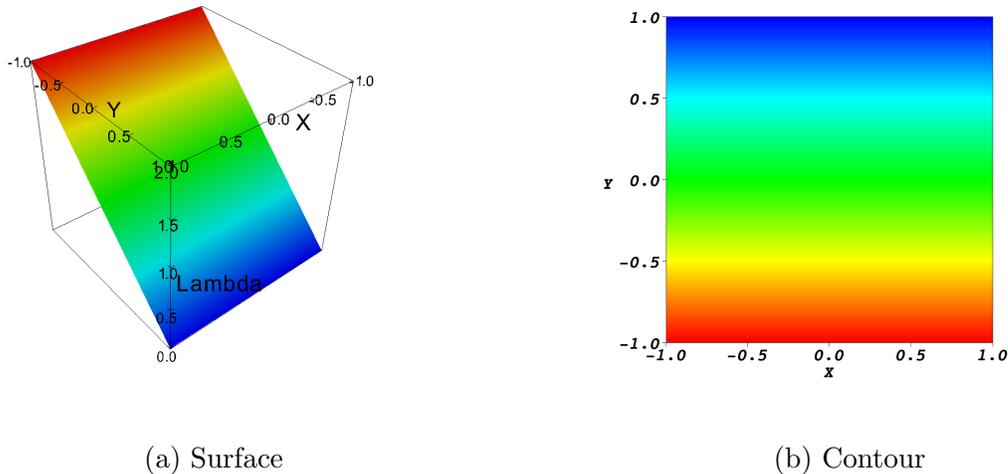


Figure 2: Fission source normalisation gives rise to a linear correction.

Application of this normalisation therefore results in the first order Taylor expansion being exact because all higher derivatives are zero. Computable linear corrections can thus be found that do not require high order derivatives, such as the Hessian, to be computed.

2.2 Derivatives of the Eigenvalue

In order to differentiate the eigenvalue defined in Eqn. 5 subject to the corresponding normalisation constraint defined in Eqn. 4 we differentiate the ratio of the functional to the constraint:

$$\frac{\partial}{\partial \Psi} \left(\frac{F_{\text{FS}}(\Psi)}{C_{\text{FS}}(\Psi)} \right) \quad (6)$$

The constraint is then used to eliminate the terms which appear in the denominator of the resulting expression. Note this procedure can be repeated in order to derive the higher order derivatives of the functional.

3. EIGENVALUE CORRECTION PROCEDURE

The proposed procedure for recovering the error in the eigenvalue is linear because a first order Taylor series is used. This is exact when the fission-source normalisation is applied, because the high order derivatives of the eigenvalue are all zero. Note this is not the case when the eigenvector normalisation is applied. In that case, high order derivatives exist and would need to be included in order to obtain a correction. This generally requires the Hessian to be computed which is numerically demanding. Worse still, with the eigenvector normalisation there is no information on the first order term because this is zero at a saddle point. Use of the eigenvector normalisation is therefore not recommended.

3.1 Linear Functional Correction Procedure

One can expand the functional as a Taylor series as follows:

$$\begin{aligned} F_{\text{FS}}(\Psi_{\text{exact}}) - F_{\text{FS}}(\Psi) &= \left. \frac{\partial F_{\text{FS}}}{\partial \Psi} \right|_{C_{\text{FS}}(\Psi)=1} (\Psi_{\text{exact}} - \Psi) \\ &= \mathbf{b}^T (\mathbf{A} - \lambda \mathbf{B}) (\Psi_{\text{exact}} - \Psi) \end{aligned} \quad (7)$$

in which Ψ_{exact} is the exact eigenvector corresponding to the associated exact eigenvalue that we are attempting to determine. All other terms in this expansion vanish provided that both Ψ and Ψ_{exact} satisfy the normalisation condition Eqn. 4. Likewise, one can expand the residual to first order and obtain:

