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Introduction to Meshfree and Particle Methods

Meshfree methods have several origins: on one genealogical tree are the particle methods originated by Lucy [1] and Gingold and Monaghan [2], then refined and extended by Monaghan and his coworkers [3, 4]. On the other are the generalized finite difference methods, originated by Jensen [5] and refined by Perrone, Kao, Liszka, and Orkisz [6, 7]. One of the most important papers in the emergence of these methods was the work of Nayroles, Touzot, and Villon [8]. They called the method the diffuse element method. As we shall see, there are many similarities between these methods, though the initial viewpoints appear to be decidedly different.

Remarkably, a watershed in the development of these methods occurred when they were named "meshfree" (or meshless) methods, which shows that an attractive name goes a long way. The advantage of the name meshfree is that it highlights the most compelling attribute of these methods: the absence of a mesh of elements interconnected by nodes. The generation of finite element meshes for three-dimensional problems of bodies with a variety of features is still very challenging, especially when the model must be remeshed as the solution evolves, as in solidification and dynamic fracture problems. Adaptive refinement using finite elements is also cumbersome due to compatibility requirements along element boundaries.

Both names have persisted: Larry Libersky pointed out at an early specialty meeting on these methods that the name meshfree is more marketable than meshless: we don't call foods "fatless" or soft drinks "sugarless"; they are called "fat-free" and "sugar-free"! Thus, meshfree is a more attractive name for these methods.

1.1 Definition of Meshfree Method

For the purposes of this book, we define a meshfree method as any method that constructs the approximation in terms of nodal values, where the connectivity of the nodes need not be specified explicitly, and the arrangement of the nodes is arbitrary. In fact, information like connectivity is usually extracted in meshfree methods on the fly. Thus, the major distinction from finite element methods (FEMs) is that elements are not used to construct the approximation functions. For traditional finite difference methods, the arrangement of nodes is also not arbitrary. Nodes are arranged in a highly structured manner so that their indices can identify adjacent nodes required in constructing the equations. The difference between these two approaches is crystallized in Figure 1.1 by observing how a finite element discretization contrasts with a meshfree discretization: the approximation is generally associated only with nodes in the latter. The meshfree approximation function associated with node I is denoted by Ψ_I, and the subdomain over which it is nonzero, the

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Ted Belytschko, J. S. Chen, and Michael Hillman.

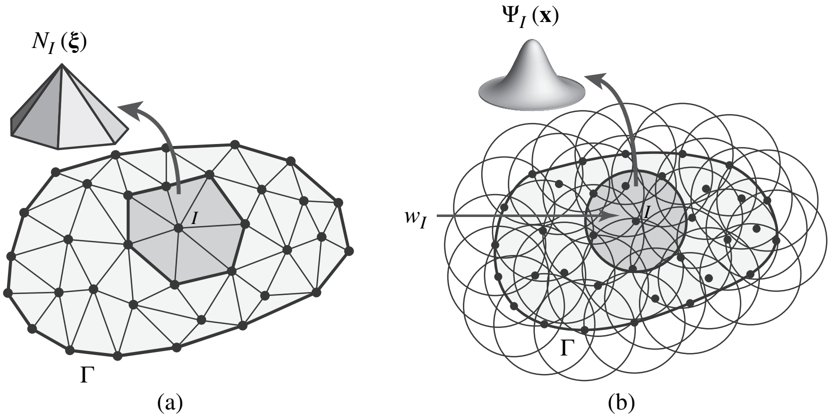


Figure 1.1 (a) Patching of finite element shape functions from local element domains and (b) meshfree approximation functions constructed directly at the nodes in the global coordinate, employing circular supports. The boundary of the domain is denoted as Γ. *Source:* Adapted from Chen and Belytschko [9], figure 1, p. 887. Reproduced with permission of Springer Nature.

support of Ψ_I, is denoted by w_I. It can be seen that the support naturally defines connectivity rather than fixed connectivity dictated by a grid or a mesh of elements. Thus, any field variable in differential equations can be approximated using a point cloud without any particular structure.

