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Introduction

1.1 Introduction

Natural phenomena can often be described mathematically in the form of systems of differential equations. To derive meaningful conclusions with quantitative understanding, accurate solutions to these systems of differential equations are required, which are often not feasible by exact formulae. Instead, approximate numerical approaches, become viable means given the complex nature of the boundary conditions, loading environments and material distributions, noting that often they approach the exact solution, given certain conditions are satisfied. This chapter presents a general procedure for numerically estimating functional fields using spectral methods. In this discussion, emphasis is given to the collocation approach in the framework of spectral methods due to its simpler implementation when compared with the well-established Galerkin and Ritz approaches within the general scope of spectral methods. The appropriate choice of polynomial basis used in the early collocation methods [1, 2] was interlinked with the distribution of the collocation points and this undesirable complexity was addressed with the introduction of the generalised differential quadrature method (DQM) [3]. This method relies on solving differential equations directly, known as the strong-form method of solution. Owing to its simplicity and ease of implementation and rapid numerical convergence, DQM was applied to problems across various disciplines of science. Despite the promising features of DQM, it may suffer from degradation of accuracy with successive differentiation operations. In this regard, the indirect approximation technique is an emerging approach to circumvent differentiation-induced errors associated with direct approximation. This chapter provides an insight into the development of numerical approximation methods and highlights the limitations that support the adoption of indirect approximation techniques.

1.2 Overview of Numerical Approximation Methods

Widely used state-of-the-art structural analyses rely on the finite element method (FEM), notwithstanding the current progress made in using large amounts of data with artificial intelligence (AI) methods, especially neural networks; see for example [4]. Both approaches can be used to model highly continuous systems, but the former has a degree of inherent continuity represented by underlying physical principles in the system, while the latter typically interpolates data from discrete points obtained from sampling. Both represent response surfaces, such as deformations,

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stresses and temperature as a discrete set of data, which lends itself to solution by matrix methods. Here, we focus on methods in which knowledge of the physics of the problem at hand can be represented mathematically, e.g. in terms of energy (or in general terms as a functional) or in terms of balance expressions, typically represented by differential equations. An energy formulation involves the integration of state variables over the domain (or structure) and so weakens continuity requirements, and is known as the *weak* method, while the solution of differential equations is accomplished on a point-by-point basis and is known as the *strong* method.

The essence of all direct methods of solutions involves representing a variable of interest (e.g. deflection, stress, temperature, flow rate, etc.) by a particular form, typically a series of basis functions, whose coefficients (or weights) can be tweaked to minimise the energy of the system or to solve the governing differential equations, subject to appropriate boundary conditions. By representing a continuous field (or function), by a series inherently converts a continuous system into a discrete one, and in the limit, for equivalence between the two, a discrete system with an infinite number of points. Here, we credit Fourier [5] with his trigonometric series representation of heat flow and latterly, Ritz, with these developments. Indeed, Ritz, in his phenomenally profound paper (see [6]) shows the conditions in which a continuous function can be represented by a series formulation, introducing terms, which we understand now as linear independence and completeness. The former can be understood by considering a two-dimensional (2D) vector space whereby a linear combination of two vectors has the significance of being able to represent any point (position vector) in the 2D vector space. Such principles extend to n-dimensional space. By 'completeness', it means that the series has all sequential terms in a series. So, considering a trigonometrical sine series, then each successive frequency would have to be included. Under these conditions, Ritz showed that an arbitrary function could be represented by a complete infinite series with linearly independent terms, known as basis functions. Of course, the conundrum created by this approach is that an infinite number of the resulting linear equations cannot be formed and therefore solved. Helpfully, Ritz also showed that as the number of terms in the series increases, the exact solution is approached. An early attempt to use this method to solve for an engineering quantity of interest was by Lord Rayleigh in his monumental text: 'Theory of Sound' [7], where in one small section he used a single sine function (one term series, if you will), to approximate the first vibration mode of excitation of a hemispherical shell, so to determine its fundamental frequency. As Calladine [8] regales, Rayleigh [9] was interested in quantifying the natural frequency of his college bell at Trinity, Cambridge, the one-term displacement function for the vibration mode captured its behaviour well except for near the bell's edges (i.e. boundaries), which should be stress free but were not with the single-term mode shape. However, the boundary layer for this problem was narrow, identified by rapidly decaying values of interior stresses to the edge [8]. Rayleigh realised if more sinusoidal terms, of higher frequency, were added, then better agreement could be achieved [10]. However, no proof or generalisation of the process seems to have emerged until Ritz [6], and hence Rayleigh–Ritz methods of direct approximation were born and used to solve systems where functionals, such as the energy of the system, could be formed. For an interesting discussion on early developments in Rayleigh–Ritz methods, the reader is referred to [11]. Inspired by Rayleigh, in the early years of the twentieth century, Timoshenko [12] solved buckling problems of isotropic plates with various loading and boundary conditions using mostly one-term shape functions for the buckling mode shape. As a result of these works, Timoshenko won the Zhuravskii Prize with Bubnov as reviewer. Indeed, in his review, Bubnov also integrated the partial differential equation (PDE) with respect to the unknown displacement, minimised the outcome, which is essentially orthogonalising the error, and in so doing created what is now known as the Galerkin method [13]. This method does not rely on a functional and can be used to solve any differential equation in the weak sense. Notably,