$$\begin{aligned} \mathcal{R}(\Psi_{\text{exact}}) - \mathcal{R}(\Psi) = -\mathcal{R}(\Psi) &\approx \frac{\partial \mathcal{R}}{\partial \Psi} (\Psi_{\text{exact}} - \Psi) \\ &= \left(\mathbf{A} - \lambda \mathbf{B} - (\mathbf{B}\Psi)\mathbf{b}^T(\mathbf{A} - \lambda \mathbf{B}) \right) (\Psi_{\text{exact}} - \Psi) \\ &= (\mathbf{A} - \lambda \mathbf{B} - \mathbf{Q}) (\Psi_{\text{exact}} - \Psi) \end{aligned} \quad (8)$$

in which $\mathbf{Q} = (\mathbf{B}\Psi)\mathbf{b}^T(\mathbf{A} - \lambda\mathbf{B})$. Note this expression contains the full rank-1 matrix $(\mathbf{B}\Psi)\mathbf{b}^T$, as this comprises the outer (tensor) product of the two vectors $(\mathbf{B}\Psi)$ and \mathbf{b}^T . This may be interpreted as an energy source/sink in the equations because \mathbf{Q} is full and this serves to make the matrix $(\mathbf{A} - \lambda\mathbf{B} - \mathbf{Q})$ problematic (potentially singular). In order to produce a correction to the eigenvector, one proceeds by inverting the above expression:

$$\Psi_{\text{exact}} - \Psi = - \left(\frac{\partial \mathcal{R}}{\partial \Psi} \right)^{-1} \mathcal{R}(\Psi) \quad (9)$$

The corresponding correction to the eigenvalue is given by:

$$\begin{aligned} F_{\text{FS}}(\Psi_{\text{exact}}) - F_{\text{FS}}(\Psi) &= - \left. \frac{\partial F_{\text{FS}}}{\partial \Psi} \right|_{C_{\text{FS}}(\Psi)=1} \left(\frac{\partial \mathcal{R}}{\partial \Psi} \right)^{-1} \mathcal{R}(\Psi) \\ &= \mathcal{R}(\Psi)^T \left(\frac{\partial \mathcal{R}}{\partial \Psi} \right)^{-T} \left(- \left. \frac{\partial F_{\text{FS}}}{\partial \Psi} \right|_{C_{\text{FS}}(\Psi)=1} \right)^T \\ &= \mathcal{R}(\Psi)^T \Psi^* \end{aligned} \quad (10)$$

where the adjoint flux Ψ^* has been introduced. This is defined as the solution vector to the system

$$\frac{\partial \mathcal{R}}{\partial \Psi} \Psi^* = \left(- \left. \frac{\partial F_{\text{FS}}}{\partial \Psi} \right|_{C_{\text{FS}}\Psi=1} \right)^T \quad (11)$$

which may be explicitly written as

$$\begin{aligned} (\mathbf{A}^T - \lambda\mathbf{B}^T - \mathbf{Q}^T)\Psi^* &= (\mathbf{A}^T - \lambda\mathbf{B}^T)\Psi^* - (\mathbf{A} - \lambda\mathbf{B})^T \mathbf{b}(\mathbf{B}\Psi)^T \Psi^* \\ &= -(\mathbf{A}^T - \lambda\mathbf{B}^T)\mathbf{b} \end{aligned} \quad (12)$$

This serves to define the adjoint eigenvector up to an unknown constant, so one might choose $(\mathbf{B}\Psi)^T \Psi^* = 0$ so that the term containing the \mathbf{Q} matrix can be dropped from the left hand side of the adjoint equation, thereby removing the explicit dependence on Ψ from this equation. When it comes to computing the correction, the Galerkin orthogonality properties of the discretisation ensure that the correction is invariant to a constant offset in the adjoint eigenvector solution, that is to say $\mathcal{R}(\Psi)^T \mathbf{b} = 0$. The resulting adjoint equation is:

$$(\mathbf{A}^T - \lambda\mathbf{B}^T)\Psi^* = -(\mathbf{A}^T - \lambda\mathbf{B}^T)\mathbf{b} \quad (13)$$

Note Eqn. 13 may alternatively be written as:

$$(\mathbf{A}^T - \lambda\mathbf{B}^T)(\Psi^* + \mathbf{b}) = \mathbf{0} \quad (14)$$

