Adaptive finite element method for eigensolutions of regular second and fourth order Sturm-Liouville problems via the element energy projection technique

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ABSTRACT

Purpose

A numerically adaptive finite element (FE) method is presented for accurate, efficient and reliable eigensolutions of regular second and fourth order Sturm-Liouville (SL) problems with variable coefficients.

Methodology

After the conventional FE solution for an eigenpair (i.e. eigenvalue and eigenfunction) of a particular order has been obtained on a given mesh, a novel strategy is introduced, in which the FE solution of the eigenproblem is equivalently viewed as the FE solution of an associated linear problem. This strategy allows the Element Energy Projection (EEP) technique for linear problems to calculate super-convergent FE solutions for eigenfunctions anywhere on any element. These EEP super-convergent solutions are used to estimate the FE solution errors and to guide mesh refinements, until the accuracy matches user-preset error tolerance on both eigenvalues and eigenfunctions.

Findings

Numerical results for a number of representative and challenging SL problems are presented to demonstrate the effectiveness, efficiency, accuracy and reliability of the proposed method.

Research limitations

The method is limited to regular SL problems, but it can also solve some singular SL problems in an indirect way.

Value

Comprehensive utilization of the EEP technique yields a simple, efficient and reliable adaptive FE procedure that finds sufficiently fine meshes for preset error tolerances on eigenvalues and eigenfunctions to be achieved, even on problems which proved troublesome to competing methods. The method can readily be extended to vector SL problems.

KEYWORDS: Eigenvalues; Adaptivity; Finite element; Energy methods; Projection schemes.

ARTICLE CLASSIFICATION: Research paper

1. INTRODUCTION

The theory presented in this paper covers the regular second and fourth order Sturm-Liouville (SL) eigenproblems to which many physical problems over a continuous spatial domain can be reduced. However, for convenience, the vibration of a non-uniform structural member is chosen as the default physical model in this paper. For brevity, Dirichlet (i.e. fixed-end) boundary conditions (BCs) are taken as the default for both second and fourth order SL problems in this paper. Also, for conciseness, whenever possible, both the second and fourth order SL problems are dealt with together by putting the fourth order case into brackets, e.g. second [fourth] order case. Additionally, in the equations parts (a) and (b) are for the second and fourth order SL cases, respectively, and the mathematical term 'eigenfunction' is frequently replaced by the physical term 'mode'.

The regular second order SL problem is to find the eigenvalues λ and eigenfunctions $u(x)$ of the second order ordinary differential equation (ODE)

$$Lu \equiv -(p(x)u')' + q(x)u = \lambda r(x)u, \quad a < x < b \tag{1}$$

subject to the default BCs

$$u(a) = 0, \quad u(b) = 0 \tag{2}$$

where: prime denotes ordinary derivative; L is the associated self-adjoint operator; (a,b) is finite; p, p', q and r are continuous on $[a,b]$; $p > 0$ and $r > 0$ on $[a,b]$.

The regular fourth order SL problem is to find the eigenvalues λ and eigenfunctions $w(x)$ of the fourth order ODE

$$Lw \equiv (p(x)w'')'' - (s(x)w')' + q(x)w = \lambda r(x)w, \quad a < x < b \tag{3}$$

subject to the default BCs

$$\begin{cases} w(a) = 0 \\ w'(a) = 0 \end{cases} \qquad \begin{cases} w(b) = 0 \\ w'(b) = 0 \end{cases} \tag{4}$$

where: p, p', p'', s, s', q and r are all continuous on $[a,b]$; $p > 0$ and $r > 0$ on $[a,b]$. Note that the same symbol L is used in Eqs. (1) and (3) to represent different self-adjoint operators, which are easily distinguishable from related contexts.

For second order SL problems, there are a number of state-of-the-art codes, e.g. SLEDGE (Pruess and Fulton, 1993), SLEIGN2 (Bailey *et al*., 2001) and components of the NAG library (Numerical Algorithms Group, 1999), of which some only find the eigenvalues. However, the fourth order SL problem is very challenging and to the

authors' best knowledge the only code that specifically solves such problems is SLEUTH (Greenberg and Marletta, 1997), which unfortunately does not impose error control on eigenfunctions and hence cannot serve as a complete eigensolver. Both packages of SLEDGE and SLEUTH use piecewise constant approximation of the variable coefficients in SL problems with shooting methods used to locate eigenvalues. The package SLEIGN2 uses the Prüfer transformation and oscillatory properties to calculate both eigenvalues and eigenfunctions.

There are some other approximate methods dedicated to SL problems. Prikazchikov and Loseva (2004) constructed a difference scheme of high order by using a special FE method for second order SL problems, Andrew (2003) proposed an asymptotic correction technique to improve the accuracy of FE solutions for second order SL problems, Yücel and Boubaker (2012) applied the Differential Quadrature Method to compute the eigenvalues of some regular fourth order SL problems, and Taher *et al*. (2013) proposed a technique based on the chebyshev spectral collocation method for the eigenvalues of fourth order SL problems. However, these methods are generally not adaptivity oriented and lack ingredients required in an adaptive package.

The authors of this paper were motivated to probe into SL eigenproblems from the structural engineering discipline by having successfully solved structural vibration problems with uniform members (Yuan *et al*., 2003; Williams and Wittrick, 1970; Wittrick and Williams, 1971, 1973), which are special cases of both second and fourth order SL problems with constant coefficients. Four of the present authors developed a recursive second order convergence method (Yuan *et al*., 2003) for accurate solution of both eigenvalues (natural frequencies) and eigenfunctions (modes) by using the exact Dynamic Stiffness Method (DSM). This critical success led to further progress in a series of research projects using the DSM (Djoudi *et al*., 2005; Yuan *et al*., 2007c, 2014).