Galerkin was a student under Bubnov and used the method for analysing the stability behaviour of multipart plated ship structures. For another interesting detailed discussion on such developments, Elishakoff et al. [14] suggest Timoshenko thought that Ritz had already suggested such an approach in his 1908 paper – indeed, there is a single equation written which resembles, but is actually not, what we now call the Galerkin method, but it was not developed or used to solve any problems by Ritz. To make this brief review more complete, we should also mention the pioneering work of Richardson [15] who in 1911 proposed the finite difference method (FDM) for solving differential equations. So until 1915, in addition to Richardson, physicists (e.g. Rayleigh), mathematicians (e.g. Ritz) and engineers (e.g. Galerkin) had appreciated that a continuous system could be represented by a finite number of discrete entities – as a key underpinning development of what evolved to be the FEM. Important developments in the late 1920s then happened independently in mathematics and engineering. First, the mathematics Where Courant made important developments [16], in which referring to Weierstrass's first theorem [17], he showed how a series of piecewise constant polynomials can represent an arbitrary continuous function. He made important connections between FDM and Rayleigh–Ritz method by showing the former could be derived as a special case of the latter, as long as only first-order derivatives were involved in the variational statement. He also solved polygonal domains using a net of triangular 'elements' by the FDM and tried to do so with higher-order polynomials but seems to have been unable to find suitable basis functions for the Rayleigh–Ritz method to be applied. Concurrently, in engineering practice, the development of faster mono-wing aeroplanes in the late 1920s led to catastrophic flutter failures due to the flexible, thin-walled constructions used. Indeed, initially, Frazer and Duncan working at the National Physics Laboratory in the UK, were researching and developing methods for analysing the aeroelastic response of such aeroplanes. They were soon joined by Collar and they developed semi-rigid elastic models (today, understood as discrete systems)-both experimentally in the lab using lumped masses and, importantly for the current context, also numerically. These authors [18–20] made extremely important developments by recognising that mechanical systems comprising discrete components lend themselves to solutions using matrix methods by computerised methods. They calculated the natural frequency of twisted and tapered propeller blades (they called them airscrews), formulating stiffness matrices. Indeed, their textbook [20] seems to be the first to describe the importance and application of matrices for solving numerical methods in engineering disciplines, as opposed to pure mathematical analysis. Later in the mid-1950s, Argyris and Kelsey [21] developed a force-based matrix method for structural analysis, while contemporaneously, Turner et al. developed a matrix method for modelling simplistic aeroplane structures, and it is one of their co-workers, Clough, who is widely credited for naming the finite element method. Interestingly, these researchers seem largely unaware of the earlier 1930s work done in the UK and give significant credit to Courant [22] for developing the idea of a continuum being broken into triangular domains for analysis. There have been many reports on the history of the FEM and related techniques – we highlight those by Leissa [11] and Felippa [23] as particularly illuminating. A further important contribution made by Rayleigh and picked up by Timoshenko is that as long as the finite series (remember, mostly containing only a single term in their examples) obey displacement-based (i.e. essential) boundary conditions, then as more series terms are added, then the exact solution is approached from above. In other words, these approximate solutions overestimated natural frequencies and buckling loads by being overly stiff, or from an alternative perspective, not having sufficient degrees of freedom to be sufficiently flexible-noting each term in the series represents another degree of freedom.

So far, our discussion has focused on variational (i.e. weak) forms of solving PDEs. We note that strong forms solve these equations on a point-by-point basis and FEMs can be derived in this way or

from a variational perspective (where only first-order derivatives occur in the variational statement [22]. However, Finlayson generalises such collocation methods, and gives an interesting history of their developments [24]. Note, Section 1.5 describes the strong-form DQM, which was developed from the 1970s.

