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Note

Laguerre Polynomials for Infinite-Domain Spectral Elements

1. Introduction

Laguerre polynomials are investigated in an effort to improve the generality of the spectral element method [1], specifically to improve accuracy in wake regions and to extend the method to efficiently solve external flow problems. Previous investigations estimated that Laguerre polynomials would have little practical use in spectral methods because of their poor ability to approximate general functions, as demonstrated by Gottlieb and Orszag [2]. Maday, Pernaud-Thomas, and Vandeven [3], however, point out that Laguerre polynomials should only be used for functions with simple behaviour at infinity. In this note, it is found that Laguerre-type elements may be used in conjunction with Legendre-type elements to resolve more accurately regions of outflow and infinite boundaries.

2. Formulation

In considering semi-infinite domains, the weighted residual form of the problem to be solved requires integrals with an upper limit of infinity as well as a weighting function of decaying type in order to relax the solution as $x \to \infty$. Consider the Helmholtz problem which is stated as $-u_{xx} + \lambda^2 u = f$ with boundary conditions $u(0) = 0$ and $u_x(x \to \infty) \to 0$. Its variational statement is written as: Find $u \in H_0^1$ such that

$$\int_0^\infty v_x u_x e^{-x} dx + \lambda^2 \int_0^\infty v u e^{-x} dx = \int_0^\infty v u_x e^{-x} dx + \int_0^\infty v f e^{-x} dx \qquad \forall v \in H_0^1, \quad (1)$$

where H_0^1 is the Sobolev space of functions which are square integrable with respect to the measure $e^{-x}dx$ and whose derivatives are square integrable with respect to the measure $e^{-x}dx$, and which vanish at the domain boundary $x = 0$. From this statement, we see that the semi-infinite domain description as defined here has the usual symmetric positive definite elliptic term, as well as an additional convective term. Numerically, the elliptic term is treated implicitly and is solved by a conjugate gradient method, whereas the convective part is treated explicitly. Note that if we were to solve a convective-diffusive problem $\nu u_{xx} + u_x = f$ with small viscosity ν,

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treating the additional convective term of the order vu_x explicitly does not cause stability problems since the u_x term dominates. The boundary condition at $x=0$ is a simple Dirichlet boundary condition $u(0)=0$, whereas the boundary condition at $x \to \infty$ must be a natural boundary condition. The discretized form of this equation is obtained by quadrature estimation of each integral.

Gauss–Radau type Laguerre quadrature is used since it accurately performs the necessary quadratures in the e^{-x} weighted norm. Quadrature is exact for any polynomial $f(x)$ of degree $\leqslant 2N$ and is written as

$$\int_0^\infty f(x)\, e^{-x} dx = \sum_{i=0}^{N} w_i f(x_i), \tag{2}$$

where the $N+1$ collocation points x_i are defined as the zeros of $xL'_{N+1}(x)$ and

$$w_i = \frac{1}{(N+1)\, L^2_{N+1}(x_i)}. \tag{3}$$

Gauss–Radau quadrature as defined above includes the boundary point $x=0$ as a collocation point and excludes the right-hand infinite boundary. (For a finite domain, Gauss–Lobatto quadrature is used since it includes both boundary points as collocation points.) The Laguerre polynomials $L_N(x)$ are defined by the ordinary differential equation

$$xL''_N(x) + (1-x)\, L'_N(x) + NL_N(x) = 0. \tag{4}$$

Applying Gauss–Radau–Laguerre quadrature to (1) gives

$$\sum_{i=0}^{N} w_p D_{pi} D_{pj} u_j = \sum_{i=0}^{N} w_i D_{ij} u_j - \lambda^2 \sum_{i=0}^{N} w_i u_i + \sum_{i=0}^{N} w_i f_i, \tag{5}$$

where the notation u_j signifies $u(x_j)$, summation is implied by repeated indices, and

$$D_{ij} = \frac{dh_j}{dx}(x_i). \tag{6}$$

In the above, u has been represented by the series

$$u(x) = \sum_{i=0}^{N} u_i h_i(x), \tag{7}$$

where the interpolation function is given as

$$h_i(x) = \frac{-xL'_{N+1}(x)}{(N+1)\, L_{N+1}(x_i)(x-x_i)} \tag{8}$$

and the associated interpolant derivative operator as

$$D_{ij}=\frac{L_{N+1}(x_i)}{L_{N+1}(x_j)}\frac{1}{(x_i-x_j)} \qquad \text{for } i\neq j \tag{9}$$