The procedure presented in this paper is based on the conventional finite element (FE) method (Bathe, 1996). This means that it no longer requires the calculation of exact dynamic stiffnesses, but instead relies on sufficiently fine meshes being found for sufficiently accurate FE solutions. The most important and substantial contribution of the present paper is its presentation of an adaptive procedure for finding such meshes. A key component in the procedure is the recently developed Element Energy Projection (EEP) technique (Yuan *et al*., 2006, 2007a, 2007b; Yuan and Zhao, 2007; Yuan and Xing, 2014), which is applied, with a novel 'technology transfer' from linear problems

to the current eigenproblem, to calculate super-convergent solutions, which are called EEP solutions in the following, for eigenfunctions during the FE post-processing stage. These EEP solutions are then used as if they were exact solutions to estimate the errors in the FE solutions and hence to further guide mesh refinements (Yuan and He, 2006; Yuan *et al*., 2008). This yields a simple, efficient, reliable and general adaptive FE procedure that is able to find sufficiently fine meshes for the accuracy of the obtained FE solutions to satisfy the user-preset error tolerances on both eigenvalues and eigenfunctions.

2. OUTLINE OF THE SOLUTION PROCEDURE

For conciseness and neatness, suppose that the leading n eigenpairs $(\lambda_k, u_k\,[w_k])$ $(k=1,\ldots,n)$ are required (although k may not necessarily be from 1) and that the user-preset error tolerance for both eigenvalues and modes is Tol. The aim of the procedure presented is to find FE solutions $(\lambda_k^h, u_k^h\,[w_k^h])$ $(k=1,\ldots,n)$ on sufficiently fine meshes π_k $(k=1,\ldots,n)$ such that

$$|\lambda_k-\lambda_k^h|\le Tol\cdot(1+|\lambda_k|) \tag{5}$$

$$\max|u_k-u_k^h|\le Tol\text{, with }\max|u_k|=1 \tag{6a}$$

$$\max|w_k-w_k^h|\le Tol\text{ with }\max|w_k|=1 \tag{6b}$$

Since the exact solutions $(\lambda_k, u_k\,[w_k])$ are not usually available, the proposed procedure uses the following stop criteria instead

$$\lambda_u-\lambda_l\le Tol\cdot(1+\max(|\lambda_l|,|\lambda_u|)),\qquad \lambda_k^h\in(\lambda_l,\lambda_u) \tag{7}$$

$$\max|u_k^*-u_k^h|\le Tol\text{, with }\max|u_k^h|=1 \tag{8a}$$

$$\max|w_k^*-w_k^h|\le Tol\text{ with }\max|w_k^h|=1 \tag{8b}$$

where the eigenvalue interval is defined by bounds (λ_l, λ_u) calculated on the mesh π_k and the more accurate u_k^* $[w_k^*]$ are EEP solutions calculated based on u_k^h $[w_k^h]$ on the mesh π_k, which will be described below. Note that once Eq. (7) is satisfied with true bounds (λ_l, λ_u), any value in (λ_l, λ_u) serves as a valid FE solution λ^h which is guaranteed to satisfy Eq. (5).

In practical computation, the solution procedure starts from the lowest eigenpair

$(\lambda_1, u_1\,[w_1])$ and successively advances until the highest eigenpair $(\lambda_n, u_n\,[w_n])$ has been found. To start with the first eigenpair, an initial mesh π_0 is specified by the user. After the adaptive solution for the first eigenpair has been completed, its final mesh π_1 is used as the initial mesh for finding the next eigenpair.

The proposed adaptive procedure achieves the above objective for each eigenpair $(\lambda, u\,[w])$ simply by implementing the following three-step adaptive strategy.

(1) FE solution. On the current mesh, the conventional FE solution $(\lambda^h, u^h\,[w^h])$ is obtained by jointly using the bisection method, the Sturm sequence property and inverse iteration, as described in Section 3.

(2) EEP solution. Based on the FE solution $(\lambda^h, u^h\,[w^h])$, the EEP solution $u^*\,[w^*]$ is calculated on each element *e*, as described in Section 4.

(3) Mesh refinement. The EEP solution $u^*\,[w^*]$ is used to calculate the maximum error on each element $\max\limits_e |u^* - u^h|$ [$\max\limits_e |w^* - w^h|$]. For those elements for which Eq. (8) is not satisfied, the error-averaging method (Yuan *et al*., 2008) is used to subdivide each into two elements, forming a new refined mesh, as described in Section 5. Then the procedure returns to the first step (i.e. the FE solution) and cycles until all elements satisfy Eq. (8).

The above three steps constitute a round of adaptive iteration. After Eq. (8) has been satisfied by a series of such adaptive iterations, the procedure further proceeds to satisfying Eq. (7) by adjusting the bounds on the sought eigenvalue.

3. FE SOLUTION

This section describes the implementation of the first step of the adaptive strategy, i.e. the conventional FE solution.

3.1 FE formulation

The element model adopted is the conventional polynomial element of degree $m>1$ [$m>3$], with length h and end nodal coordinates $\bar{x}_1$ and $\bar{x}_2$. Also let $u^h \in C^0$ [$w^h \in C^1$] denote the conventional FE solution on the given mesh π, in which C^0 is the space of continuous functions and C^1 is the space of the functions which are continuous up-to the first-order derivative. As in common practice, the shape functions

for u^h could be of either Lagrange or hierarchical type whereas those for w^h are of Hermite type.