Comparing strong and weak forms is theoretically straightforward, but their solution and practical applicability are more nuanced. It is noted that both methods are equivalent, as integrating the functional in the weak form gives the governing differential equation and essential boundary condition in the strong form. Mathematically, the contrast concerns integration or higher-order differentiation for weak and strong forms, respectively. As such, the difference lies in the implementation, i.e. discretisation and solution process of both schemes. The lower-order differential operators required within weak formulations allow lower orders of continuity or smoothness in the domain, which is attractive for modelling complex geometries. On the other hand, where there are highly fluctuating fields within a domain, the higher continuity required by strong formulations becomes attractive, but the higher degree of continuity required leads to less model versatility.

Currently, our comparison has focused on overall mathematical and physical reasoning. Now, we consider their respective solution methods. Both methods rely on assuming a series representation of the variables of interest. Mathematically, this is well understood by appealing to Weierstrass's first theorem, Ritz's contribution, and more recently, in terms of spectral methods [25–27] of series representations of the variables at hand (see Section 1.4 for more information on Spectral Methods). FEMs rely on breaking up the domain of interest into one-dimensional, 2D or 3D spatial elements in which the low-order polynomials approximate a variable of interest. Lowest-order continuity, which is termed C^0, which only requires the value of the function (and none of its derivatives to be continuous) occurs at element boundaries. This low degree of continuity allows large problems to be solved with a high degree of flexibility leading to global stiffness matrices with low rank, that are characterised by low bandwidths, in other words, the matrices are sparse. There are efficient iterative matrix solution methods for such models. To obtain converged solutions, many elements are required, which is so-called *h*-refinement). Of course, it is possible to use fewer elements with a greater degree order of polynomials (*p*-refinement), but versatility decreases and matrix solution methods become more difficult as fuller matrices develop. Continuity at an element boundary is less than the continuity within an element and more accurate solutions can be obtained by increasing the number of elements (*h*-refinement) or by raising the order of polynomial within an element (*p*-refinement), or indeed by a mixture of both – *hp*-refinement (see [28]). The huge success of classical FEM codes is not that they capture the physics particularly well, it is in the fact that the low-order continuity imbued by both use of piecewise low-order polynomials and element boundaries gives rise to sparse matrices, as already mentioned, which can be solved efficiently while simultaneously giving great applicability to complex geometric problems. Their inherent model versatility captures complex geometries and is facilitated by low continuity elements. So for example, FEM meshes allow complex geometries to be modelled by using piecewise continuous elements of relatively low order. As well as model versatility, the reduction in model continuity offered by FEM leads to system matrices that are banded in structure, also satisfying natural boundary conditions, which allows for efficient computational solution methods to be applied. Fewer elements but with greater *p*-refinement lead to fuller matrices and more expensive matrix manipulation methods. In contrast, strong-form methods capture the inherent degree of continuity of a problem.

In drawing a conclusion to this discussion, it should be said that both weak and strong methods discretise a continuous domain and convert an energy (or other scalar functional) into a simple discretised algebraic system of equations that are solved using matrix methods. Strong-form methods

capture a higher degree of continuity within a strong form element or domain of interest, leading to fuller matrices (noting the off-diagonal terms represent the enhanced continuity) in comparison with the low degree of continuity and sparse matrices of FEM. So which is best? Well it depends! It depends on the problems at hand, considering geometric complexity and gradients of variables of interest. From our experiences, strong-form methods capture the physics of the problem best with *p*-refinement and boundaries are placed where there is a break in higher-order continuity. Ultimately, combined weak–strong-form appeals in which strong form elements are used in regions of high gradients and conventional FEM near complex boundaries. However, such mixed techniques are not currently available and buoyed by the fact that *p*-refinement coupled with strong-form captures physical continuity most effectively, this book is dedicated to deriving strong-form methods of solving differential equations.

1.3 Numerical Approximation

Mathematical models describing physical phenomena capture the behaviour of nature (to a large extent) in the form of mathematical equations constructed as differential equations (e.g. ordinary differential equations (ODEs), PDEs or integral equations. In an engineering context, these ODEs and PDEs must be solved to retrieve relevant information that can facilitate design and analysis of the phenomena under study. Exact formulae or closed-form solutions satisfying the governing equations are rarely feasible, sometimes not even possible. As such, numerical approximation becomes inevitable.