$$=\frac{1}{2} \qquad \text{for } i=j\neq 0 \tag{10}$$

$$=-\frac{N}{2} \qquad \text{for } i=j=0. \tag{11}$$

We note that it may be useful in other contexts to use the Laguerre functions defined by

$$\phi_n(x)=e^{-x/2}L_n(x) \tag{12}$$

as an expansion basis instead of the Laguerre polynomials alone. Much of the formulation is the same as presented here. The proper norm in that case would be

$$\|u\|^2=\int_0^\infty u(x)^2\,dx \simeq \sum_{i=0}^{N} w_i u(x_i)^2 \tag{13}$$

which is similar to the present formulation only the e^{-x} behaviour is included in the pointwise value instead of the norm evaluation.

Laguerre elements can be used consistently with other type elements such as Legendre. This is due to the fact that the boundary terms in the variational formulation cancel automatically as follows: consider the Helmholtz problem where Legendre spectral elements are used for the domain $[-a; 0]$ and the Laguerre for $[0; \infty[$. The boundary terms are from the Legendre part $-vu_x]_{-a}^{0}$ and from the Laguerre part $-vu_x e^{-x}]_0^\infty$. The terms at $x=0$ cancel, providing a weak C^1 condition automatically at the element interface and avoiding the need for any special patching techniques. The remaining boundary terms are determined by boundary conditions at $-a$ and ∞.

3. Results

The method is tested in several situations which reveal some interesting points of this formulation. The first is a question of numerics which is particular to the Laguerre formulation. The second is concerned with the correct boundary condition formulation that should be used at the infinite boundary.

The Laguerre spectral element formulation involves calculations of polynomials of large orders with large arguments since the x_j behave approximately as $x_j \sim (j+1)^2/(N+1)$ for $j \geqslant 1$, which are multiplied by the weights which become exponentially small as N increases, since $w_j \sim ((N+1)\,x_j^{2N+2})^{-1}$. These numbers

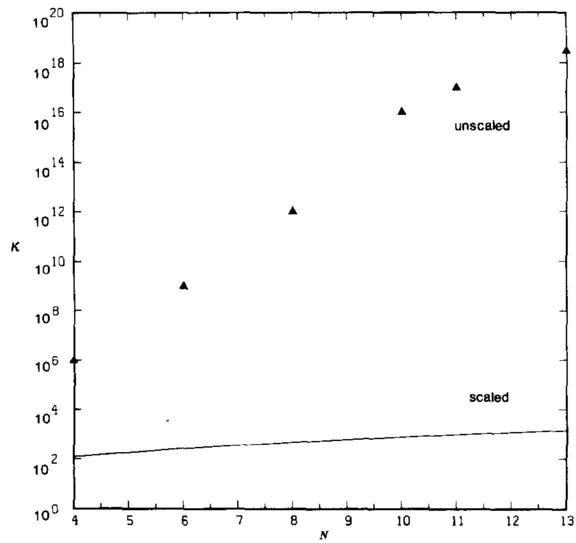

FIG. 1. Log-linear plot of condition number vs polynomial order N for the scaled and unscaled cases.

lead to problems in the machine calculations and accuracy is lost. The Laguerre-discretized (second-order derivative) operator matrix is found to have a condition number which increases exponentially with N. Upon rescaling the operator matrix with a diagonal matrix of the Laguerre weights, the growth of the condition number is limited. This is illustrated in Fig. 1, where the condition number is plotted against N in a log-linear fashion for the scaled and unscaled cases.