For the current mesh π, the standard FE formulation leads to a linear eigenproblem of the form (Bathe, 1996)

$$\mathbf{KD} = \lambda \mathbf{MD} \tag{9}$$

where $\mathbf{D}$ is the so-called mode vector, and both $\mathbf{K}$ and $\mathbf{M}$ are square and symmetrical constant matrices with $\mathbf{M}$ being also positive definite. Given an arbitrary trial value λ_a (shift value), the above problem can be equivalently written in the shifted form (Bathe, 1996)

$$\mathbf{K}_a \mathbf{D} = \mu \mathbf{MD} \quad \text{with } \mathbf{K}_a = \mathbf{K} - \lambda_a \mathbf{M},\ \mu = \lambda - \lambda_a \tag{10}$$

Eq. (10) is taken as the eigenproblem to be solved in the remainder of this paper.

3.2 Divide-and-Conquer

For the sake of reliability, Eq. (10) is solved by a two-phase *Divide-and-Conquer* (DC) strategy (Yuan *et al*., 2003) as follows.

(i) *Divide phase.* Quickly isolate an eigenvalue interval (λ_l, λ_u) containing the sought eigenvalue (initially the first one λ_1^h) on the current mesh by using the bisection method via the Sturm sequence property;

(ii) *Conquer phase.* Find the eigenpair $(\mu^h, \mathbf{D}^h)$ by using inverse iteration to obtain the conventional FE solution $(\lambda^h, u^h[w^h])$ with $\lambda^h \in (\lambda_l, \lambda_u)$.

3.3 J-count based on Sturm sequence property

According to the well-known Sturm sequence property (Wilkinson, 1965), the total number of eigenvalues below λ_a for Eq. (10) can be calculated by the following *J-count* formula

$$J(\lambda_a) = s\{\mathbf{K}_a\} \tag{11}$$

Here $s\{\mathbf{K}_a\}$ is the sign count of $\mathbf{K}_a$, which equals the number of negative leading diagonal elements of the upper triangular matrix $\mathbf{K}_a^{\Delta}$ obtained from $\mathbf{K}_a$ by ordinary Gaussian elimination. One of the usages of the *J-count* is, at the *Divide phase*, to incorporate it into the bisection method (Williams and Wittrick, 1970) to search for bounds (λ_l, λ_u) on the sought *k*-th eigenvalue λ_k such that $J(\lambda_u) \geq k$ and $J(\lambda_l) < k$.

Another usage is to compute the number of eigenvalues N_r in a given eigenvalue interval (λ_l, λ_u) as

$$N_r = J(\lambda_u) - J(\lambda_l) \tag{12}$$

Using the *J-count*, the *Divide phase* is performed as follows. Bisection is used simply to find an interval (λ_l, λ_u) containing the sought eigenvalue λ_k and then the interval (λ_l, λ_u) is further narrowed by the bisection method until either (a) $N_r = 1$ in (λ_l, λ_u) or (b) $N_r > 1$ in (λ_l, λ_u) but the interval is narrow enough to satisfy the stop criterion of Eq. (7). In case (b), all N_r (>1) eigenvalues in (λ_l, λ_u) are considered to be coincident for the current mesh. In the following analysis, case (a) is considered as the default case with case (b) only briefly addressed.

When an appropriate interval (λ_l, λ_u) has been identified, the procedure switches from the *Divide phase* to the *Conquer phase* which solves Eq. (10) by inverse iteration for the eigenpair $(\mu^h, \mathbf{D}^h)$.

3.4 Inverse iteration

Suppose that during the *Divide phase* an eigenvalue interval (λ_l, λ_u) has been identified by the bisection method. In case (a), i.e. when $N_r = 1$, the initial λ_a is set as $\lambda_a = \frac{1}{2}(\lambda_l + \lambda_u)$. This ensures that the nearest eigenvalue to λ_a is the one within (λ_l, λ_u) and hence guarantees that the desired eigenvalue μ is the numerically smallest of all the eigenvalues of Eq. (10) and so can be safely and efficiently solved for by using inverse iteration (Yuan *et al*., 2003) which guarantees convergence on the eigenpair $(\mu, \mathbf{D})$ for which the absolute eigenvalue is least. The inverse iteration is terminated when

$$\left|\mu^{(i+1)} - \mu^{(i)}\right| < Tol \quad \text{and} \quad \max\left|D_j^{(i+1)} - D_j^{(i)}\right| < Tol \tag{13}$$

Here $D_j^{(i)}$ is the *j*-th component in $\mathbf{D}$ at the *i*-th inverse iteration step and $\mathbf{D}$ is normalized by $\max_j |D_j| = 1$. In case (b), i.e. when $N_r > 1$, Eq. (10) is solved with $\lambda_a = \frac{1}{2}(\lambda_l + \lambda_u)$ by using subspace iteration to find the N_r absolutely smallest eigenpairs simultaneously.

Note that both the inverse and subspace iterations involve factorization of $\mathbf{K}_a$,

which implies the *J-count* at λ_a for the current mesh can easily be found without additional computation. Hence it is immediately known whether λ_a is a new upper or lower bound and the eigenvalue interval (λ_l, λ_u) is updated accordingly.

After the above inverse iteration converges, an FE solution $(\mu^h, \mathbf{D}^h)$ (i.e. $(\lambda^h, \mathbf{D}^h)$ with $\lambda^h = \lambda_a + \mu^h$) of Eq. (10) is obtained. However, the current mesh may not be sufficiently fine and so the accuracy of this FE solution needs to be checked by a more accurate solution, namely the EEP solution, which is discussed in the following section.

4. EEP SOLUTION

This section firstly introduces a recently developed Element Energy Projection (EEP) technique for extracting super-convergent solutions from conventional FE solutions of linear boundary value problems (BVPs). It then presents a novel technology transfer of the EEP technique from linear BVP to SL problems, enabling the desired error checking for the FE solution of SL problems.