1.2 Key Approximation Characteristics

Meshfree methods possess several key characteristics that make them a highly unique class of numerical methods for solving differential equations. First, by the definition we have laid out, the approximation is formed without the need for a mesh or grid, and the connectivity is instead defined naturally. Meshfree approximations can also be constructed with arbitrary smoothness, and they can be much smoother or rougher than the finite element shape functions. In fact, the order of continuity and completeness can be made independent from one another in most meshfree methods, as opposed to finite element or isogeometric analysis, where increasing continuity requires increasing the polynomial order (completeness).

With smoother approximations, quantities involving derivatives such as strains in continuum mechanics and fluxes in heat transfer are also much smoother. This attribute increases the accuracy of the solution when the approximated function is smooth. Since solutions of diffusion equations and elasticity are usually very smooth when the material coefficients are continuous, this advantage applies to many useful classes of problems. Several of these properties, and other special properties are detailed in Chapter 3 "Meshfree Approximations."

Utilizing the smoothness of the approximation, it is also possible to solve the strong form of a problem directly without resorting to the weak formulation. Second-order derivatives are often required; these are simple to compute based on the smoothness of the meshfree shape functions and can also be approximated very efficiently. Chapter 9 "Strong Form Collocation Meshfree Methods" describes these approaches. This advantage of smoothness also applies to the weak formulation of thin beams, plates, and shells, where the global continuity required is easily achieved without the substantial effort required in FEM.

The ease of adaptive refinement is another attractive feature of meshfree methods. In finite elements, approximation functions are constructed in a local parent domain, and thus, compatibility is required along the element boundaries in local adaptive refinement. On the other hand, meshfree methods only rely on nodal locations in the global coordinates to construct the approximation, and enforcing compatibility is avoided in adaptive refinement.

A major distinction between meshfree and finite element approximations is that meshfree shape functions are usually not interpolants. Finite elements are usually interpolatory, and in fact, they are Lagrange interpolants for most of the commonly used elements. On the other hand, meshfree approximation functions are usually not, and we will instead call them simply approximation functions or shape functions. They are sometimes called interpolation functions, but this terminology ignores the fundamental definition of interpolants. This property of meshfree approximations makes the direct application of boundary conditions on the primary variable, often called essential boundary conditions or Dirichlet boundary conditions, more difficult. Chapter 2 “Preliminaries: Strong and Weak Forms of Diffusion, Elasticity and Solid Continua” lays out constrained variational principles to weakly enforce Dirichlet conditions such as the Lagrange multiplier method, the penalty method, and Nitsche’s method. Special techniques can also be introduced to construct meshfree shape functions so that the traditional strong approach can be employed, which are described in Chapter 5 “Construction of Kinematically Admissible Shape Functions.”

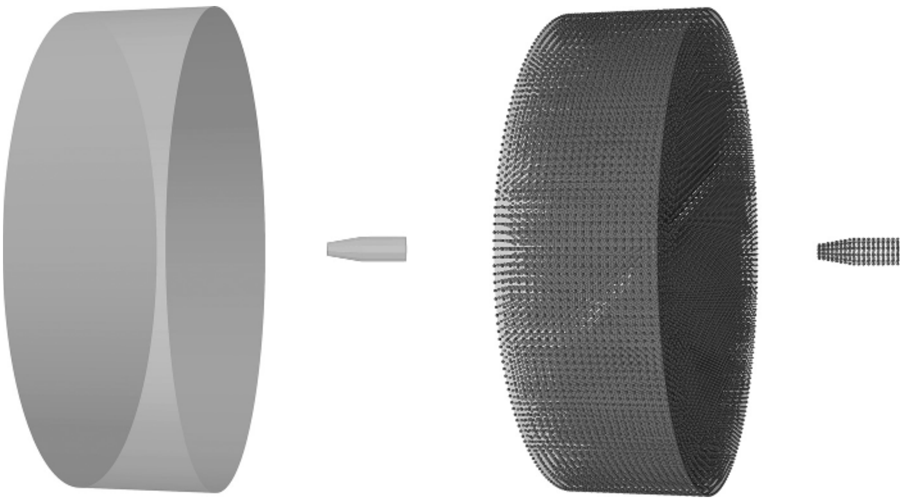
Another fundamental difference between meshfree and finite element methods is the relationship between the support of the shape functions and the subdomains over which quadrature is carried out. The element and quadrature domains are the same in finite elements, which unifies the approximation of field variables and numerical integration. This is clearly not the case for meshfree methods as the supports are defined simply by the nodes themselves, as seen in Figure 1.1b. At the same time, this offers some unique possibilities for meshfree quadrature, yet implementing a practical approach is nontrivial. Numerical integration for meshfree methods is discussed in Chapter 6, “Quadrature in Meshfree Methods.”