The simple one-dimensional solution to the Helmholtz equation $-u_{xx} + \lambda^2 u = f$ is compared to the exact solution xe^{-x} for $f = (2 + (\lambda^2 - 1)x)e^{-x}$, $\lambda = 1$, and $N = 13$, in Fig. 2. As expected, the error at the outlying points of the domain is very large. Only 10 points are shown here for reasons of scaling the plot. However, if the error is measured in terms of the following weighted H^1 error norm,

$$\varepsilon = \|u - u_{\text{exact}}\|_{e^{-x}} + \left\|\frac{du}{dx} - \frac{du_{\text{exact}}}{dx}\right\|_{e^{-x}}, \tag{14}$$

where the $\|\cdot\|_{e^{-x}}$ norm is defined as

$$\|u\|^2_{e^{-x}} = \int_0^\infty u(x)^2 e^{-x} dx \simeq \sum_{i=0}^{N} w_i u(x_i)^2, \tag{15}$$

it is only 7.10^{-4} for this case. $\|\cdot\|_{e^{-x}}$ is the proper norm since the Laguerre polynomials are orthogonal in this weighted norm. The importance of the error at the outlying points is diminished as measured by (14), (15), since the corresponding weight values become exponentially small. Figure 3 exhibits the continuity of the solution

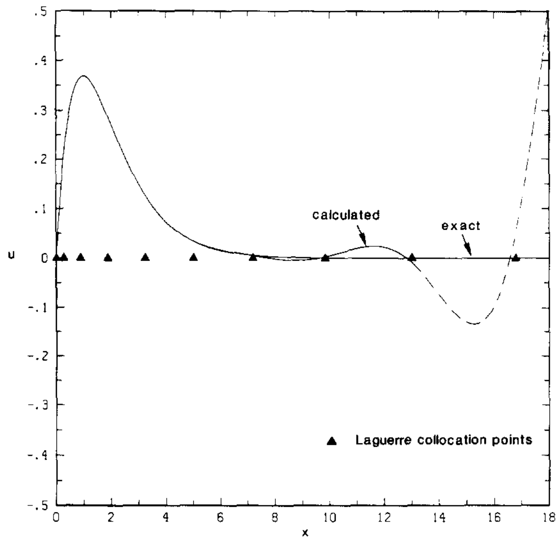

FIG. 2. Comparison of exact and calculated solutions to $-u_{xx}+\lambda^2 u=f$ with $\lambda=2$, $f=(2+(\lambda^2-1)x)e^{-x}$, and $N=13$. Dashed line indicates where the solution is no longer useful.

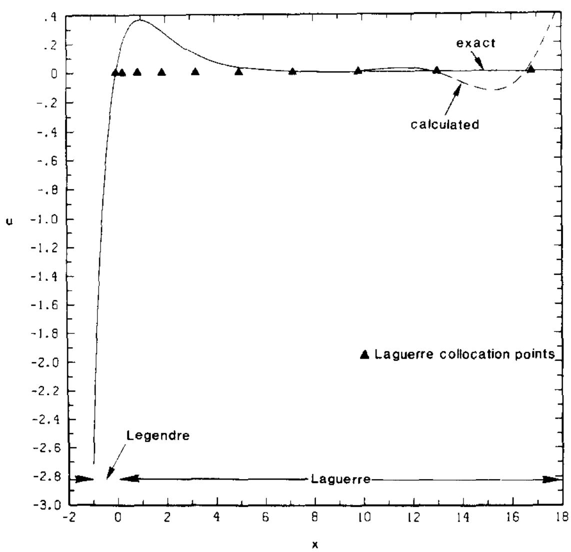

FIG. 3. Comparison of exact and calculated solutions to $-u_{xx}+\lambda^2 u=f$ with $\lambda=2$, $f=(2+(\lambda^2-1)x)e^{-x}$, using one Legendre element and one Laguerre element; $N=13$, for both elements. Dashed line indicates where the solution is no longer useful.

at $x=0$ when a coupled Legendre–Laguerre formulation is used on the same problem on the domain $[-1;\infty[$ with the boundary condition $u(-1)=-e$. $N=13$ was used in both elements here, but the last four points of the Laguerre element are again not shown. The error norm for the case of coupled Legendre–Laguerre spectral element domains is defined as

$$\varepsilon=\left(\|u-u_{\text{exact}}\|_{\text{Leg}}+\left\|\frac{du}{dx}-\frac{du_{\text{exact}}}{dx}\right\|_{\text{Leg}}\right)(x\in[-1;0])$$
$$+\left(\|u-u_{\text{exact}}\|_{e^{-x}}+\left\|\frac{du}{dx}-\frac{du_{\text{exact}}}{dx}\right\|_{e^{-x}}\right)(x\in[0;\infty[),\qquad (16)$$

where the Legendre norm is the usual L_2 norm over the interval $[-1;0]$, evaluated similarly by Legendre quadrature. The error norm for this problem is found to decrease exponentially with increasing N as shown in Fig. 4 and has the value $\varepsilon=7.10^{-4}$ for the case of Fig. 2.

