Chapter 1

Introduction

The Finite Element Method (FEM) is a well-established numerical method which has been applied to boundary value problems in different fields of engineering and the applied sciences. In spite of its numerous advantages and unparalleled success, there is an on-going thrust in the development and application of new numerical tools which hold promise for certain classes of problems, such as crack growth, plate bending, large deformations, higher-order partial differential equations (PDEs), moving phase boundaries, and modeling of multi-scale phenomena. To this end, the emergence of *meshless methods*, a new paradigm for the solution of partial differential equations, has engendered significant interest and is viewed as a step in the right direction.

The term *meshless methods* refers to Galerkin methods in which the *approximant* is constructed solely on the basis of a set of scattered nodes in $\mathbb{R}^d$ ($d = 1, 2, 3$), with no notion of an element structure required to construct the *approximant*. At the outset, we make the pointed distinction between interpolants and approximants—for the former, the function passes through the nodal data, while it is not so in the case of the latter. An element structure is used to construct finite elements which interpolate nodal data. This in essence can be viewed as the key feature that distinguish finite element methods from meshless methods; it is to be noted that in a Galerkin implementation, a background cell structure is used in both classes of methods for the purpose of numerical integration.

Some of the prominent and widely-used methods that fall under the rubric of meshless methods are: Smoothed Particle Hydrodynamics (Lucy, 1977; Gingold and Monaghan, 1977), Diffuse Element Method (DEM) ((Nayroles, Touzot, and Villon, 1992), Element-Free Galerkin (EFG) (Belytschko, Lu, and Gu, 1994), Material Point Method (MPM) (Sulsky, Chen, and Schreyer, 1994), Reproducing Kernel Particle Method (RKPM) (Liu, Jun, and Zhang, 1995), Finite Point Method (Oñate, Idelsohn, Zienkiewicz, Taylor, and Sacco, 1996), Partition of Unity Method (PUM) (Melenk and Babuška, 1996), and H-p Clouds (Duarte and Oden, 1996). Although differing in forms and construction, most of these methods are strikingly similar in many respect which enables one to view them under a common theoretical framework. Apart from the challenges confronting meshless methods in the realm of solid and fluid mechanics today, it is envisaged that meshless methods could shed light on the mathematical structure and composition of existing finite element methods. As with any Galerkin method, the main ingredients that would demonstrate the robustness of these methods lie in the selection of conforming spaces with good approximability and stability, which would lead to convergence for a broad class of problems in computational mechanics.

Smoothed particle hydrodynamics is a particle method that was pioneered by Lucy (1977) and Gingold and Monaghan (1977) in the late 1970s. The applications of SPH have primarily been focused in the area of hydrodynamics and in the simulation of astrophysical phenomena. Of late, there has been some interest in developing modifications of SPH for elliptic PDEs that arise in computational mechanics. Even though SPH is not a Galerkin method, its particle-nature renders it as a truly meshless method, and in that sense, it is indeed a desirable end for all meshless methods.

In comparison to SPH, a parallel, but yet distinctly different path was taken by Nayroles, Touzot, and Villon (1992) who proposed the Diffuse Element Method. In DEM, moving least squares (MLS) approximations (Lancaster and Salkauskas, 1981) are used to construct the approximant. Belytschko, Lu, and Gu (1994) modified DEM and substantiated it with supportive examples from solid mechanics and heat conduction to call their implementation as the Element-Free Galerkin method. EFG has been applied to a wide range of problems in solid mechanics, with particular emphasis in the area of computational fracture mechanics, such as two-dimensional and three-dimensional crack growth modeling (Belytschko et al., 1996). In proposing a reproducing kernel method, Liu, Jun, and Zhang (1995) used the continuous kernel (convolution integral) as their starting point. A discrete approximation of the continuous kernel is developed, and by correcting the discrete kernel so as to satisfy the linear reproducing conditions, a linearly complete approximation is realized. If the same weight function with identical support radius for all nodes is used, the MLS approximant is the same as the corrected discrete kernel approximation used in RKPM (Belytschko et al., 1996). In essence, there is no distinction between EFG and RKPM since the approximants are identical; the differences, if any, stem from algorithmic and implementational issues that are adopted in the two methods. The primary focus of RKPM has been in solving computational fluid mechanics problems governed by the compressible Navier-Stokes equations. We remark that contrary to that suggested by its name and the acronym used, RKPM in its current form is a meshless method and not a particle method.

A significant contribution to the mathematical structure and to the understanding of meshless methods was put forth by Melenk and Babuška (1996) and Duarte and Oden (1996). In proposing the partition of unity method, Melenk and Babuška (1996) recognized that meshless methods based on MLS approximations are specific instances of partitions of unity. The essence of PUM lies in the fact that a conforming space is easily constructing by using any system of local approximation spaces without any loss in the approximation properties. As is well-known, creating conforming finite element spaces (C^k, $k > 0$) is a non-trivial task, and in light of this, PUM provides greater flexibility in the choice of local nodal basis functions that can be tailored to the structure of the partial differential equation under consideration. *H*-*p* clouds (Duarte and Oden, 1996) use moving least squares approximation as a partition of unity to locally enrich approximation spaces. In *H*-*p* clouds, local approximation spaces are constructed by multiplying a partition of unity by polynomials or other classes of functions, such as $\sqrt{r}$ for crack problems to cite an example. The ease of *p*-adaptivity in *H*-*p* clouds is particularly attractive and is a very promising element of the method. In the Finite Point Method, Oñate et al. (1996) used a weighted least-squares approximation scheme in conjunction with point collocation to solve fluid mechanics problems. In an attempt to obviate issues involving numerical dissipation of Eulerian methods and mesh distortion of purely Lagrangian methods, Sulsky, Chen, and Schreyer (1994) used a Lagrangian mesh that follow particles and an Eulerian mesh defined over the computational domain in the implementation of the Material Point Method. The interested reader can refer to the review article by Belytschko et al. (1996) and the references therein for further details on meshless methods.