Consequently, $\Psi^* + \mathbf{b}$ is a generalised eigenvalue of the operator \mathbf{A}^T with respect to the matrix \mathbf{B}^T corresponding to the eigenvalue λ , scaled to satisfy $(\mathbf{B}\Psi)^T(\Psi^* + \mathbf{b}) = 1$. For a symmetric (self adjoint) pair of operators this implies that $\Psi^* = \alpha\Psi - \mathbf{b}$ where α is a constant which must be determined from the normalisation condition:

$$0 = (\mathbf{B}\Psi)^T\Psi^* = (\mathbf{B}\Psi)^T(\alpha\Psi - \mathbf{b}) = \alpha\Psi^T\mathbf{B}\Psi - 1 \quad (15)$$

which implies that $\Psi^* = (\Psi^T\mathbf{B}\Psi)^{-1}\Psi - \mathbf{b}$. For asymmetric operators one must solve the above equation in order to determine the adjoint eigenvector. Finally, one is in a position to update the functional using the following expression:

$$F_{\text{FS}}(\Psi_{\text{exact}}) = F_{\text{FS}}(\Psi) + \mathcal{R}(\Psi)^T\Psi^* \quad (16)$$

If the same spatial basis functions are used for the forward and adjoint solutions, in conjunction with a Galerkin weighted discretisation of the forward and adjoint problems, then the Galerkin orthogonality properties of the residual will lead to zero correction. Consequently, one must use a more finely resolved and/or higher order solution for the adjoint eigenvectors appearing in the correction term. In the present work this shall be referred to as $\Psi_{h/2}^*$ in which h refers to a mesh spacing. This results in a correction term that is computable:

$$\begin{aligned} F_{\text{FS}}(\Psi_{\text{exact}}) &= F_{\text{FS}}(\Psi) + \mathcal{R}_{h/2}(\Psi_h)^T(\Psi_{h/2}^* - \Psi_h^*) \\ &= F_{\text{FS}}(\Psi) + (\Psi_{h/2}^* - \Psi_{h \rightarrow h/2}^*)^T(\mathbf{A}_{h/2} - \lambda_h\mathbf{B}_{h/2})\Psi_{h \rightarrow h/2} \end{aligned} \quad (17)$$

where $h \rightarrow h/2$ represents the prolongation of the solution onto the finer mesh and/or higher order basis functions denoted by $h/2$. Typically, the finely resolved adjoint solution would be obtained via use of an C^1 continuous bicubic spline.

3.2 Adjoint Problem

One could also define a functional from the adjoint eigenvalue:

$$F_{\text{FS}}^*(\Psi^*) = \lambda^* = \mathbf{b}^T\mathbf{A}^T\Psi^* (= \lambda) \quad (18)$$

with the following constraint

$$C_{\text{FS}}^*(\Psi^*) = \mathbf{b}^T\mathbf{B}^T\Psi^* = 1 \quad (19)$$

Repeating the previous derivation with the transposed operators, interchanging the definition of the forward and adjoint solutions, leads to the following procedure. One starts by solving the adjoint problem with the above normalisation of the adjoint eigenvector Ψ^* .

$$\mathcal{R}^*(\Psi^*) = (\mathbf{A}^T - \lambda^* \mathbf{B}^T) \Psi^* = \mathbf{0} \quad (20)$$

One then solves the associated primal problem

$$(\mathbf{A} - \lambda \mathbf{B})(\Psi + \mathbf{b}) = \mathbf{0} \quad (21)$$

subject to the normalisation $(\mathbf{B}^T \Psi^*)^T \Psi = 0$ and then computes the correction to the adjoint eigenvalue:

$$F_{\text{FS}}^*(\Psi_{\text{exact}}^*) = F_{\text{FS}}^*(\Psi^*) + \mathcal{R}^*(\Psi^*)^T \Psi \quad (22)$$

where an improved forward solution will be required in order to calculate the correction. This procedure will produce a defect correction for the adjoint eigenvalue in agreement with that derived based on the forward solution, provided an identical technique for deriving the higher order solution is used. Note that the alternative pair of adjoint and forward eigenvectors have a different normalisation to that used for the forward correction.