For the sake of generality, a differential equation representing a physics or an engineering problem is represented as

$$\mathcal{L}_1(u) + a = 0, \tag{1.1}$$

where $\mathcal{L}_1$ is the differential operator (ordinary/partial), u is the primary variable for the differential equation and a can be a constant or a function of the domain variable. The associated boundary condition can be represented as

$$\mathcal{L}_2(u) = b, \tag{1.2}$$

where $\mathcal{L}_2$ is the differential operator and when applied to u yields b at the system boundary, which can be a variable or a constant. Now, the first step towards numerical approximation is to assume a form for the variable u which satisfies the field equation (Equation 1.1) along with the boundary condition (Equation 1.2). Therefore, assuming the variable u as a sum of basis or trial functions φ as

$$u \approx u^a = \sum_{i=0}^{N} \alpha_i \varphi_i, \tag{1.3}$$

where u^a is the approximation of function u, φ_i and α_i are the ith basis function and unknown coefficient, respectively. According to Boyd [29], building upon the highly influential work of Ritz [6], these basis functions must possess certain properties like ease of computation, rapid convergence, linear independence and completeness. Upon substituting the approximate solution u^a in Equations 1.1 and 1.2, residual function can be obtained for domain (R_Ω) and boundary (R_Γ) as

$$\mathrm{R}_\Omega = \mathcal{L}_1(u^a) + a, \quad \mathrm{R}_\Gamma = \mathcal{L}_2(u^a) - b. \tag{1.4}$$

These residual functions are identically zero for exact solutions; therefore, the aim of different numerical approximation techniques is to minimise the residuals sufficiently subject to the refinement of field discretisation. If the basis functions are chosen in such a way that they satisfy the

specified boundary condition, then the residual over the domain can be forced to approach zero in an average sense by

$$\int_{\Omega} \widehat{w}_i \mathrm{R}_{\Omega} = \int_{\Omega} \widehat{w}_i (\mathcal{L}_1(u^a) + a) = 0, \quad \text{for} \quad i = 0, 1, 2, \ldots, n, \tag{1.5}$$

where $\widehat{w}_i$ are the weighting functions. Equation 1.5 results in $n+1$ algebraic equations, which could be simultaneously solved to obtain unknown coefficients α_i. This general scheme of approximation is known as the method of weighted residuals (MWR) [30]. The choice of basis and weighting functions forms the criteria that distinguishes different numerical schemes.

1.4 Spectral Methods

Spectral methods are a class of numerical approximation techniques known for their high spatial accuracy at low computational cost. These methods are preferred in applications where high accuracy in numerical estimates is required at a relatively low computational cost. These methods have successfully demonstrated promising utility in applications such as heat transfer [31], computational fluid dynamics [32], numerical weather prediction [33, 34], seismic response in geological structures [35] and many more.

Spectral methods are considered to be global methods, unlike FEM and FDM, which are local methods. Local methods employ low-order interpolating polynomials as basis functions, which are defined locally within a sub-interval in the global domain or *element* and are zero over the rest of the domain. This process implies that numerical computation, at a point in the global domain, relies on the information provided by neighbouring points and hence necessitates a fine mesh to approximate a function with significant spatial and temporal variations. Consequentially, considerable computational resources are required to achieve accurate approximation using low-order polynomials. On the contrary, spectral methods approximate a function using globally defined higher-order polynomials as basis or trial functions. Numerical approximation of the function is accomplished using contributions from all points in the global domain, which results in a more accurate estimation at comparatively lower computational cost than local methods.

Finlayson and Scriven [30] argued that most of the approximation techniques can be categorised as special cases of MWR on the basis of choice of weight functions adopted. From this perspective, spectral method can be implemented via three approaches, namely, Galerkin, Tau and collocation [25]. Although it is worth mentioning, Boyd [26] categorised spectral methods into two groups, interpolating methods (based on collocation and non-interpolating methods (based on Galerkin and Tau approaches). Nevertheless, the distinguishing feature still remains the choice of weight functions employed to realise the implementation of the method and the residual minimisation technique.

1.4.1 Galerkin and Tau Approach

In the Galerkin approach [36], the basis functions φ_i are adopted as weight functions $\widehat{w}_i$ and the integral of the weighted residual (Equation 1.5) is made zero for every weight function, after performing integration-by-parts, leading to $N + 1$ algebraic equations and finally solving the system for unknown coefficients α_i. The Tau approach is similar to the Galerkin approach with the only difference being the non-conformity of basis functions at the boundaries, i.e. the basis functions, which are essentially weight functions, need not satisfy the boundary conditions a priori and therefore a separate set of equations are supplemented along with the field equations to implement

boundary conditions. Lanczos [2] developed the Tau approach by employing Chebyshev polynomials as weight functions and later Orszag [37] applied it to analyse stability of plane Poiseuille flow and reported accurate results with less computational effort. The method was further developed by Ortiz and co-workers by exploring the equivalence of the method with other numerical approximation techniques [38–40].