4.1 EEP formulae for linear BVP

Consider the second [fourth] order BVP of Eq. (1) [Eq. (3)] with $\lambda r(x)u$ [$\lambda r(x)w$] being replaced by a 'load' term $f(x)$ [$f(x)$] and its FE solutions for u [w] which, for convenience, are called displacements in this section. It is well known that for elements of degree m the FE solution u^h [w^h] gains, for sufficiently smooth problems and solutions, a super-convergence $O(h^{2m})$ [$O(h^{2(m-1)})$] at the element end nodes [25, 26], while the FE solutions of u^h [w^h] at element interior points only gain convergence $O(h^{m+1})$ [$O(h^{m+1})$] (Douglas, 1974; Strang and Fix, 1973).

In earlier studies led by the first author (Yuan *et al*., 2006, 2007a, 2007b; Yuan and Zhao, 2007; Yuan and Xing, 2014), it has been found that the well-known projection theorem (Strang and Fix, 1973) in FE mathematical theory almost holds true for a single element of degree $m\,(>1)$ [$m\,(>3)$]. Accordingly, based on a series of related conceptual studies, the EEP method has been developed for computation of both super-convergent displacements and derivatives at any interior point for FE solution of linear BVPs. The EEP formulae were developed in both simplified and condensed forms. This paper uses the simplified form, due to its simplicity, convenience and

efficiency, the formulae of which are presented as follows

$$u^* = u^h + \frac{h}{p}\left(\overline{N}_1 \int_{\bar{x}_1}^{\bar{x}} (f - Lu^h)\,\overline{N}_2 \mathrm{d}x + \overline{N}_2 \int_{\bar{x}}^{\bar{x}_2} (f - Lu^h)\,\overline{N}_1 \mathrm{d}x \right) \tag{14a}$$

$$\begin{aligned} pw^* = pw^h &+ J_2^0\,(\bar{x}_1 - \bar{x})^3/6 + J_2^1\,(\bar{x}_1 - \bar{x})^2/2 \\ &- J_1^0\,(\bar{x}_2 - \bar{x})^3/6 - J_1^1\,(\bar{x}_2 - \bar{x})^2/2 \end{aligned} \tag{14b}$$

Here: $\overline{N}_i \ \ (i = 1,2)$ are the linear shape functions; $(\,)^*$ represents EEP value at the interior point $\bar{x} \in (\bar{x}_1, \bar{x}_2)$ with $h = \bar{x}_2 - \bar{x}_1$; and

$$J_1^\alpha = \int_{\bar{x}_1}^{\bar{x}} (f - Lw^h)\,\overline{N}_2^\alpha \mathrm{d}x, \ \ J_2^\alpha = \int_{\bar{x}}^{\bar{x}_2} (f - Lw^h)\,\overline{N}_1^\alpha \mathrm{d}x, \ \ \alpha = 0,1 \tag{15}$$

with $\overline{N}_i^\alpha \ \ (i = 1,2, \alpha = 0,1)$ being conventional cubic Hermite shape functions.

Mathematical analyses (Yuan and Zhao, 2007; Yuan and Xing, 2014; Zhao *et al*., 2007; Yuan *et al*., 2015) have proved that for both the second and fourth order cases u^* and w^* gain in general a super-convergence of at least $O(h^{m+2})$ in maximum norm, i.e. $\max\limits_{a<x<b} \left| u - u^* \right| < Ch^{m+2}$ [$\max\limits_{a<x<b} \left| w - w^* \right| < Ch^{m+2}$]. It is also worth mentioning that the calculations of Eq. (14) are performed at the post-processing stage, and involve only some definite integration.

Since the accuracy of the EEP solution u^* [w^*] is at least one order higher than that of u^h [w^h], for elements of degree $m > 1$ [$m > 3$], a very simple strategy for error estimation is to use u^* [w^*] instead of the exact solution u [w] to estimate the errors in u^h [w^h]. This estimate tends to become more accurate and reliable as the mesh becomes finer ($h \to 0$) and hence can be used to guide mesh refinement.

4.2 EEP technology transfer to SL problems

The EEP formulae are powerful and valuable but a key question remains unanswered: namely, they are for linear BVPs, so how can they be applied to SL problems which essentially have a special nonlinear form due to the obviously nonlinear term $\lambda r(x)u$ [$\lambda r(x)w$]? The answer is as follows.

Note that Eq. (10) is solved as the shifted form of Eq. (9), so that at the final stage of the inverse iteration the obtained solution $(\mu^h, u^h\,[w^h])$ is the best FE solution on the current mesh to the shifted ODE eigenproblem

$$L_{\lambda_a} u \equiv -(p(x)u')' + q(x)u - \lambda_a\, r(x)u = \mu r(x)u, \quad a < x < b \tag{16a}$$

$$
\begin{aligned}
&u(a)=0, \quad u(b)=0 \\
&\text{with } u \text{ being normalized as } \max_{a<x<b}|u(x)|=1 \\
&L_{\lambda_a} w \equiv (p(x)w'')'' - (s(x)w')' + q(x)w - \lambda_a r(x)w = \mu r(x)w, \quad a<x<b \\
&w(a)=0, \quad w'(a)=0, \quad w(b)=0, \quad w'(b)=0 \\
&\text{with } w \text{ being normalized as } \max_{a<x<b}|w(x)|=1
\end{aligned}
\tag{16b}
$$