In this thesis, we assess the potential and capabilities of a recently developed numerical method—coined as Natural Neighbor Finite Elements (Traversoni, 1994) or Natural Element Method (Braun and Sambridge, 1995). A detailed description of its implementation for PDEs is given by Braun and Sambridge (1995), who refer to the method as Natural Element Method (NEM), which is the name we choose to use here. The application of NEM to the solution of elliptic boundary value problems in solid mechanics is explored.

The interpolation scheme used in NEM is known as natural neighbor (n-n) interpolation. Natural neighbor interpolation (Sibson, 1980; Sibson, 1981) is a multivariate data interpolation scheme (Alfeld, 1989), which has primarily been used in data interpolation and modeling of geophysical phenomena. For some of the previous works and typical applications of natural neighbor interpolation, see Watson and Philip (1987), Watson (1988), Gold (1989), Farin (1990b), Owens (1992), Watson (1992), Traversoni (1993), Piper (1993), Watson (1994), Traversoni (1994), Brown (1994), Jones, Owens, and Perry (1995), Robinson (1995), Braun, Sambridge, and McQueen (1995), Braun and Sambridge (1995) and Perez and Traversoni (1996). Natural neighbor interpolation relies on concepts such as Voronoi diagrams (Voronoi, 1908) and Delaunay tessellations (Delaunay, 1934) in computational geometry (Shamos, 1978; Preparata and Shamos, 1985; O'Rourke, 1994), to construct the interpolant. In spite of its fairly simple and appealing structure, sound theoretical basis for construction, and desirable smoothness properties, n-n interpolation has received little attention in the area of multivariate data interpolation, when compared to other schemes such as Shepard's interpolant (Shepard, 1968), moving least squares approximants (Lancaster and Salkauskas, 1981), radial basis functions (Rippa, 1984; Powell, 1987), or Hardy's multiquadrics (Hardy, 1971). Recent work on n-n interpolation (Braun, Sambridge, and McQueen, 1995) and its application to the modeling of complex fluid-structure interaction phenomena (Braun and Sambridge, 1995) does indicate the merits of the method for the solution of PDEs and suggests that it could be a promising numerical tool in the realm of computational mechanics.

We assume the discrete model of a body $\Omega \subset \mathbb{R}^2$ consists of a set of distinct nodes N, and a polygonal description of the boundary $\partial\Omega$. In the natural element method, the trial and test functions are constructed using natural neighbor interpolants. These interpolants are based on the Voronoi tessellation of the nodal set N. The Voronoi tessellation is a unique geometric structure that partitions the domain into disjoint nodal regions on the basis of shortest Euclidean distances. The interpolants are smooth everywhere, except at the nodes where they are C^0. The NEM interpolant is strictly linear between adjacent nodes on the boundary of the convex hull, which facilitates imposition of essential boundary conditions. In the application of NEM to elliptic PDEs that arise in solid mechanics, a displacement-based Galerkin implementation is used. The trial and test functions in the weak (variational) form are constructed using natural neighbor interpolants. The solution of the discrete system of linear equations $\mathbf{Kd} = \mathbf{f}$ is carried out to obtain the nodal vector $\mathbf{d}$.

Parts of this thesis have been submitted for publication. A significant portion of Chapters 2 and 3 is to appear in Sukumar, Moran, and Belytschko (1998); parts of Chapter 4 are in Sukumar and Moran (1998); and Sukumar (1998) which is based on Chapter 5, is currently in preparation. The outline of this thesis follows.

In Chapter 2, some of the essential elements of a Galerkin method and its approximability, stability, and convergence for elliptic boundary value problems are presented. Prerequisites from functional analysis are first presented, and then in the interest of a general framework, the abstract variational problem is considered. The Galerkin solution for linear elliptic PDEs is described.

In Chapter 3, a brief description of Voronoi diagrams and Delaunay triangles is first given. Then, an extensive discussion on natural neighbor interpolants that are used in the natural element method is presented. A detailed description of the construction, properties, and computational procedure to evaluate natural neighbor shape functions is outlined.

Chapter 4 focuses on the application of the natural element method in two-dimensional linear elasticity. First, the treatment of material discontinuities is addressed, and then the modeling of non-convex bodies (straight cracks) using NEM is described. Various applications of NEM in two-dimensional solid mechanics, which include problems with homogeneous deformation (patch tests), steep gradients, strain discontinuity (bimaterial interface), as well as those with singularities (crack-tip fields) are presented. The results for the field variables as well as convergence studies are compared to exact (analytical) solutions and to FEM solutions, wherever appropriate.

In Chapter 5, the construction of Farin's (1990) C^1 natural neighbor interpolant is presented, and a computational methodology for its application to PDEs is proposed. The application of the C^1 natural neighbor interpolant to the biharmonic equation with Dirichlet boundary conditions is presented. An eigenanalysis is carried out to ascertain the properties of the discrete approximation spaces and the stability of the C^1 numerical method.

In Chapter 6, we present a displacement-pressure mixed formulation for NEM in linear elasticity. The governing equations (strong form) with validity for both, the compressible and incompressible case are stated. The variational statement for the mixed formulation and the resulting discrete system of equations are derived. Applications of the mixed natural element method to problems in compressible and near incompressible elasticity are presented.

In Chapter 7, a summary of some of the main results obtained in this work are presented, with some concluding remarks on the potential and promise of the natural element method in computational mechanics.