

EFFECT OF HYPERBOLIC INTERPOLATION IN THE FINITE ELEMENT SOLUTION OF AN EIGENVALUE PROBLEM

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ABSTRACT

In this paper hyperbolic interpolation has been used instead of Lagrange interpolation in solving an eigenvalue problem by using finite element method. The result shows that there is a good agreement between the eigenvalues obtained by using hyperbolic interpolation and the exact eigenvalues.

Keywords: Eigenvalue problem, finite element method, Lagrange interpolation, hyperbolic interpolation.

1. Introduction

The method of separation of variables gives rise to eigenvalue problem from boundary value problem. The different types of eigenvalue problems [1-3] can also be solved by finite element method. In general Lagrange interpolation is used as an approximation of the solution of these types of problems. Galerkin Weighted Residual procedure is used to deduce the finite element model of eigenvalue problem. In this study hyperbolic shape functions have been used to compare the results with exact values and the results obtained by Lagrange's interpolation. For this first we derive the hyperbolic shape functions of order n and particularly discuss linear, quadratic and cubic hyperbolic functions in the subsequent sections.

The steady state form of the Schrödinger equation [1] for the electron in the hydrogen atom moving in the Coulomb potential of the proton

$$\frac{-\hbar^2}{2m} \nabla^2 \psi_n(r) - \frac{e^2}{r} \psi_n(r) = E_n \psi_n(r) \quad (1)$$

$\psi_n(r)$ is the wave function of the electron in the stationary state with energy E_n .

The equation (1) is made dimensionless by rescaling the radial coordinates r by a_0 (the Bohr radius) and dividing the equation by the energy unit of a Rydberg

$$R_0 (=13.6\text{eV}) \quad \text{where} \quad R_0 = \frac{-\hbar^2}{2ma_0^2} = \frac{e^2}{2a_0} \quad (2)$$

For convenience the same symbol r is retained for the radial coordinates after rescaling and the symbol λ is used for the reduced energy. For spherically symmetric state the radial part of the equation (1) becomes:

$$\left(-\frac{d^2}{dr^2} - \frac{2}{r} \frac{d}{dr} - \frac{2}{r} \right) \psi(r) = \lambda \psi(r) \quad (3)$$

$$\text{The boundary condition is } \psi(r) \rightarrow 0 \text{ as } r \rightarrow \infty \quad (4)$$

Analytical solution of this equation [5],

$$\psi(r) = \sqrt{\left[\left(\frac{2}{na_0} \right)^3 \frac{(n-l-1)!}{2n\{(n+l)!\}^3} \right]} \exp\left[\frac{-r}{na_0} \right] \left(\frac{2r}{na_0} \right)^l L_{n+l}^{2l+1} \left(\frac{2r}{na_0} \right) \quad \text{where } \lambda = \frac{1}{n^2} \quad (5)$$

This eigenvalue equation (3) was solved by Ram Mohan et al. [4] using finite element method with Lagrange interpolation. In this study, finite element method has been modified with hyperbolic interpolation and implemented to solve the eigenvalue problem. Linear, quadratic and cubic elements have been used to calculate the eigenvalues using finite element method with the hyperbolic interpolation. The results obtained by us for linear, quadratic and cubic elements using hyperbolic interpolations are compared with the analytical results. Ram Mohan et al. [4] compared the lowest four eigenvalues with exact solutions. Eigenvalues obtained by finite element method using hyperbolic interpolation shape functions for different ranges are in good agreement with the exact results.

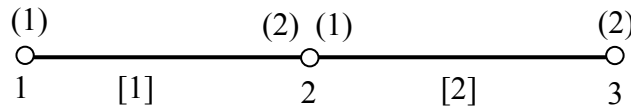


Figure 1: Local and global nodal point numbering for linear element

For quadratic element with three points (x_1, y_1) , (x_2, y_2) and (x_3, y_3) the hyperbolic interpolation is $y = H_1 y_1 + H_2 y_2$ (6)

where

$$H_1 = \frac{\sinh(x-x_2)\sinh(x-x_3)}{\sinh(x_1-x_2)\sinh(x_1-x_3)}, \quad H_2 = \frac{\sinh(x-x_1)\sinh(x-x_3)}{\sinh(x_2-x_1)\sinh(x_2-x_3)},$$

$$H_3 = \frac{\sinh(x-x_2)\sinh(x-x_1)}{\sinh(x_3-x_1)\sinh(x_3-x_2)} \quad (7)$$