3.3 Local Smoothing

Due to the Galerkin orthogonality, one will find Eqn. 16 results in zero correction. An alternative approximation to the error in the eigenvalue is derived in Eqn. 17. However, this requires a locally enriched solution to be defined on a fine mesh of spacing $h/2$ and the forward solution, calculated on a coarse mesh of spacing h , to be prolonged on to the fine mesh. The difference between the prolonged solution and the enriched solution may then be used on the fine mesh in order to define a non-zero correction. Typically, a cubic ($p=3$) polyhedral element type is used to define the enriched solution, and the prolongation operator $\mathbf{O}(h \rightarrow h/2)$ projects the linear element solution Ψ_h onto the cubic element to obtain the prolonged solution. This operation may be written as

$$\Psi_{h \rightarrow h/2} = \mathbf{O}(h \rightarrow h/2) \Psi_h \quad (23)$$

in which $\Psi_{h \rightarrow h/2}$ is the prolonged solution. Note this will be linear in terms of its convergence. Therefore the operator $\mathbf{O}(h \rightarrow h/2)$ is a 16×4 matrix that operates on the linear solution (which is a vector of length 4) and produces a new vector, $\Psi_{h \rightarrow h/2}$ which is of length 16 and comprises the prolonged eigenvector values at each of the 16 nodes of the cubic finite element. The improved solution, denoted by $\Psi_{h/2}$, is obtained by evaluating a bicubic surface at the coordinates of these nodes. This is done by taking the linear solution Ψ_h which is known at the 4 corners, and calculating the x and y gradients and the cross-derivative at the 4 corners using finite differences. These quantities are placed in the vector \mathbf{b} , of length 16. One then solves the matrix equation

$$\mathbf{M}\mathbf{c} = \mathbf{b} \quad (24)$$

for the vector of coefficients \mathbf{c} . The matrix \mathbf{M} is define in [8] and is not derived herein. The bicubic surface

$$S(x, y) = \sum_{j=0}^3 \sum_{i=0}^3 c_{ij} x^i y^j \quad (25)$$

is finally evaluated at the 16 nodes to obtain the enriched solution $\Psi_{h/2}$. Fitting a two-dimensional bicubic spline through the eigenvector in this manner produces solutions that are three times differentiable and C^1 continuous across element boundaries. The enriched solution $\Psi_{h/2}$ is therefore much smoother than the underlying solution $\Psi_{h \rightarrow h/2}$ that bounds it. One may then evaluate the difference between the prolonged and improved solution, that is to obtain $(\Psi_{h/2} - \Psi_{h \rightarrow h/2})$, at each of the 16 nodes within the cubic element and place this in Eqn. 17 to apply defect corrections to the eigenvalue λ .

4. NUMERICAL RESULTS

Results are presented in this section on a series of two dimensional elliptic problems in Cartesian geometry using continuous finite elements. Use is made of the fission source normalisation defined in Eqn. 4. All the problems are calculated on a regular orthogonal mesh, as the correction scheme uses a bicubic fit discussed in section 3.3 that is designed for regular spacing of the interpolation points. Correction on unstructured grids is left as a future topic.

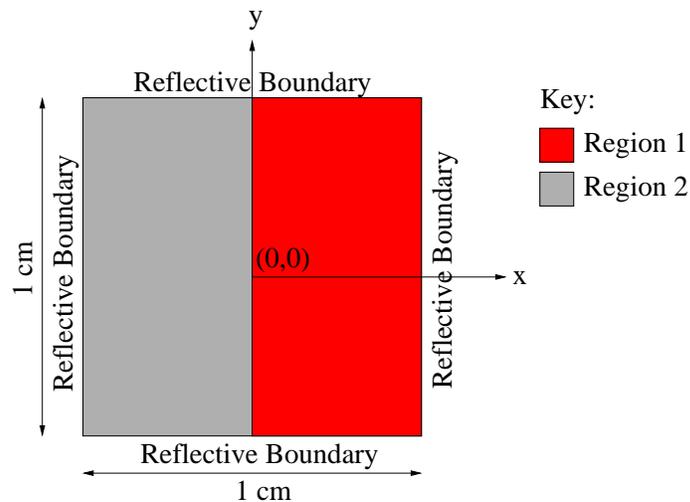


Figure 3: Problem I domain.