The absence of a mesh circumvents element distortion and entanglement issues, making meshfree methods quite suitable for arbitrarily large deformations and distortions in Lagrangian continuum mechanics. Chapter 7 “Nonlinear Meshfree Methods” summarizes their implementation in this class of problems, leveraging several of the special properties of meshfree approximations.

1.3 Meshfree Computational Model

A meshfree computational model consists of a set of nodes and a description of the model’s surfaces. We will call the set of nodes and the boundary description the *grid*, so as to avoid the word “mesh” in a “meshfree method.” It can be seen in Figure 1.1b that the arrangement of the nodes can be quite arbitrary, although uniform nodal distributions are often used when domain geometry is regular. The boundaries can be described by a variety of methods, for example, level set functions and CAD methods. It is noteworthy that in contrast to FEM, the geometric description of the body must usually be given, rather than the geometry defined directly by the mesh topology.

The generation of a meshfree grid for computational analysis is shown in Figure 1.2. Starting with a geometric definition of the model, points are generated inside the volumes while the surface definitions are retained. Nodes can be generated to fill the volume in a variety of ways. A simple way is to simply use a triangulation of the associated domain, retaining only the vertices. In fact, any finite element meshing technology can be employed, with only the nodes retained from the mesh



(a) (b)

Figure 1.2 Constructing a meshfree computational grid for a bullet penetration analysis: (a) CAD geometry and (b) the meshfree grid, which fills the CAD volumes with nodes and retains the surfaces for applying boundary conditions.

generation. On the other hand, relying on meshing technology is not necessary or even desirable, as meshfree methods obviate meshing which is a key advantage. A wide variety of sphere and ellipsoidal packing algorithms exist [10], which can be used to avoid meshing altogether. In addition, triangulation algorithms or Voronoi diagrams can be used to obtain nodal volumes, and thus the only requirement for discretization is the generation of nodes.

1.4 A Demonstration of Meshfree Analysis

Figure 1.3 demonstrates several key characteristics of a meshfree solution. A penetration analysis associated with a meshfree grid (see Figure 1.2) is performed for a concrete target. The computation proceeds without the difficulties of element distortion and entanglement. The material break-up and ensuing multi-body contact with free surface formation can be handled by node-based algorithms (see Chapter 7). As the analysis proceeds, a meshfree error detector [11] embedded in the meshfree approximation indicates where additional accuracy is needed, and points are added in these areas on-the-fly with multiple levels of adaptive refinement. The refinement is performed simply by inserting additional points without issues such as "hanging nodes" as in FEM. Thus, the framework of meshfree analysis provides a flexible tool for challenging scientific and engineering problems.