Putting $x = \frac{x_1 + x_2}{2} + \frac{x_2 - x_1}{2} \xi$ where $x_2 = \frac{x_1 + x_3}{2}$ (8)

$$H_1 = \frac{\sinh\left(\frac{x_2 - x_1}{2} \xi\right) \sinh\left(\frac{x_2 - x_1}{2} (\xi - 1)\right)}{\sinh\left(\frac{x_2 - x_1}{2}\right) \sinh(x_2 - x_1)} \quad (9)$$

$$H_2 = \frac{\sinh\left(\frac{x_2 - x_1}{2} (1 + \xi)\right) \sinh\left(\frac{x_2 - x_1}{2} (\xi - 1)\right)}{\sinh\left(\frac{x_2 - x_1}{2}\right) \sinh(x_2 - x_1)} \quad (10)$$

$$H_3 = \frac{\sinh\left(\frac{x_2 - x_1}{2} \xi\right) \sinh\left(\frac{x_2 - x_1}{2} (1 + \xi)\right)}{\sinh\left(\frac{x_2 - x_1}{2}\right) \sinh(x_2 - x_1)} \quad (11)$$

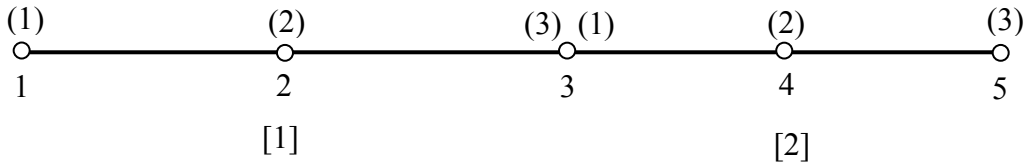


Figure 2: Local and global nodal point numbering for quadratic element

$[i]$ are the element number

(i) are the node number of the element

i are the global node number of the element

Element [1] is related with global node no. 1 and 2.

Element [2] is related with the global node no. 2 and 3.

For cubic element with four points $(x_1, y_1), (x_2, y_2), (x_3, y_3)$ and (x_4, y_4)

$$H_1 = \frac{\sinh(x - x_2)\sinh(x - x_3)\sinh(x - x_4)}{\sinh(x_1 - x_2)\sinh(x_1 - x_3)\sinh(x_1 - x_4)} \quad (12)$$

$$H_2 = \frac{\sinh(x - x_1)\sinh(x - x_3)\sinh(x - x_4)}{\sinh(x_2 - x_1)\sinh(x_2 - x_3)\sinh(x_2 - x_4)} \quad (13)$$

$$H_3 = \frac{\sinh(x - x_1)\sinh(x - x_2)\sinh(x - x_4)}{\sinh(x_3 - x_1)\sinh(x_3 - x_2)\sinh(x_3 - x_4)} \quad (14)$$

$$H_4 = \frac{\sinh(x - x_1)\sinh(x - x_2)\sinh(x - x_3)}{\sinh(x_4 - x_1)\sinh(x_4 - x_2)\sinh(x_4 - x_3)} \quad (15)$$

On substitution

$$x = \frac{x_1 + x_4}{2} + \frac{x_4 - x_1}{2} \xi \quad \text{and} \quad x_2 = \frac{2x_1 + x_4}{3}, \quad x_3 = \frac{x_1 + 2x_4}{3} \quad (16)$$

$$H_1 = \frac{\sinh\left(\frac{x_4 - x_1}{2}\right)\left(\frac{1}{3} + \xi\right)\sinh\left\{\frac{x_4 - x_1}{2}\left(-\frac{1}{3} + \xi\right)\right\}\sinh\left(\frac{x_4 - x_1}{2}\right)(-1 + \xi)}{\sinh\left(\frac{x_1 - x_4}{3}\right)\sinh\frac{2}{3}(x_1 - x_4)\sinh(x_1 - x_4)} \quad (17)$$