The domain of problem I is illustrated in Fig. 1. The first problem comprises two material regions. Region 1 is a pure absorber in the range $-0.5 \leq x \leq 0.0$, $-0.5 \leq y \leq 0.5$. Region 2 contains a fission source of $\sigma_f = 10.0$ and is in the range $0.0 \leq x \leq 0.5$, $-0.5 \leq y \leq 0.5$. The removal cross-section of both regions is $\sigma_a = 10.0$. The domain of this problem is illustrated in Fig. 3, and the materials used are defined in Table I.

Region	σ_a	σ_f
1	10.0	0.0
2	10.0	10.0

Table I: Definition of materials in problem I

Results for problem I are shown in Fig. 4, in which eigenvalue error is plotted against number of elements along the x-axis for improving mesh resolution. The eigenvalue error is defined as $\epsilon = \frac{\lambda - \lambda_{exact}}{\lambda_{exact}}$, in which λ is the eigenvalue obtained on a coarse mesh using linear (p=1) and quadratic (p=2) continuous finite elements and λ_{exact} is that obtained on a very fine mesh using the same method. The error in the uncorrected eigenvalue is calculated for both the p=1 and p=2 element type. The eigenvalue obtained using the p=1 element type is corrected. The error in this corrected result is also plotted. Correction dramatically improves the convergence rate of the p=1 eigenvalue estimate, by recovering a high proportion of the error on the coarse mesh. The corrected result does not converge as fast as the p=2 eigenvalue, but is significantly better than the p=1 eigenvalue without correction. The error is obtained using the enriched solution, based on a bicubic interpolation as discussed in section 3.3.

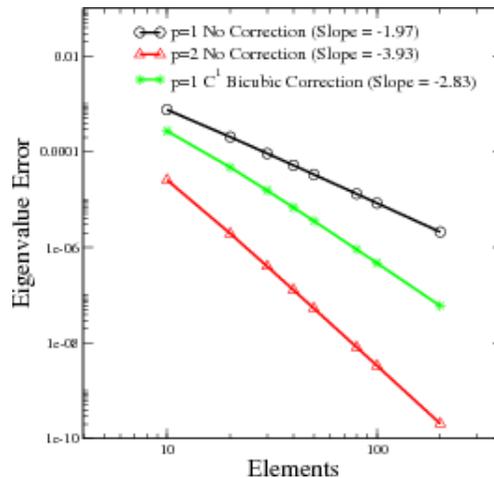


Figure 4: Problem I eigenvalue correction.

Correction increases the magnitude of the slope from 1.97 (uncorrected) to 2.83 (corrected), recovering an order of convergence in the eigenvalue.

A second problem comprising a source in the top right corner of the domain is considered as the next test case. In this problem, region 1 contains a fission source of $\sigma_f = 10.0$. This is defined in the ranges $0.0 \leq x \leq 0.5$ and $0.0 \leq y \leq 0.5$. Region 2 comprises an absorber of absorption cross-section $\sigma_a = 10.0$. The domain of problem II is illustrated in Fig. 5.