The converged FE solution $(\mu^h, u^h\,[w^h])$ implies that no further improvement in accuracy will be gained by more inverse iterations unless the mesh is further refined. It is at this stage that the linear problem based EEP technology can be directly transferred to SL problems. Specifically, the FE solution $(\mu^h, u^h\,[w^h])$ of Eq. (10) can be viewed as an FE approximation to that of the linear BVP

$$
\begin{aligned}
&L_{\lambda_a} u = f(x), \quad a<x<b, \text{ with } f(x)=\mu^h r(x) u^h \\
&u(a)=0, \quad u(b)=0
\end{aligned}
\tag{17a}
$$

$$
\begin{aligned}
&L_{\lambda_a} w = f(x), \quad a<x<b, \quad \text{with } f(x)=\mu^h r(x) w^h \\
&w(a)=0, \quad w'(a)=0, \quad w(b)=0, \quad w'(b)=0
\end{aligned}
\tag{17b}
$$

with the corresponding FE formulation being

$$
\mathbf{K}_a\mathbf{D}=\mathbf{P} \quad \text{with} \quad \mathbf{P}=\mu^h \mathbf{M}\mathbf{D}^h \tag{18}
$$

This is justified because the FE solution of the linear BVP of Eq. (17) on the current mesh is exactly the same u^h $[w^h]$. Based on this formulation, the corresponding EEP solution u^* $[w^*]$ can be calculated by using Eq. (14) with L and f replaced by L_{λ_a} and $\mu^h r(x)u^h$ $[\mu^h r(x)w^h]$ respectively, and subsequently can be used to check whether u^h $[w^h]$ is good enough compared with u^* $[w^*]$. The underlying rationale is simply that if the FE solution u^h $[w^h]$ is not good enough for the linear BVP of Eq. (17), neither is it for the original SL problem of Eq. (16), and vice versa. All of the numerical examples so far have confirmed the error estimate is indeed valid and reliable for the original SL problem of Eq. (16).

5. MESH REFINEMENT

5.1 Error checking

Suppose each element on the current mesh is divided into a grid of M equal

subintervals. For the $M-1$ interior grid points on a typical element, the ordinary FE solutions u_j^h [w_j^h] and the EEP solutions u_j^* [w_j^*] at the *j*-th interior point ($j=1,2,\cdots,M-1$) are calculated. Then the errors at the $M-1$ interior points are calculated and checked to see if all of them satisfy the given tolerance, i.e.

$$e_j^* = \left| u_j^* - u_j^h \right| \le Tol \quad (j=1,2,\cdots,M-1) \tag{19a}$$

$$e_j^* = \left| w_j^* - w_j^h \right| \le Tol \quad (j=1,2,\cdots,M-1) \tag{19b}$$

Usually it is more than sufficient to set M in the range $4 \le M \le 8$.

5.2 Elememt subdivision

If Eq. (19) is not satisfied for any *j*, the corresponding element needs to be subdivided into two sub-elements by inserting an interior node at the j_a -th point, calculated by

$$j_a = \text{int}\left(\sum_{j=1}^{M-1} j \cdot (e_j^*)^2 \Big/ \sum_{j=1}^{M-1} (e_j^*)^2 \right) \tag{20}$$

This subdivision approach is called the error-averaging method (Yuan *et al*., 2008), with the areas of error squared on the two sides of point j_a roughly equal to each other.

With the above mesh refinement completed, a new mesh π^* results and then another round of adaptive iteration is conducted on the new mesh with the shift value λ_a unchanged. This adaptive iteration proceeds repeatedly for a sequence of adaptively refined meshes until a sufficiently fine mesh π is found, such that the FE solution u^h [w^h] fully satisfies Eq. (19).

The case of subspace iteration can be implemented similarly, without substantial difficulties. Once subspace iteration converges with a set of N_r FE solutions, the processes of EEP solution, error checking and mesh refinement are applied to each solution. If the current mesh is not sufficiently fine for any of them, a new mesh is generated based on that solution and is used in another round of adaptive iteration. Such adaptive iteration is repeated until a mesh that is sufficiently fine for all N_r solutions is found.

If the FE solution u^h [w^h] fully satisfies the tolerance *Tol* on all elements as defined in Eq. (8) (or in the discrete form of Eq. (19)), the procedure of mesh refinement is terminated. However, the eigenvalue $\lambda^h = \lambda_a + \mu^h$ thus obtained may not

yet be accurate enough, and so the procedure continues to adjust the bounds until Eq. (7) is also fully satisfied.

After a round of the above adaptive iteration, the outcome is a number of useful results with rich and important information, e.g. an FE solution $(\mu^h, \mathbf{D}^h)$ (or $(\lambda^h, \mathbf{D}^h)$) with a *J-count* at λ_a on a previous mesh and a finer mesh. Then comprehensive use of these results can guide and guard successive adaptive iterations so that they approach the exact eigenpair of the sought order quickly and safely. There are some auxiliary techniques in computation, e.g. checking and adjusting eigenvalue bounds, dealing with negative eigenvalues. They are all well handled by common practice and thus a detailed description is not given here.

6. NUMERICAL EXAMPLES

The proposed method was implemented in a Fortran 90 code and was tested by computing the first fifty eigenpairs for a batch of 44 SL eigenproblems (Greenberg and Marletta, 1997; Pruess *et al*., 1994). For all the examples, it was found that the present method produced satisfactory results, with both eigenvalues and modes fully satisfying the preset error tolerances. In this section, four representative and challenging examples are chosen to demonstrate the effectiveness of the proposed method. All of these examples were run with *Tol* = 10^{-9} on a LENOVO Notebook computer with a Pentium M 2.8GHz CPU, with about 14 decimal digits of floating point numbers used. The polynomial elements used in these examples had degree $m = 3$ [$m = 5$] for all second [fourth] order SL problems.

The error of the computed eigenvalue λ^h is measured by

$$\varepsilon_\lambda = \frac{\left|\lambda - \lambda^h\right|}{1 + \left|\lambda\right|} \tag{21}$$

where λ is the exact eigenvalue. For problems where the exact eigenvalue is unknown λ is replaced by the result produced by SLEDGE/SLEUTH and the corresponding error given by Eq. (21) was denoted by ε_λ^*.