Exponential convergence of the error norm does not occur for cases of the Helmholtz equation where $\lambda<0.5$ for the above formulation. This is attributed to the treatment of the natural boundary condition at ∞. From the variational form (1), the boundary term $ve^{-x}u_x]^{\infty}$ is used to generate the natural boundary condition at infinity of $u_x(x\rightarrow\infty)=0$. The Helmholtz equation admits homogeneous solutions of the form $e^{-\lambda x}$ and $e^{+\lambda x}$ and hence the product boundary term is of the form $ve^{-x}e^{+\lambda x}]^{\infty}$. For $\lambda-1<0$ this product is zero $\forall v$ and hence growing modes can still exist. Furthermore, for well-posedness it is necessary that the homogeneous

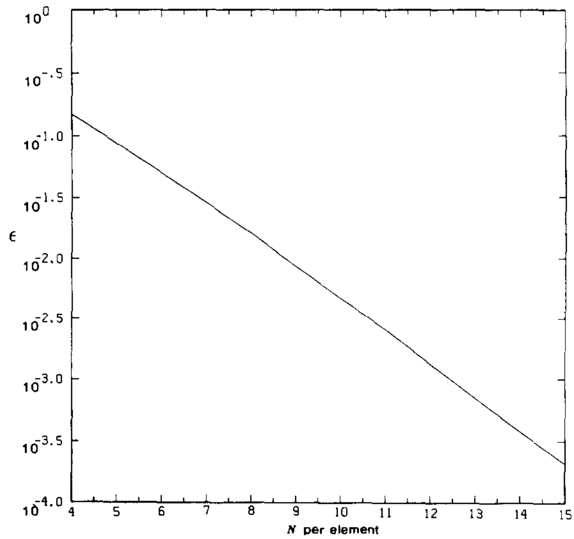

FIG. 4. Convergence plot of error norm vs polynomial order N per element for the coupled Legendre–Laguerre solution to $-u_{xx}+\lambda^2u=f$, with $\lambda=2$, $f=(2+(\lambda^2-1)x)e^{-x}$.

solution not belong to H_0^1. Following Maday *et al.*'s definition of the Sobolev spaces $H^p_{e^{-\alpha x}}$ [3], this implies at worst that the integral $\int_0^\infty e^{+2\lambda x} e^{-x} dx$ must not converge; that is, $2\lambda - 1 > 0$. Thus for cases where $\lambda < 0.5$ this boundary condition is not sufficient and convergence behaviour is poor or unobtainable. Instead, a modified Laguerre formulation is used, defined by a simple rescaling of the weighting function to $e^{-\alpha x}$. This corresponds to redefining the space of functions to $H^1_{\alpha,0}$, the space of functions which are square integrable with respect to the measure $e^{-\alpha x} dx$ and whose first derivatives are similarly integrable. Quadrature is then rewritten as

$$\int_0^\infty f(x)\, e^{-\alpha x} dx = \frac{1}{\alpha} \sum_{i=0}^{N} w_i f\left(\frac{x_i}{\alpha}\right), \tag{17}$$

where α is chosen to suppress the growing modes in the problem. The variational problem becomes: Find $u \in H^1_{\alpha,0}$ such that

$$\int_0^\infty v_x u_x e^{-\alpha x} dx + \lambda^2 \int_0^\infty v u e^{-\alpha x} dx = \int_0^\infty v u_x e^{-\alpha x} dx + \int_0^\infty v f e^{-\alpha x} dx \qquad \forall v \in H^1_{\alpha,0}. \tag{18}$$

Using the same arguments as above, the requirement for convergence becomes $2\lambda - \alpha > 0$.