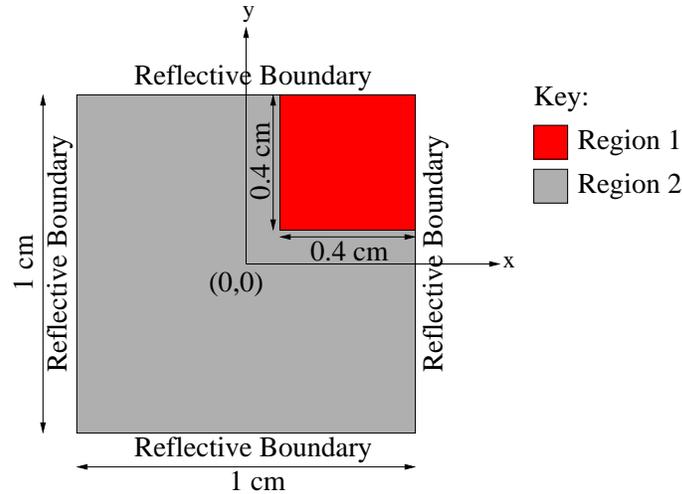


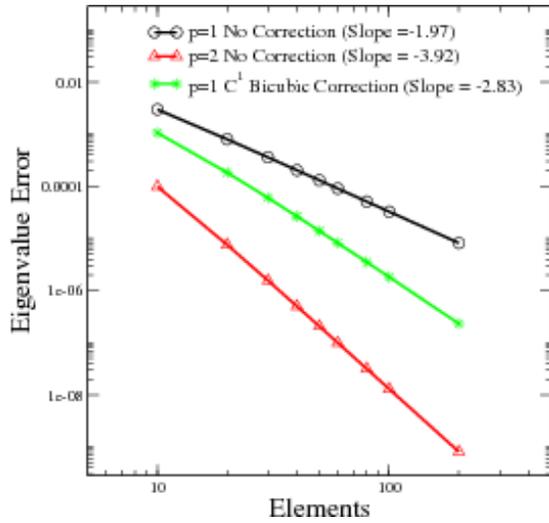
Figure 5: Problem II domain.

The materials used in this problem are defined in Table II

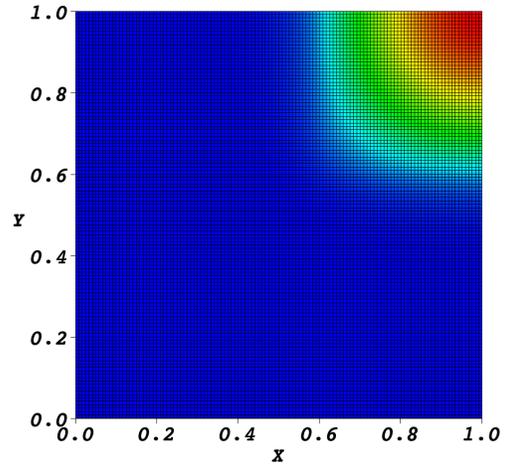
Region	σ_a	σ_f
1	10.0	10.0
2	10.0	0.0

Table II: Definition of materials in problem II

The error in both corrected and uncorrected eigenvalue is plotted against number of elements as done for the previous problem. These plots are included in Fig. 6(a). Uncorrected eigenvalues are shown for both a $p=1$ and a $p=2$ element type, and the $p=1$ corrected eigenvalue is shown. A contour plot of the eigenvector is included in Fig. 6(b) to illustrate the particles being absorbed very sharply as they diffuse from the source region. The gradient in the solution is sharp around the boundary of the source making this a very challenging problem. However, the adjoint based correction scheme performs consistently well in this problem, again recovering an order of convergence with respect to the uncorrected $p=1$ solution. This improves the magnitude of the slope from 1.97 ($p=1$ uncorrected) to 2.83 ($p=1$ corrected). The convergence rate of the corrected eigenvalue is still not as good as that of an uncorrected eigenvalue obtained using a $p=2$ element. However, a $p=2$ solution is far more intensive to obtain computationally.



(a) Correction



(b) Eigenvector

Figure 6: Problem III correction and eigenvector contour graphic.

A final test problem is considered that is designed to test error recovery when multiple sources are present. Problem III, the domain of which is illustrated in Fig. 7, comprises four source "pins" inside a moderate absorber.