To calculate the error of a computed eigenfunction $u^h(x)$ [$w^h(x)$], the domain was divided into n_p =1000 uniform subintervals for all examples. Then the error between $u^h(x)$ [$w^h(x)$] and the exact one $u(x)$ [$w(x)$] was calculated from

$$\varepsilon_u = \max_{i=0,1,\ldots,n_p} \left| \frac{u(x_i)}{u(x_j)} - \frac{u^h(x_i)}{u^h(x_j)} \right| \quad \text{with } \left|u(x_j)\right| = \max_{k=0,1,\ldots,n_p} \left|u(x_k)\right| \tag{22a}$$

$$\varepsilon_w = \max_{i=0,1,\ldots,n_p} \left| \frac{w(x_i)}{w(x_j)} - \frac{w^h(x_i)}{w^h(x_j)} \right| \quad \text{with } \left|w(x_j)\right| = \max_{k=0,1,\ldots,n_p} \left|w(x_k)\right| \tag{22b}$$

where the use of $|u(x_j)|$ [$|w(x_j)|$] implies that normalization was based on the discrete values $u(x_k)$ [$w(x_k)$] of the exact solution. For those second order SL problems whose exact eigenfunctions were not available, $u(x_k)$ was replaced by values calculated by SLEDGE and the corresponding error given by Eq. (22a) was denoted by ε_u^*. For the fourth order SL problems, because SLEUTH does not impose error control on eigenfunctions and hence their accuracy is too poor to compare with the present method. For all calculated errors, the machine accuracy was assumed to be 10^{-14} and errors smaller than this will not be shown.

Example 1 (Second order SL Problem)

$$\begin{cases} p(x) = e^{10}/\cosh(10x), \quad r(x) = 100\pi^2 e^{10}\cosh(10x)/\sinh^2 10 \\ q(x) = 0, \quad a = 0, \quad b = 1, \quad u(a) = 0, \quad u(b) = 0 \end{cases} \tag{23}$$

The analytical solution of this example is

$$\lambda_k = k^2,\ u_k(x) = \sin\left(k\pi \frac{\sinh(10x)}{\sinh 10} \right),\ k = 1,2,... \tag{24}$$

Figure 1 shows the variation of functions $p(x)$ and $r(x)$. It is obvious that $p(x)$ decreases rapidly while $r(x)$ increases rapidly. This corresponds to an axial free vibration problem of a fixed bar with the ratio of stiffness to mass varying from very large to very small. To illustrate the adaptivity effects, the first three eigenpairs were calculated with *Tol*=10^{-3}, and the variations of the eigenfunctions and the corresponding final meshes are shown in Figures 2 and 3 respectively. It can be seen that the adaptive process can automatically and properly arrange more elements for the sharply varied parts of these eigenfunctions. To get further tastes for the adaptivity effects, the final number of elements, the errors of the computed eigenfunctions, the maximum $h_{\max}$ and minimum $h_{\min}$ of element sizes on the final meshes and the number of adaptive steps are given in Table 1. It is seen that the errors of the adaptive FE results are fully

controlled within the preset *Tol* in the maximum norm, and the big difference between $h_{\max}$ and $h_{\min}$ well reflects the capability of generating extreme irregular meshes by the present method. For *Tol* = 10^{-9}, the eigenvalue errors ε_λ and eigenfunction errors ε_u of the proposed method and SLEDGE are shown in Figure 4(a) and it can be seen to agree with the user-preset error tolerance for both eigenvalues and eigenfunctions very well.

Example 2 (Second order SL Problem): Coffey-Evans equation

$$\begin{cases} p(x) = r(x) = 1, \quad q(x) = -2\beta\cos 2x + (\beta \sin 2x)^2 \\ \beta = \begin{Bmatrix} 20 \\ 50 \end{Bmatrix}, \quad a = -\dfrac{\pi}{2}, \quad b = \dfrac{\pi}{2}, \quad u(a) = 0, \quad u(b) = 0 \end{cases} \tag{25}$$

The Coffey-Evans equation is well known to be a very difficult one. Even though the mathematical theory guarantees that for the separated boundary conditions there are no multiple eigenvalues for regular second order SL problems, the triple well of the Coffey-Evans potential produces triplets of eigenvalues which can be made arbitrarily close by deepening the well, i.e. by increasing β. The number of triplets increases as β increases. For $i \le 2$ and β = 20, or for $i \le 6$ and β = 50, the i-th triplet occurs as eigenvalue numbers $4i - 1$, $4i$ and $4i + 1$. The first two of the triplets can be seen in Table 2, which illustrates how the triplets become much tighter as β is increased from 20 to 50 and also that they become less tight as i increases. Note that the β = 50 case is a very difficult one for some other software (Pryce, 1993). The computed results given by the present method and by SLEDGE are given in Figure 4(b) and can be seen to agree very well with each other except for the eigenfunctions corresponding to the triplets. When using 14 decimal digit precision, neither method could give acceptable solutions for these exceptional cases, due to the difficulty of separating the modes in each triplet.

Example 3 (Fourth order SL Problem)

$$\begin{cases} p(x) = \dfrac{9}{64}x^6, \quad s(x) = \dfrac{27}{128}x^4, \quad q(x) = -\dfrac{1215}{1024}x^2, \quad r(x) = \dfrac{64\pi^4}{9x^6} \\ a = 1, \quad b = 2, \quad w(a) = 0, \quad w''(a) = 0, \quad w(b) = 0, \quad w''(b) = 0 \end{cases} \tag{26}$$

The exact solution of this example is

$$\lambda_k = k^4, \; w_k(x) = x^{\frac{3}{2}} \sin(k\pi(\frac{4}{3x^2} - \frac{1}{3})), \; k = 1,2,... \tag{27}$$

The eigenvalue errors ε_λ and eigenfunction errors ε_w for both the present method and

SLEUTH are shown in Figure 4(c). It can be seen that some of the eigenvalues from SLEUTH are not sufficiently accurate and the eigenfunctions from SLEUTH are completely unacceptable for the given tolerance.