1.4.2 Collocation Approach

The collocation approach, a subset of spectral methods, also known as the pseudospectral method, seems to have originated in the works of Slater [41] and Kantorovich and Krylov [42] but it was Frazer et al. [1] who developed it as a generalised framework for implementation to the problems governed by ODEs. In this approach, the residual function is satisfied exactly at specific points in the domain known as collocation points. This is achieved by assuming Dirac delta functions as the weights, i.e. $\widehat{w}_i = \delta(x - x_i)$, where x_i is the collocation points. As the number of collocation points is increased, the residual vanishes progressively on the entire domain [30]. This approach was pursued further by many researchers owing to the simplicity of its implementation as no integration was required, which was its most attractive feature [29, 43].

Frazer et al. [1] used various basis functions and equally spaced points for the implementation of the collocation approach for several problems and compared the results with Galerkin and least squares methods. It was the work of Lanczos [2], where it was argued that the appropriate choice of basis functions and the distribution of the collocation points is imperative to the numerical accuracy and convergence of the approximation. Lanczos [2] used Chebyshev polynomials as basis functions and collocated them at their roots (in the so-called Chebyshev collocation method) and this selection of basis and collocation points were further pursued by Clenshaw [44], Clenshaw and Norton [45] and Wright [46] to solve linear and nonlinear ODEs. Villadsen and Stewart [47] further extended this method to PDEs under the name orthogonal collocation because of the fact that orthogonal polynomials were used as basis functions for approximation and the collocation points selected were the roots of these orthogonal polynomials. This, in a sense, is equivalent to the Galerkin approach if the integral of the weighted residual is evaluated via numerical integration using optimal quadrature points [29, 47]. It was concluded that the use of roots of Chebyshev polynomials as the collocation points instead of a uniform distribution yields better minimisation of the residual since the Runge phenomenon [48] is suppressed for the points stretched towards boundaries [29]. Villadsen and Stewart [47] reported improvement in the accuracy by selecting roots of Jacobi polynomials as the collocation points and selecting functional values of the field variables at collocation points ($u^a(x_i)$) as unknown coefficients α_i where x_i are the set of collocation points. This change in the selection of unknown coefficients made the procedure more explicit, finite difference-like, and made it easier to automate the process for general implementation to a wide variety of problems [43]. The orthogonal collocation method was subsequently expanded for different classes of collocation points particularly in the field of chemical engineering [49–54].

Parallel to the development of the orthogonal collocation, Orszag [55] presented the comparison of numerical accuracy of the collocation method, known as pseudospectral and Galerkin (spectral) methods, respectively, for selected initial value problems and later, the monograph by Gottlieb and Orszag [25] gave the first comprehensive mathematical evaluation of the theory of spectral methods [56]. A great deal of literature concerning different aspects related to spectral methods was produced and it is neither possible, nor intended, to review spectral methods in their entirety. However, the reader is referred to some excellent texts describing the method, solution strategies, applications and limitations [29, 32, 56–59].

The reliance of the numerical accuracy and convergence of collocation methods on the appropriate choice of basis functions and distribution of collocation points was acknowledged in the form of another simple yet efficient pseudospectral method known as the DQM. Later, a generalised version, known as the generalised differential quadrature (GDQ) was proposed to resolve this issue of choice of basis functions and distribution of collocation points.

1.5 Differential Quadrature Method

Bellman et al. [60, 61] introduced an efficient numerical discretisation technique to obtain solutions for problems governed by high-order ordinary and PDEs by approximating the spatial derivative of a function using a linear weighted sum of all the functional values in the domain. This technique is known as: the DQM. As its name suggests, the motivation of the approach was derived from the concept of numerically approximating the definite integral of a function by an integral quadrature.

Evaluation of an integral of a function $\int_a^b f(x)\mathrm{d}x$ is often encountered in the mathematical formulation of many problems and it is often not possible to obtain an exact solution. As we know, $\int_a^b f(x)\mathrm{d}x$ is the area under the curve $f(x)$ with the bounds $a \leq x \leq b$, this area can be approximated by assuming it to be a linear weighted sum as:

$$\int_a^b f(x)\mathrm{d}x = w_1 f_1 + w_2 f_2 + \cdots + w_n f_n = \sum_{i=1}^{n} w_i f_i, \tag{1.6}$$

where $w_1, w_2, \ldots, w_n$ are the weighting coefficients and $f_1, f_2, \ldots, f_n$ are the functional values at the discrete points in the domain. Based on the concept of integral quadrature, Bellman and Casti [60] proposed that the first-order derivative of the function f with respect to x at a grid point can be represented by a linear sum of all of the functional values with in the entire domain by

$$\left.\frac{\partial f}{\partial x}\right|_{x_i} = \sum_{j=1}^{N} a_{ij} f(x_j), \quad \text{for } i = 1, 2, \ldots, N, \tag{1.7}$$