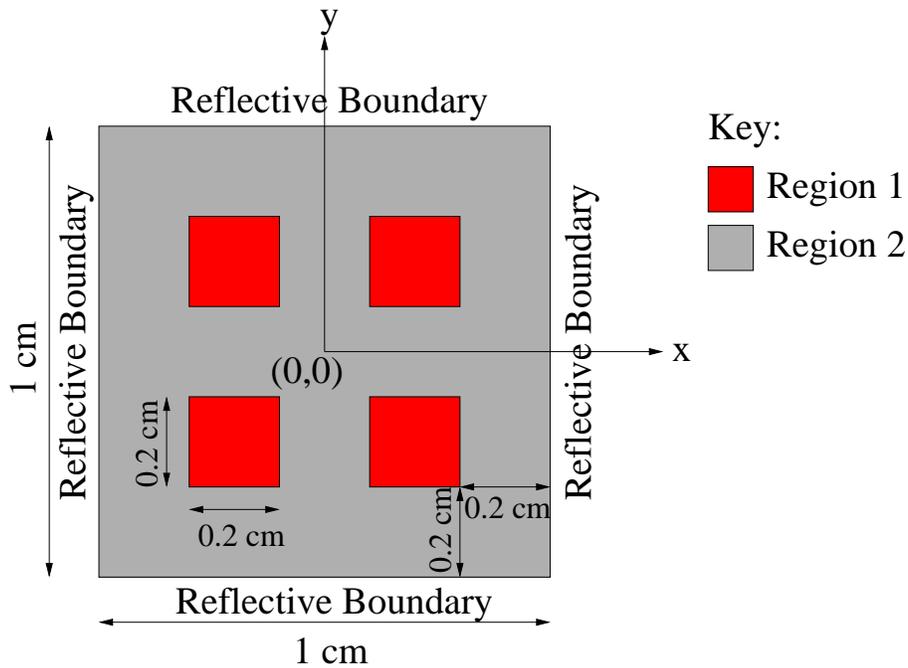


Figure 7: Problem III domain.

The source pins (region 1) are each of dimension 2 cm x 2cm, and located with their centres

positioned at coordinates $x,y=(2.5,2.5)$, $(7.5,2.5)$, $(2.5,7.5)$, $(7.5,7.5)$ within the domain. The material they comprise of has a fission cross-section $\sigma_f = 10.0$ and absorption cross-section $\sigma_a = 10.0$. The absorber (region 2) has no sources present and an absorption cross-section of $\sigma_a = 10.0$. There is no scattering in this problem. It is noted that scattering would make this test case a more demanding problem. However, scattering effects are left as the topic of further work. The materials are defined in Table III.

Region	σ_a	σ_f
1	10.0	10.0
2	10.0	0.0

Table III: Definition of materials in problem III

Results for problem III are presented in Fig. 8. As with the previous problems, eigenvalue error has been plotted against the number of elements along the x-axis of the mesh. The error in the uncorrected eigenvalue is demonstrated for a $p=1$, $p=2$ and $p=3$ element type. The $p=1$ eigenvalue is corrected with the bicubic spline in the same manner as the previous problems.