Example 4 (Fourth order SL Problem): a simplified Cahn-Hilliard equation

$$\begin{cases} p(x) = 1.1 - x^2, \quad s(x) = -20, \quad q(x) = 0, \quad r(x) = 1 \\ a = -1, \quad b = 1, \quad w(a) = 0, \quad w'(a) = 0, \quad w(b) = 0, \quad w'(b) = 0 \end{cases} \tag{28}$$

The eigenvalue differences between the present method and SLEUTH are shown in Figure 4(d) and some selected eigenvalues computed by the present method are listed in Table 2. It is obvious that the difference of the first and third eigenvalues between our method and SLEUTH exceeds the error tolerance. For this problem, the present code was additionally compiled with quadruple precision (about 28 decimal digits) using Intel Visual Fortran 11, and was run with a stricter tolerance $Tol = 10^{-15}$. Comparison with these results showed that our first and third eigenvalues satisfy the error tolerance $Tol = 10^{-9}$. This implies that for the first and third eigenvalues SLEUTH are not accurate enough to satisfy the error tolerance.

7. CONCLUDING REMARKS

A new adaptive FE method for accurate, efficient and reliable computation of both the eigenvalues and eigenfunctions of regular second and fourth order SL eigenproblems has been presented. Comprehensive utilization of the EEP technique with a number of other auxiliary techniques (including the Sturm sequence property and both inverse and subspace iterations) has yielded a simple, efficient and reliable adaptive FE procedure that finds sufficiently fine meshes for the user-preset error tolerances to be achieved. Numerical results, including ones known to be particularly troublesome, have shown that the present method always completely satisfied the required error tolerances for both eigenvalues and eigenfunctions. The present paper is limited to regular SL problems, but with some numerical treatments, as done by SLEUTH, the present method can also solve some singular SL problems in an indirect way. Looking forward, a very welcoming and encouraging feature of this method is that it can readily be extended to vector SL problems since the EEP formulae for corresponding linear system of ODEs are well available already, which will be addressed in other papers.

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Table 1 Adaptive iteration results of Example 1 (Tol=10^{-3})

k	Final number of elements	$\max\|u-u^h\|$	$h_{\max}$	$h_{\min}$	Adaptive steps
1	9	0.95E-6	0.4375	0.0234	4
2	14	0.77E-6	0.3281	0.0117	1
3	18	0.61E-6	0.3281	0.0059	2

Table 2 Selected eigenvalues λ_k computed by the present method for Example 2 and Example 4

k	Example		
	2 ($\beta = 20$)	2 ($\beta = 50$)	4
1	0.000000000	0.000000000	-77.89968895
2	77.91619568	197.9687265	-43.13822158
3	151.4627783	391.8081915	81.02449670
4	151.4632237	391.8081915	703.9992915
5	151.4636690	391.8081917	2182.636239
6	220.1542298	581.3771092	4991.260833
7	283.0948147	766.5168273	9702.727093
8	283.2507438	766.5168273	16985.85788
9	283.4087354	766.5168275	27605.35265
10	339.3706657	947.0474916	42421.71719
15	452.6311750	1458.746557	216276.6366
20	613.2813296	1771.935291	679173.3123
25	833.3807330	2058.412167	1646345.342
30	1105.794050	2417.288116	3392822.470
35	1429.249568	2657.771476	6253427.131
40	1803.251190	2979.923959	10622773.15
45	2227.567985	3375.290131	16955265.18
50	2702.079745	3830.263314	25765098.42