$$H_2 = \left(\frac{\sinh\left\{\left(\frac{x_4 - x_1}{2}\right)(1 + \xi)\right\}\sinh\left\{\left(\frac{x_4 - x_1}{6}\right)(\xi - 1)\sinh\left\{\left(\frac{x_4 - x_1}{2}\right)(\xi - 1)\right\}\right\}}{\sinh\left(\frac{x_4 - x_1}{3}\right)\sinh\left\{\left(\frac{x_1 - x_4}{3}\right)\right\}\sinh\left\{\frac{2}{3}(x_1 - x_4)\right\}} \right) \quad (18)$$

$$H_3 = \left(\frac{\sinh\{(x_4 - x_1)(1 + \xi)\}\sinh\left\{\left(\frac{x_4 - x_1}{6}\right)(3\xi + 1)\sinh\left\{\left(\frac{x_4 - x_1}{2}\right)(\xi - 1)\right\}\right\}}{\sinh\left\{\frac{2}{3}(x_4 - x_1)\right\}\sinh\left\{\frac{x_4 - x_1}{3}\right\}\sinh\left(\frac{x_1 - x_4}{3}\right)} \right) \quad (19)$$

$$H_4 = \left(\frac{\sinh\left\{\left(\frac{x_4 - x_1}{2}\right)(1 + \xi)\right\}\sinh\left\{\left(\frac{x_4 - x_1}{6}\right)(3\xi + 1)\sinh\left\{\left(\frac{x_4 - x_1}{6}\right)(3\xi - 1)\right\}\right\}}{\sinh(x_4 - x_1)\sinh\left\{\frac{2}{3}(x_4 - x_1)\right\}\sinh\left\{\frac{x_4 - x_1}{3}\right\}} \right) \quad (20)$$

Figure 3 figure 4 and figure 5, shows the comparison between the Lagrange interpolation shape functions and hyperbolic interpolation shape functions for the range 0 to 1. Shape functions for linear element are shown in figure 1; where h_1, h_2 denote the hyperbolic

shape functions and l_1, l_2 denote the shape functions for Lagrange interpolations respectively.

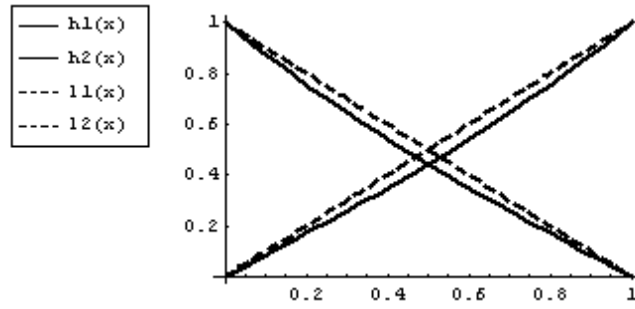


Figure 3: Linear Lagrange and corresponding hyperbolic interpolation shape functions

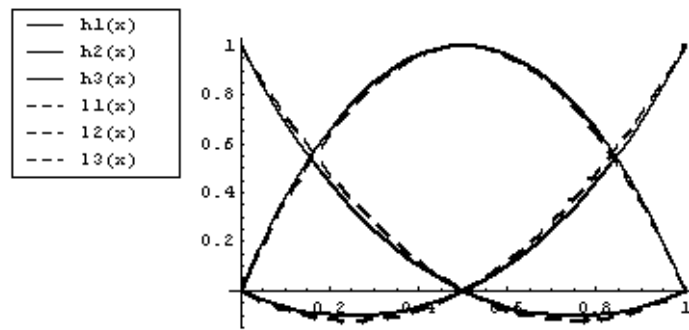


Figure 4: Quadratic Lagrange and corresponding hyperbolic interpolation shape functions;

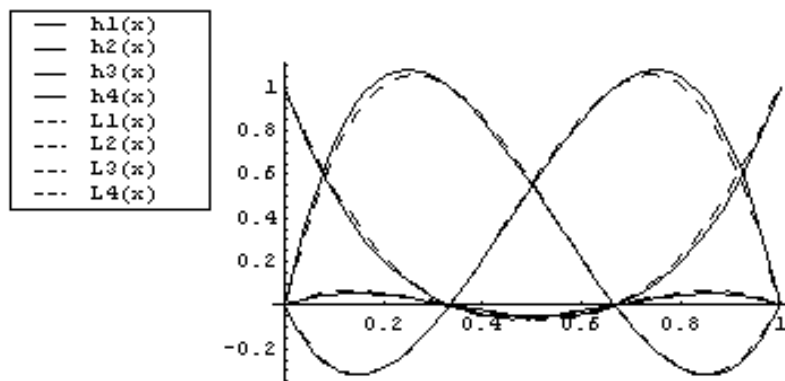


Figure 5: cubic Lagrange and corresponding hyperbolic interpolation shape functions