where a_{ij} and $f(x_j)$ represent the weighting coefficients and functional values of the collocation points in the domain, respectively. Bellman and Casti [60] applied DQM to fluid flow problems and reported high numerical accuracy with relatively low computational cost. Later, Mingle [62] studied nonlinear transient heat conduction phenomena using DQM and Civan and Sliepcevich [63] applied DQM to transport phenomena problems. DQM was introduced to the field of structural mechanics by Jang et al. [64] and Bert et al. [65], where higher-order differential equations governing flexural and dynamic behaviour of beam and plate structures were solved. These works motivated the exploration of DQM as an efficient numerical technique for problems in structural mechanics and is well accounted for in the first review on DQM by Bert and Malik [66].

1.5.1 Determination of Weighting Coefficients

Determining the weighting coefficients a_{ij} is the most important step in the DQM approximation process. Bellman et al. [61] suggested two different methods to evaluate these weighting coefficients. The first way is to assume polynomial basis functions of the form x^k for $k = 0, 1, \ldots, N-1$

for the approximation of the function $f(x)$. Substituting into Equation 1.7 yields a set of N linear algebraic equations,

$$\sum_{j=1}^{N} a_{ij} x_j^k = k x_i^{k-1} \quad \text{for } i = 1, 2, \ldots, N, \qquad k = 0, 1, \ldots, N-1. \tag{1.8}$$

Equation 1.8 results in a matrix of Vandermonde form and can be solved for a_{ij}. However, Vandermonde matrices are inherently ill-conditioned and the inversion becomes cumbersome as the number of collocation points increases particularly when $N > 13$ [27, 67]. The second approach proposed by Bellman et al. [61] is similar to the first in terms of implementation, the only difference being the choice of basis function and the distribution of collocation points. The basis function adopted is $L_n(x)/(x - x_k)L_N^{(1)}(x_k)$, where $L_N(x)$ is the Nth-order Legendre polynomial and $L_N^{(1)}(x)$ is the first derivative of $L_N(x)$. Collocation points were chosen to be the roots of shifted Legendre polynomials and a simple algebraic formulation was obtained for a_{ij} as:

$$a_{ij} = \frac{L_N^{(1)}(x_i)}{(x_i - x_j)L_N^{(1)}(x_j)} \quad \text{for} \quad i \neq j, \quad a_{ii} = \frac{1 - 2x_i}{2x_i(x_i - 1)} \tag{1.9}$$

although the second approach is simpler, it restricts the choice of collocation points, thereby severely limiting its application to engineering problems.

Later, Shu and Richard [3] proposed GDQ based on a Lagrange polynomial basis in order to overcome the limitations of previous approaches for evaluation of weighting coefficients, corresponding to arbitrary order of derivatives. If $a_{ij}^{(m)}$ represents weighting coefficients corresponding to the mth-order derivative, Shu's general recurrence formula can be expressed as:

$$a_{ij}^{(m)} = m\left(a_{ij}^{(1)} a_{ii}^{(m-1)} - \frac{a_{ij}^{m-1}}{x_i - x_j}\right),$$
$$\text{for } i, j = 1, 2, \ldots, N, \quad m = 2, 3, \ldots, N-1,$$
$$a_{ii}^{(m)} = -\sum_{j=1, j\neq i}^{N} a_{ij}^{(m)}, \tag{1.10}$$

where $a_{ij}^{(1)}$ are the weighting coefficients for the first-order derivative and are calculated as

$$a_{ij}^{(1)} = \frac{M^{(1)}(x_i)}{M^{(1)}(x_j)(x_i - x_j)}, \quad \text{for} \quad i \neq j,$$
$$M^{(1)}(x_i) = \prod_{j=1, j\neq i}^{N} (x_i - x_j). \tag{1.11}$$

It is worth mentioning that these recurrence formulae by Shu [68], unlike previous counterparts, are not restricted to a specific distribution of collocation points.

DQM enables the solution of the governing differential equation in strong form, i.e. the equations are explicitly satisfied at each collocation point. This approach is contrary to traditional FEM or Galerkin approaches, where the governing equations are integrated over the domain to obtain the

weak form and approximately satisfied over the domain in an average sense. This feature facilitates the capture of rapidly varying stress gradients, especially towards boundaries, with relatively little computational effort, as natural, along with essential boundary conditions, are imposed at the boundaries on a point-by point-basis. Now, due to the one-to-one correspondence between collocation points and functional values, only one equation can be satisfied at each collocation point. As a result, the application of DQM to structural mechanical problems poses a challenge with regards to the implementation of dual boundary conditions and to address this issue several researchers have proposed additional numerical procedures.