This method is found to be successful, giving exponential convergence when α is chosen properly, that is, in a range found to be in the neighbourhood of 2λ and with $\alpha < 2\lambda$. Equation (17) indicates that the modified Laguerre formulation is simply a rescaling of the quadrature points distribution that gives better resolution for each case, i.e., each λ. In all cases the error norm is reduced by several orders of magnitude as illustrated in Fig. 5. This figure shows the error norm for the modified Laguerre formulation as a function of α for the case $\lambda = 0.1$ and $N = 21$. Note that the error norm is a minimum in the vicinity of $\alpha = 0.18$, whereas the solution was unobtainable for the usual Laguerre ($\alpha = 1$). This is consistent with the findings of Maday *et al.* [3], which show that the larger the coefficient α, the smaller the approximation error is. For $\alpha = 0.2 = 2\lambda$ and increasing, the error grows rapidly, which verifies our convergence requirement of $\alpha < 2\lambda$. Though the error is still poor ($O(10^{-1})$) even for the optimum α, this is a result of the function we are trying to approximate: xe^{-x}. Rescaling with an α (or equivalently λ) which is smaller than 1, actually makes it harder to approximate a function like xe^{-x} as $x \to \infty$. More points are required in these cases, but the boundary condition is no longer responsible for the error since it is correctly posed.

With the understanding of its above-described properties, the Laguerre formulation is found to be a useful way to treat unbounded regions in the spectral element method. Infinite boundaries were previously treated by domain truncation and algebraic, as well as exponential, mapping techniques [4, 5, 6] and more recently by orthogonal rational basis functions [7, 8]. Boyd [4] has shown that exponential mappings are uniformly poor tools for semi-infinite mappings since the transformed

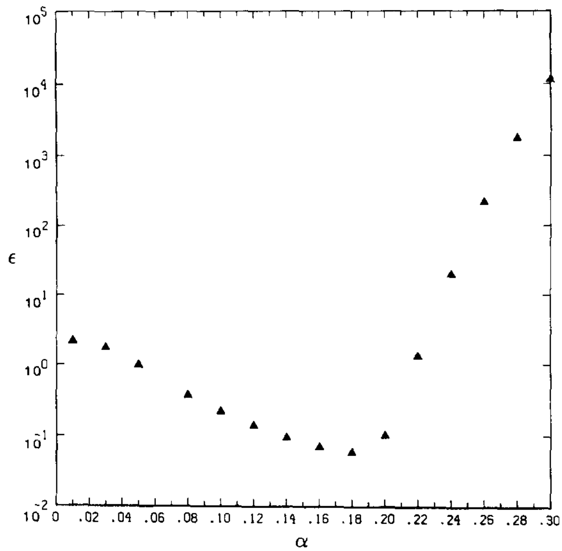

FIG. 5. Plot of modified Laguerre error norm vs α for $\lambda = 0.1$ and $N = 21$.

functions exhibit strong singularities, giving poor convergence. In agreement with Grosch and Orszag's numerical experiments [5], Boyd has shown that domain truncation is best for functions that decay rapidly and algebraic mappings are best for functions with singularities. In either case, however, convergence depends on parameters whose optimum values are only determined by knowing the asymptotic behaviour of the function. In the present method, one must also use a parameter α which may be found by knowing the asymptotic behaviour of the function or more practically by reasonable estimation from error estimates from a previous choice of α. The Laguerre formulation replaces exponential mapping by using the e^{-x} weighting function, which diminishes the importance of the error at the outlying points near infinity. The present method provides a variational formulation consistent with our finite domain techniques, compatible in particular with Legendre elements, providing exponential convergence for infinite domains.

4. CONCLUSIONS

In summary, it has been demonstrated that Laguerre polynomials may be used in the spectral element formulation for the solution of partial differential equations, particularly in regions of outflow or infinite boundaries. Their consistency with Legendre elements enables their use without any special treatment of the boundary interface. The only extra work involved is in the calculation of a new convection-type term which may be treated explicitly. Rescaling of the discretized operator matrix with the weights of the Laguerre functions is necessary since the condition number is found to increase exponentially with increasing polynomial order. Exponential convergence of the solution is obtained provided a natural boundary condition is imposed at ∞. A modified Laguerre formulation involving a rescaled weighting function may be used to suit each problem in suppressing growing modes in the numerical scheme.

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