3. Formulation of Eigenvalue Problem

Consider a general class of one dimensional eigenproblems governed by the following second order ordinary differential equation

$$-\frac{d}{dx}\left(p(x)\frac{dU}{dx}\right) + q(x)U = \lambda r(x)U, \quad a < x < b \quad \text{with b.c } U(b) = 0 \quad (21)$$

Let $\tilde{U} = \sum_{j=1}^n a_j H_j(x)$ be the trial approximation for a typical element e .where

a_j are constants to be determined. $H_j(x)$ are the hyperbolic basis function's described in the previous section and n is the degrees of freedom. Then the Galerkin residual equation for the element e is

$$\int_e -\left[\frac{d}{dx}\left(p(x)\frac{d\tilde{U}}{dx}\right) + q(x)\tilde{U} - \lambda r(x)\tilde{U}\right] H_i(x) dx = 0 \quad i = 1, 2, 3, \dots, n \quad (22)$$

Now integrating by parts and with minor simplifications we have

$$\sum_{j=1}^n \left[\int_e \frac{dH_i(x)}{dx} p(x) \frac{dH_j(x)}{dx} \right] a_j + \sum_{j=1}^n \left[\int_e H_i(x) q(x) H_j(x) \right] a_j - \lambda \sum_{j=1}^n \left[\int_e H_i(x) r(x) H_j(x) \right] a_j = 0 \quad (23)$$

$i = 1, 2, 3, \dots, n$ which can be written in conventional matrix form

$$[K]\{a\} - \lambda[M]\{a\} = \{0\} \quad (24)$$

where

$$K_{ij} = \int_e \frac{dH_i(x)}{dx} p(x) \frac{dH_j(x)}{dx} dx + \int_e H_i(x) q(x) H_j(x) dx, \quad M_{ij} = \int_e H_i(x) r(x) H_j(x) dx \quad (25)$$

where K and M represent the stiffness matrix and the mass matrix, respectively.

3.1 Numerical example: Ram-Mohan et al. [4] solved the eigenvalue problem

$$-\frac{1}{x^2} \frac{d}{dx} \left(x^2 \frac{dU}{dx} \right) - \frac{2}{x} U = \lambda U \quad \text{with b.c. } U(20) = 0 \quad (26)$$

with domain having limit 0 to 20 taking 20 linear elements.

Multiplying the equation by the weight function v and integrating from 0 to 20 we obtain

$$\int_0^{20} \left[-\frac{d}{dx} \left(x^2 \frac{dU}{dx} \right) - 2xU \right] v dx = \int_0^{20} \lambda x^2 U v dx \quad (27)$$

and then

$$\int_0^{20} \left(x^2 \frac{dv}{dx} \frac{dU}{dx} - 2xvU \right) dx = \int_0^{20} \lambda x^2 v U dx \quad (28)$$

Considering the linear element from $x = x_1$ to $x = x_2$ writing $U = H_1 U_1 + H_2 U_2$ (29)

and using the Galerkin approach with $v = H_1$ and $v = H_2$, the elements of the stiffness

$$matrix \text{ are obtained as } k_{ij} = \int_{x_2}^{x_1} \left(x^2 \frac{dH_i}{dx} \frac{dH_j}{dx} - 2xH_i H_j \right) dx \text{ with } i, j = 1, 2 \quad (30)$$

Using the substitution the same substitution as before

$$dx = \frac{h}{2} d\xi \text{ where } x_2 - x_1 = h = \text{length of an element} \quad (31)$$

$$k_{ij} = \int_{-1}^1 \left[\left(\frac{x_1 + x_2}{2} + \frac{x_2 - x_1}{2} \xi \right)^2 \frac{dH_i}{d\xi} \frac{d\xi}{dx} \frac{dH_j}{d\xi} \frac{d\xi}{dx} - 2 \left(\frac{x_1 + x_2}{2} + \frac{x_2 - x_1}{2} \xi \right) H_i H_j \frac{h}{2} d\xi \right] \quad (32)$$

For the first element

The elements of the mass matrix are

$$M_{ij} = \int_{x_1}^{x_2} x^2 H_i H_j dx \quad (33)$$

$$= \int_{-1}^1 \left[\left(\frac{x_1 + x_2}{2} + \frac{x_2 - x_1}{2} \xi \right)^2 H_i H_j \frac{h}{2} d\xi \right] \quad (34)$$

The global stiffness equation $KU = \lambda MU$ for two linear elements.