1.5.2 DQM Implementation of Dual Boundary Conditions

Accuracy and convergence of the DQM[1] solution highly depends on the satisfactory implementation of the boundary conditions. Because DQM solves governing equations in strong form, each collocation point yields one equation in the global system of equations. For problems having a single boundary condition, the method is straightforward, i.e. a discrete boundary condition is satisfied at a corresponding boundary point. However, for problems where more than one condition is required at the boundaries, for example, in the case of the Euler–Bernoulli beam equation, different approaches have been reported in literature that guarantee appropriate implementation of dual boundary conditions, as now discussed.

Bert et al. [65] proposed the δ-technique to eliminate difficulties in implementing two conditions at a single boundary point. The essential conditions are satisfied explicitly at the boundary points and the natural boundary conditions are implemented at the points adjacent to the boundary at a δ distance. The accuracy of the results depends on the magnitude of the distance, because the natural condition is not strictly implemented at the boundary. Therefore, a small value of δ ensures better enforcement of natural boundary conditions, thereby yielding more accurate results. However, if the magnitude of δ exceeds a critical value, the DQM weight coefficient matrices become highly ill-conditioned and result in oscillations of the numerical solution [67].

To overcome the drawbacks of the δ-technique, Wang and Bert [69] proposed a new approach to implement dual boundary conditions by modifying the weight coefficient matrices. In this approach, the essential boundary conditions are explicitly implemented at the boundary points, whereas the natural boundary conditions are satisfied by making the rows of the weight coefficient matrix corresponding to the boundary points be zero. This approach guarantees an accurate estimate as boundary conditions are exactly satisfied at the boundary. However, it was reported by Malik and Bert [70] that the method cannot be implemented for non-homogeneous boundary conditions, particularly for clamped and free edge restraints. In this regard, Shu and Du [71] proposed an approach to implement combinations of simply supported and clamped edge conditions where essential boundary conditions are directly implemented at the boundary whereas natural conditions are discretised using DQM. These discretised natural conditions at opposite ends or boundaries, yield the functional values at the points adjacent to the boundary, which are then substituted back into field equations. The major drawback with this approach is its implementation for mixed-derivative boundary conditions in which the entire domain contributes to the approximation at a particular grid point.

Du et al. [72, 73] introduced the idea of separating the points for field equations and boundary conditions so as to ease implementation. The essential and natural boundary conditions are discretised at the boundary points and then replace the field equations at the boundary and adjacent

1 Although referring to the differential quadrature method as 'the DQM' is grammatically correct, it is cumbersome to the ear, so we just adopt 'DQM' from now on.

points. Later, Shu and Du [74] extended this idea of separation of domains into interior points where governing field equations are discretised and boundary and adjacent interior points where essential and natural boundary conditions are enforced, respectively. This approach is highly versatile as arbitrary combinations of edge restraints can be implemented; however, it was shown that the method seems to be sensitive to boundaries having a free corner and can be resolved by further clustering of grid points towards the boundaries.

Other techniques incorporating two degrees of freedom at each end point or at boundary points were also proposed [75–77] and are summarised and discussed in detail [78, 79]. Given the numerous implementations to treat dual boundary conditions, it can be concluded that this complication is inherent to DQM in its original form and the satisfaction of boundary conditions requires different approaches for different problems under consideration.

1.6 Errors Incurred in Numerical Differentiation

Problems in structural mechanics require evaluation of higher-order derivatives of the field variables, which translates into inputs for computing variables of interest, including normal and transverse shear stresses. These stresses are of critical importance in the design methodology of structural components and are vital variables driving the design, manufacturing and optimisation of engineering structures. Thus, it is quite evident that the estimation of these higher-order variables, with sufficient numerical accuracy, is of paramount importance.

As noted [67, 80], the process of numerical differentiation is susceptible to error accumulation and the error deteriorates with an increase in the order of differentiation. In this regard, Breuer and Everson [81] studied the error associated with estimation of the derivative of a function when approximated using Chebyshev polynomials collocated on Gauss–Lobatto points. It was reported that significant errors accrue during the computation of derivatives owing to the finite numerical precision, i.e. round-off errors and these errors increase with a greater number of polynomials used in the approximation. Also, the spatial distribution of this *derivative error* was examined, and it was reported that the distribution is not uniform throughout the domain. The derivative error was reported to be worst in the vicinity of the boundaries, meaning that the derivatives computed using Chebyshev polynomials are least accurate at the end points. Specifically, as noted, the error grew linearly with the number of polynomials within the interior of the domain and quadratically near the boundaries.