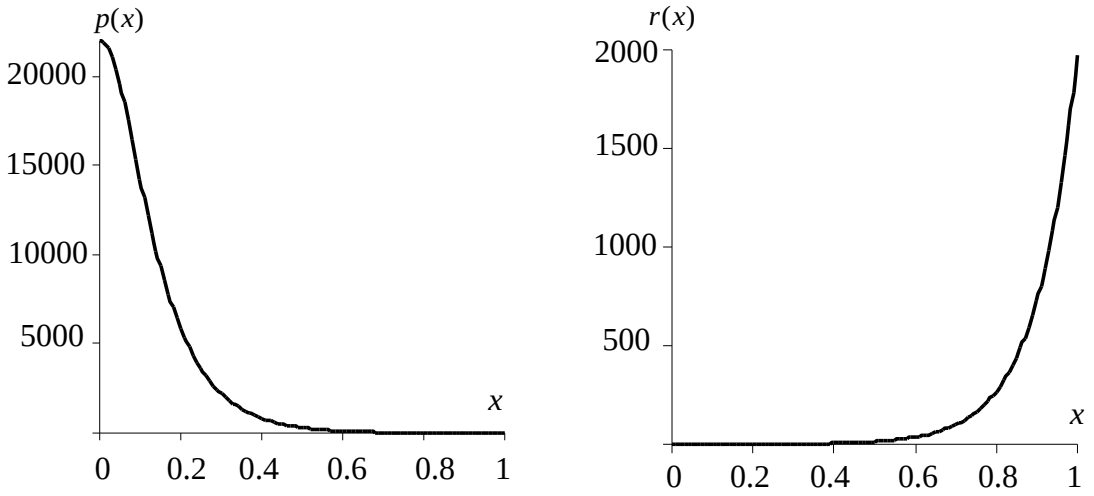

Fig. 1 Variation of the coefficients of Example 1

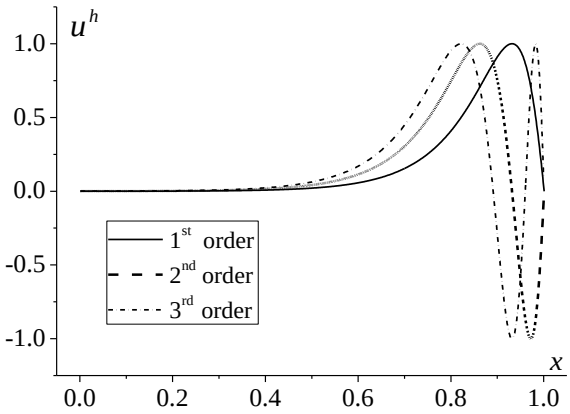

Fig. 2 First three eigenfunctions of Example 1

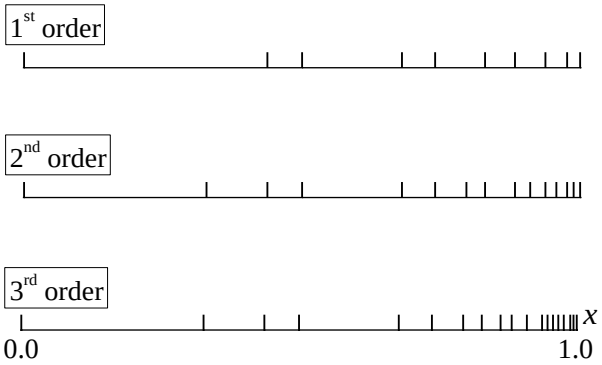

Fig. 3 Final meshes of first three eigenpairs of Example 1 (Tol=10^{-3})

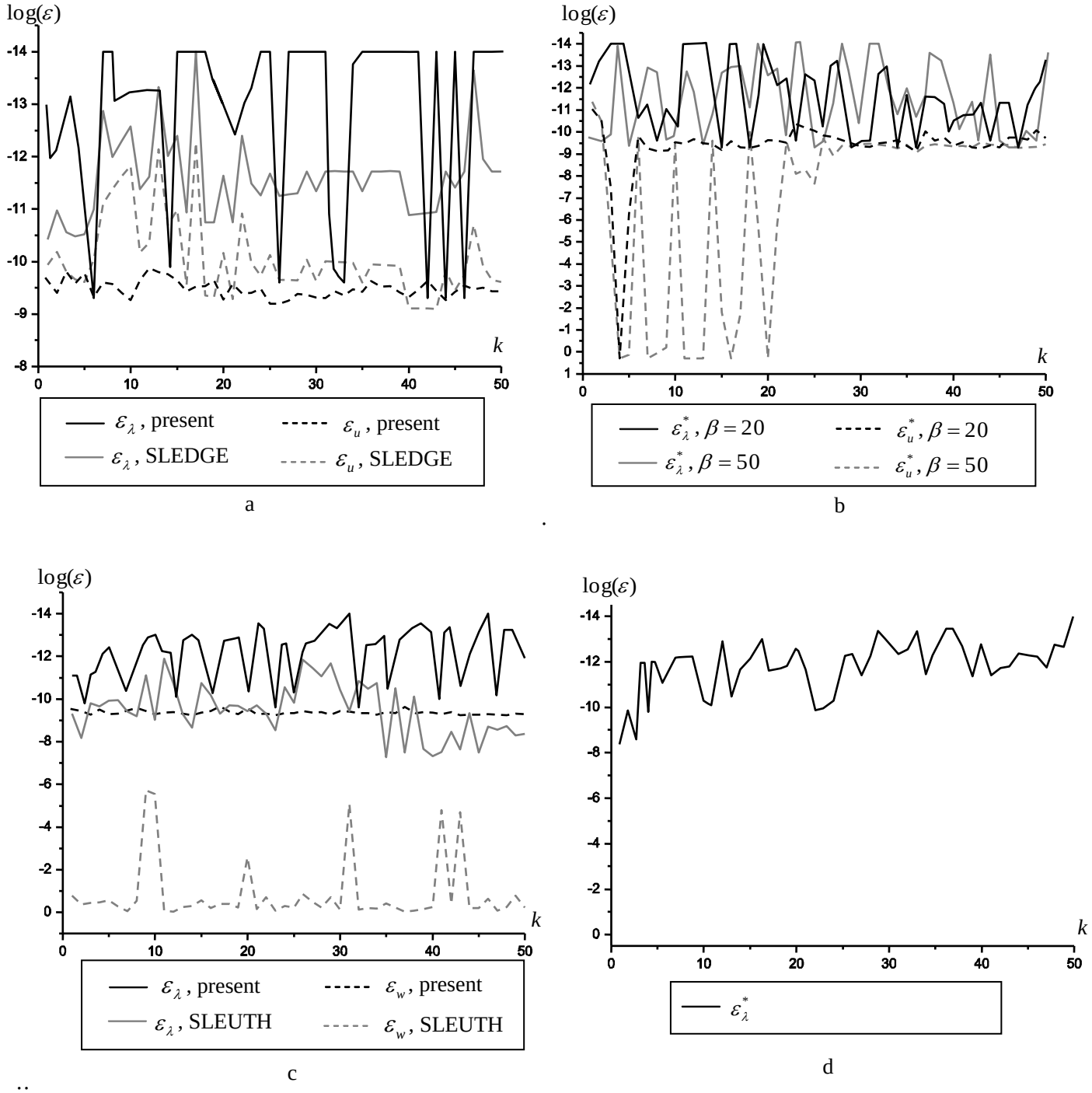

Fig. 4 Relative errors and differences, ε_λ and ε_λ^* for the *k*-th eigenvalue, ε_u [ε_w] and ε_u^* for the *k*-th eigenfunction, for (a) Example 1, (b) Example 2, (c) Example 3, (d) Example 4