For 20 linear elements global stiffness matrix K and the global mass matrix M will be a 21×21 matrix.

The matrix eigenvalue equation is $KU = \lambda MU$. The equation is solved by Jacobi's method, to find the eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_{20}$.

Eigenvalue problem in equation (3) is solved using standard Jacobi method. Jacobi method is preferable when all the eigenvalues and eigenvectors are required. This method calculates negative, zero, or positive eigenvalues. All integrations are performed using 5-point Gauss quadrature. Numerical computations are performed using **FORTAN** programming languages.

4. Result and Discussion

Relative errors have been shown between Lagrange's and exact eigenvalues as well hyperbolic and exact eigenvalues in Table I, Table II and Table III. In Table I the eigenvalues calculated using 20 elements show discrepancy with the analytical results. Again in Table I the eigenvalues calculated using 20 elements for the range 20 using hyperbolic interpolation gives smaller percentage error than those of Lagrange's interpolation for the same. Also it has been observed that as the number of elements and the ranges increased, the percentage error also increased in case of hyperbolic interpolation. To improve the accuracy of the results the degree of interpolation function has been increased. Eigenvalues obtained from Table II shows less discrepancy.

From table III it is seen that, smaller number of elements are not in good agreement. It has also been observed that from percentage relative error in Table III is smaller for both Lagranng and hyperbolic interpolation than those of Table I and Table II. Thus Table III agrees well with exact eigenvalues than those of Table I and Table II.

We conclude that the eigenvalues illustrated in Table III are more compatible to those computed in Table II and Table I.

Table I. Eigenvalues obtained by using linear Lagrange and Hyperbolic interpolation for different ranges

Quantum Number n	Energy (Rydberg) Lagrange interpolation	Energy (Rydberg) Hyperbolic Interpolation	Range	Number of elements	Exact eigenvalues	Relative Error Between Exact & Lagrange %	Relative Error Between Exact & Hyperbolic %
1	-0.941709	-1.003040	20	20	-1.000000	5.8290	0.3040
2	-0.238261	-0.250049			-0.250000	4.6956	0.0196
3	-0.092925	-0.099322			-0.111111	16.367	10.610
4	0.047545	0.034866			-0.062500	176.07	155.78
1	-0.999992	-0.999109	50	50	-1.000000	0.0010	0.0891
2	-0.249999	-0.249078			-0.250000	0.0004	0.3688
3	-0.111111	-0.110304			-0.111111	0.0000	0.7000
4	-0.062409	-0.061600			-0.062500	0.1456	1.4400
1	-0.999999	-1.000053	50	100	-1.000000	0.0001	0.0053
2	-0.250000	-0.249999			-0.250000	0.0000	0.0000
3	-0.111111	-0.111110			-0.111111	0.0000	0.0000
4	-0.062408	-0.062399			-0.062500	0.1472	0.1616
1	-0.999993	-0.997429	100	100	-1.000000	0.0010	0.2571
2	-0.249999	-0.249833			-0.250000	0.0001	0.0668
3	-0.111111	-0.111065			-0.111111	0.00000	0.0414
4	-0.062500	-0.062480			-0.062500	0.0000	0.0320

Table II. Eigenvalues obtained by using Lagrange and Hyperbolic interpolation using quadratic element for different domain.