One of the remedial procedures adopted to reduce the derivative error is preconditioning of the functions using weights [81]. The weights helped in damping of the errors, particularly at the boundaries, resulting in a more uniform distribution of the errors in the domain and also reduction in the maximum error. Additionally, it has been suggested that the number of differentiation operations should be reduced, and numerical integration must be adopted in the problem formulation as it is less prone to error accumulation. In addition, since the error is also associated with an increase in the number of collocation points, domain decomposition coupled with spectral methods was also suggested as a viable method. Finally, a trade-off was suggested between truncation error, which decreases with greater spatial resolution, and round-off-error, which increases with the number of collocation points.

In the same vein, Shu [67] presented error propagation associated with functional and derivative approximations of a function, while Ojo et al. [80] explained this error propagation with the increase in the order of derivatives employing Chebyshev grid representation. It is worth noting, as indicated in [80], that DQM magnifies the derivative error with the first-order derivative error

varying quadratically with the highest order of the polynomial and successive differentiation operations further deteriorate the error geometrically. Similar observations regarding accumulation of error as a result of numerical differentiation were observed by Mai-Duy and Tran-Cong [82, 83] using radial basis functions networks for functional approximation. It was observed that the norm of error associated with the numerical estimation of the function amplifies with each successive differentiation operation. For example, for the function considered in [82], the difference between the norm of error associated with a functional approximation and its second derivative is of the order $\mathcal{O}(10^4)$. However, it must be emphasised, that the amplification of the error in the derivative does not emanate from the round-off-error, as was the case reported in [81], but from the propagation of an error associated with the functional estimate itself.

1.7 Indirect Approximation Approach

In order to circumvent the compounding of error induced by differentiation operations, Mai-Duy and Tran-Cong [82] proposed an indirect approximation approach known as Indirect Radial Basis Functions Networks. The strategy adopted for indirect approximation is to start the approximation procedure by expressing higher derivatives of a function in terms of some finite basis and then recover the lower-order functions by successive integration operations. In this way, any inherent inaccuracy associated with the process of numerical differentiation would be better controlled by integration operations, leading to improved accuracy of the functional estimate. Also, it is recommended [82] that, for better accuracy, the approximation should start with the highest derivative of the function present in the problem rather than from the lower derivative so as to avoid any numerical differentiation operation.

Drawing motivation from the work of Mai-Duy and Tran-Cong [82, 83], another method was proposed by Wu and Ren [84] using DQM based on the interpolation of the highest derivative (DQIHD). As the name suggests, the highest derivative of the function is approximated using Lagrange polynomials and lower derivatives and the function itself is obtained by integration. Though it was claimed that the DQIHD method is based on DQM, no clear mathematical reasoning was presented by the authors in this regard, except for the use of Lagrange polynomials as basis functions. Furthermore, the description of errors associated with indirect approximation was not discussed, neither in [82, 83] nor in [84]. As such, it is not clear how to gauge the performance of this indirect approach for system approximation. It must also be noted that, owing to the constants of integration, the discretised equations naturally result in an under-determined system and this aspect of the method is left unaddressed. Additionally, it should be noted that contrary to the claim of solving the buckling problem for a thin isotropic plate, all examples in [84] concerned static analysis. In summary, many aspects related to the implementation and performance of indirect approximation have been left unexplained in the literature.

1.8 Conclusion

This chapter explores the historical development of numerical approximation methods that drive the modelling of physical systems. While focusing on methods which mathematically capture the physics of the problem at hand in the form of differential equations, the attributes of weak and strong methods are explained in terms of versatility, accuracy, efficiency and applicability. The application of global methods employing higher-order polynomials is further explored with specific emphasis on collocation methods, drawing a distinction between different approaches based on the

choice of weight functions and residual minimisation techniques. Remarkably, the introduction of the GDQ method mitigates the constraints over the choice of basis functions and distribution of collocation points. As such, ODEs and PDEs can be solved more efficiently. Despite its fidelity, the accuracy of the GDQ approach, like other direct collocation techniques, is often influenced by differentiation-induced numerical errors, especially when approximating higher-order derivatives. This drawback motivated the development of an indirect approximation procedure whereby higher-order derivatives of a function are directly approximated and lower-order derivatives are recovered via integration, potentially leading to the minimisation of differentiation-induced errors. In this regard, the Indirect Radial Basis Functions Networks and Differential Quadrature based on Interpolation of the Highest Derivative are promising approaches that reduce reliance on differentiation and leverage on integration for improved accuracy. However, the practical implementation and error characterisation of indirect approximation methods in general remain inadequately addressed, underscoring the need for further analysis to validate their efficacy and exploit these techniques for diverse engineering applications. In the next chapter, a mathematical framework for the inverse DQM is presented.

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