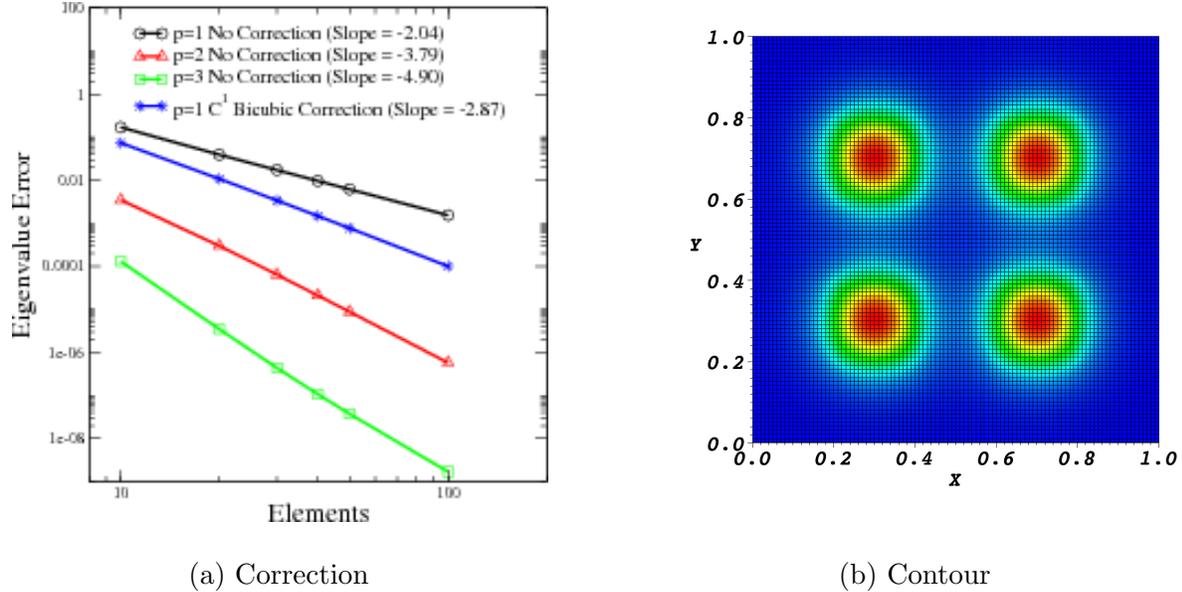


Figure 8: Problem III correction and eigenvector contour graphic.

Correction using the bicubic fit again improves the convergence rate of the $p=1$ eigenvalue, in this test case the magnitude of the slope increases from 2.04 ($p=1$ uncorrected) to 2.87 ($p=1$ corrected). This rate is not as good as that of the higher order elements, which in this problem are found to have slope magnitudes of 3.79 ($p=2$ uncorrected) and 4.90 ($p=3$ uncorrected). However,

use of the $p=2$ and $p=3$ element types in this calculation is far more intensive numerically than using a $p=1$ element with the defect correction, as found with the previous problems. A contour graphic of the eigenvector solution is included to illustrate the profile of the flux in the vicinity of the four pins.

5. CONCLUSIONS

An adjoint based approach to removing the error in eigenvalue calculations is presented. The scheme, which uses a first order Taylor analysis of the eigenvalue functional and residual of the governing equation, derives an approximation to the error. A defect correction on the solution is then performed in which the approximation to the error is removed from the solution. Significant improvements to the convergence rate of the eigenvalue are achieved via this approach. This is demonstrated using Galerkin weighted continuous finite elements on a series of demanding two dimensional elliptic problems in Cartesian (X-Y) geometry. This formulation can also be applied to hyperbolic problems (work in progress) as well as other types of discretisation in general geometries. It may also be applied to other types of functional besides the eigenvalue. Suggested applications of this approach are to define an error metric that may be used to automate mesh adaptivity in addition to improving bulk functional estimates on coarse computational grids.

ACKNOWLEDGEMENTS

The work herein has been undertaken as part of a PhD in the Applied Modelling and Computation Group, Imperial College London. The authors wish to acknowledge that this PhD is being funded by AWE plc and has used time and resources supplied by the Computational Physics Group at AWE plc.

REFERENCES

1. D. A. Venditti and D. L. Darmofal. Grid Adaptation for Functional Outputs: Application to Two-Dimensional Inviscid Flows. *Journal of Computational Physics.*, **176**, pp. 40-69 (2002).
2. D. A. Venditti and D. L. Darmofal. Anisotropic Grid Adaptation for Functional Outputs: Application to Two-Dimensional Viscous Flows. *Journal of Computational Physics.*, **187**, pp. 22-46 (2003).
3. D. A. Venditti and D. L. Darmofal. Adjoint Error Estimation and Grid Adaptation for Functional Outputs: Application to Quasi-One-Dimensional Flow. *Journal of Computational Physics.*, **164**, pp. 204-227 (2000).
4. N. A. Pierce and M. B. Giles. Adjoint and Defect Error Bounding and Correction for Functional Estimates. *Journal of Computational Physics.*, **200**, pp. 769-794 (2004).
5. M. B. Giles and N. A. Pierce and E. Suli. Progress in Adjoint Error Correction for Integral Functionals. *Computing and Visualization in Science.*, **6**, pp. 113-121 (2004).

6. M. Ainsworth and J. T. Oden. A Posteriori Error Estimation in Finite Element Analysis. *Computer Methods in Applied Mechanics and Engineering.*, **142**, pp. 1-88 (1997).
7. P. W. Power *PhD Thesis:Error Measures for Finite Element Ocean Modelling.* Imperial College, London United Kingdom (2007).
8. W. H. Press, S. A. Teukolsky, W. T. Vetterling and B. P. Flannery *Numerical Recipes The Art of Scientific Computing Third Edition.* Cambridge University Press, New York & USA (2007).