Quantum Number n	Energy (Rydberg) Lagrange Interpolation	Energy (Rydberg) Hyperbolic Interpolation	Range	Number of elements	Exact eigenvalues	Relative Error Between Exact & Lagrange %	Relative Error Between Exact & Hyperbolic %
1	-0.9989508	-1.0196911	20	20	-1.000000	0.1049	1.9690
2	-0.2498442	-0.2506893			-0.250000	0.0623	0.2757
3	-0.0997724	-0.0988970			-0.111111	10.204	10.990
4	0.033427	0.0366957			-0.062500	153.48	158.71
5	0.225756	0.2330899			-0.040000	664.39	682.72
1	-0.998950	-1.019691	50	50	-1.000000	0.1050	1.9690
2	-0.249870	-0.250716			-0.250000	0.0520	0.2864
3	-0.111069	-0.110605			-0.111111	0.0378	0.4554
4	-0.062389	-0.061881			-0.062500	0.1776	0.9904
5	-0.035713	-0.034987			-0.040000	10.717	12.532
1	-0.999920	-1.001783	50	100	-1.000000	0.008	0.1783
2	-0.249991	-0.250069			-0.250000	0.0036	0.0276
3	-0.111108	-0.111078			-0.111111	0.0027	0.0297
4	-0.062407	-0.062371			-0.062500	0.1488	0.2064
5	-0.035728	-0.035677			-0.040000	10.68	10.807
1	-0.099895	-1.019691	100	100	-1.000000	0.1050	1.9690
2	-0.249870	-0.250716			-0.250000	0.0520	0.2864
3	-0.111069	-0.110605			-0.111111	0.0378	0.4554
4	-0.062481	-0.061985			-0.062500	0.0032	0.8240
5	-0.039990	-0.039584			-0.040000	0.0250	1.0400
1	-0.999919	-1.001783	100	200	1.000000	0.00811	0.1783
2	-0.249990	-0.250069			-0.250000	0.0040	0.0276
3	-0.111108	-0.111078			-0.111111	0.0018	0.0297
4	-0.062498	-0.062464			-0.062500	0.0032	0.0576
5	-0.039999	-0.039972			-0.040000	0.0025	0.0700

Table III. Eigenvalues obtained by using Lagrange and Hyperbolic interpolation using cubic element for different domain.

Quantum Number n	Energy (Rydberg) Lagrange Interpolation	Energy (Rydberg) Hyperbolic Interpolation	Range	Number of elements	Exact eigenvalues	Relative Error Between Exact & Lagrange %	Relative Error Between Exact & Hyperbolic %
1	-0.999992	-1.003040	20	20	-1.000000	0.0008	0.3040
2	-0.249973	-0.250049			-0.250000	0.0108	0.0196
3	-0.099836	-0.099322			-0.111111	10.14	10.610
4	0.033427	0.034866			-0.062500	153.48	155.78
5	0.225756	0.228553			-0.040000	425.20	671.38
1	-0.999992	-0.999109	50	50	-1.000000	0.0008	0.0891
2	-0.249999	-0.249078			-0.250000	0.0001	0.0922
3	-0.111111	-0.110304			-0.111111	0.0000	0.7260
4	-0.062409	-0.061600			-0.062500	0.1456	0.3688
5	-0.035730	-0.034951			-0.040000	10.675	12.622
1	-0.999999	-1.000053	50	100	-1.000000	0.0001	0.0053
2	-0.250000	-0.249999			-0.250000	0.00000	0.0004
3	-0.111111	-0.111110			-0.111111	.00000.	0.0009
4	-0.062408	-0.062399			-0.062500	1472	0.1616
5	-0.035730	-0.035727			-0.040000	10.751	10.680
1	-0.999993	-0.997429	100	100	-1.000000	0.0007	0.2571
2	-0.249999	-0.249833			-0.250000	0.0004	0.0668
3	-0.111111	-0.111065			-0.111111	0.0000	0.0414
4	-0.062500	-0.062480			-0.062500	0.0000	0.0320
5	-0.039999	-0.039990			-0.040000	0.0250	0.0250

Conclusion

This paper has presented the finite element method with hyperbolic interpolation shape functions and eigenvalues have been calculated by using this modified finite element method with hyperbolic interpolation for linear, quadratic and cubic elements. Results obtained using these methods are compared with the analytically obtained results. It is clear from the tables that eigenvalues obtained by using Lagrange's interpolation gives better accuracy and it is widely used although the new approach of using hyperbolic interpolation can be compatible to the use of Lagrange's shape functions.

We conclude from this paper that results and the percentage error from hyperbolic interpolation is thus closer to those obtained by Lagrange's interpolations shape functions. The fact that hyperbolic interpolation shape functions can provide better results in the solution of an eigenvalue problem has not been appreciated earlier and we expect to see a greater use of the finite element method in the solution of physical problems with modified interpolation functions in the future.

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