1.5 Classes of Meshfree Methods

Meshfree methods have been developed under two general branches of formulations which are covered in this book:

1) **The Galerkin meshfree methods based on the weak form of partial differential equations (PDEs).** While no mesh is needed in the construction of the approximation, domain integration

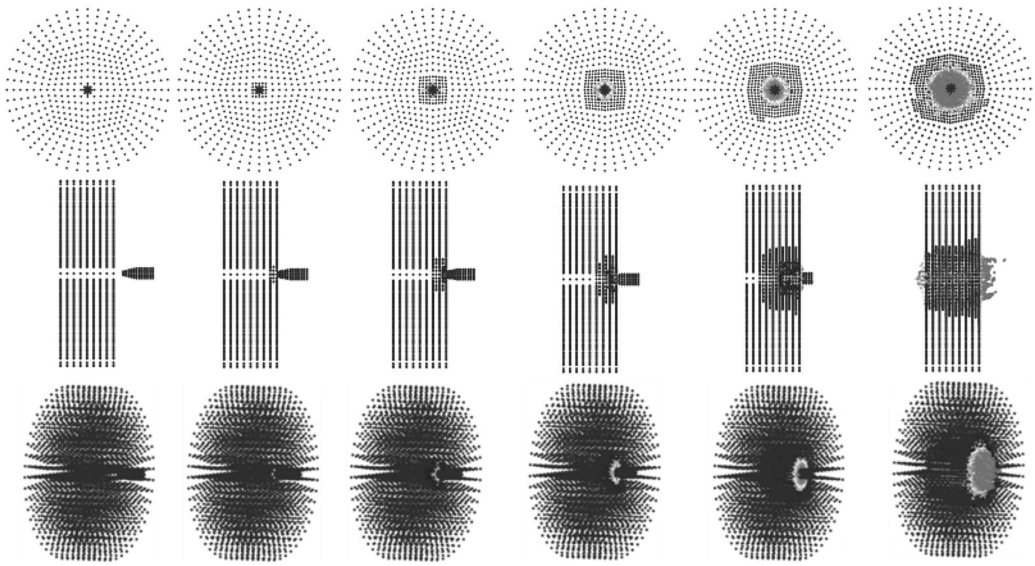


Figure 1.3 Meshfree simulation of a bullet penetration event with adaptive model refinement. Top to bottom: back view, side view, and a front perspective; left to right: as the simulation proceeds.

is required, and special techniques to enforce essential boundary conditions are needed. Domain integration and enforcement of boundary conditions are discussed in Chapters 4–6; and

2) **The collocation meshfree methods based on the strong form of PDEs.** Because of the ease in constructing smooth meshfree approximations, PDEs can be solved using the strong form directly at collocation points without special domain integration and essential boundary condition procedures, as will be presented in Chapter 9.

Table 1.1 shows the wide variety of the meshfree methods that have been proposed; Table 1.2 lists the common acronyms for these methods. Essentially, one may classify these methods based on the approximation and how it is employed to solve the governing equations at hand. As can be seen, meshfree methods have generally been developed using the classical weak formulation.

In this book, we do not go into too much detail on the meshfree implementation of Peridynamics [27] or optimal transportation meshfree methods [48], which are based on governing equations other than the classical differential ones. We also do not include the Lagrangian–Eulerian type methods of particle in cell [56, 57] and material point methods [12, 13], which employ Lagrangian points with an Eulerian computational mesh. Instead, we refer the interested reader to the review by Li and Liu [58] for a broad overview that includes meshfree methods that do not strictly fall under the categories of Galerkin or collocation.

We will focus primarily on meshfree methods of the Galerkin type that employ shape functions with compact support, which are covered in Chapters 3–8. Some collocation methods and approximation functions with both global and compact supports will be discussed in Chapter 9. A compact support is essential if the governing equations are to be sparse; large systems of equations that are not sparse are extremely expensive. This observation also applies to solutions by explicit time integration. When the supports are not compact, the acceleration at any node depends on the nodal values of all nodes of the model. This makes the computation of the acceleration very expensive.

Table 1.1 Various Galerkin and collocation-based meshfree methods.

			Solution scheme (Discretization)	
			Weak form	**Strong form**
Approximation	Local Polynomial	Eulerian mesh with Lagrangian points	MPM [12, 13], PFEM-2 [14, 15]	
		Reconstructed	PFEM [16, 17]	
		Discontinuous/meshless	FPM [18]	
	Moving least squares and reproducing kernel	Direct derivatives	EFG [19], RKPM [20, 21]	FP [22], RKCM [23, 24]
		Diffuse/implicit derivatives	DEM [8]	GRKCM [25, 26], GFD [5, 7]
		Non-local derivatives		PD [27], ULPH [28], RKPD [29]
		Smoothed derivatives	SCNI [30], RKGS [31]	GSCM [32]
		Enriched	XEFG [33, 34]	
		Petrov–Galerkin	MLPG [35], VCI [36]	
		Eulerian mesh with Lagrangian points	Improved MPM [37]	
		Reconstructed meshfree	SLRKPM [38, 39]	
	Partition of unity	Polynomial enrichment	*hp*C [40, 41], MFS [42]	
		General enrichment	PUM [43, 44], PPU [45]	
	MaxEnt	Lagrangian	MaxEnt [46, 47]	
		Reconstructed	OTM [48]	
	Natural neighbor	Lagrangian	NEM [49, 50]	
		Reconstructed	MFEM [51]	
	Radial basis functions		RPIM [52]	RBCM [53, 54]
	Kernel approximation		SPH [1, 2]	MPS [55]

Table 1.2 Common acronyms of meshfree methods.

DEM	Diffuse element method
EFG	Element-free Galerkin
FPM	Fragile points method
FP	Finite point
GFD	Generalized finite difference
GRKCM	Gradient reproducing kernel collocation method
GSCM	Gradient smoothing collocation method
*hp*C	*h-p* clouds
MaxEnt	Maximum entropy
MFEM	Meshless finite element method
MFS	Method of finite spheres
MLPG	Meshless local Petrov–Galerkin
MPM	Material point method
MPS	Moving particle semi-implicit
NEM	Natural element method
OTM	Optimal transportation meshfree
PD	Peridynamics
PFEM	Particle finite element method
PFEM-2	Particle finite element method, second generation
PPU	Particle partition of unity
PU	Partition of unity
RBCM	Radial basis collocation method
RKCM	Reproducing kernel collocation method
RKGS	Reproducing kernel gradient smoothing
RKPD	Reproducing kernel peridynamics
RKPM	Reproducing kernel particle method
RPIM	Radial point interpolation method
SCNI	Stabilized conforming nodal integration
SLRKPM	Semi-Lagrangian reproducing kernel particle method
ULPH	Updated Lagrangian particle hydrodynamics
VCI	Variationally consistent integration
XEFG	Extended element-free Galerkin

The situation is akin to molecular dynamics. Potentials that depend on all atoms in a system are very slow, whereas potentials that only involve the nearest neighbors are very fast.

1.6 Applications of Meshfree Methods

Meshfree methods are particularly well-suited for large deformation applications where FEM fails due to mesh entanglement and other mesh-related issues. They have been applied to many different solid mechanics problems such as large deformation of hyperelastic materials [59, 60], metal forming [61, 62], geotechnical analysis [63, 64], earthmoving [38], explosive and magnetic welding [65], and additive manufacturing [66]. Figure 1.4 demonstrates a meshfree simulation of a landslide due to the 1989 Loma Prieta earthquake with substantial fluid-like motion of material undergoing plastic flow. Figure 1.5 shows a simulation of the explosive welding process (which is featured on the cover of this book), with a comparison of the experimentally observed steady-state interfacial wave.

Fracture mechanics is another area where meshfree methods offer a unique strength. Early on, it was recognized that meshfree formulations such as the element-free Galerkin method could offer an effective alternative to finite elements in modeling fracture by cutting the particle influence across a crack and further provide easy adaptive refinement to attain accuracy near crack tips [68, 69]. The cracking particle method [70] offers one such unique implementation. Alternatively, enrichment of the approximation functions for crack tip singularities can be embedded in the approximation [71, 72], or added extrinsically [71, 73] as in the extended finite element method. Figure 1.6 shows different fracture mechanisms developed in the meshfree simulation of a concrete unit-cell specimen subjected to tension and shear.

The naturally conforming properties of meshfree approximations allow adaptivity to be performed in a much more effective manner than conventional FEM. Nodes can be inserted or removed with ease, and error indicators have been formulated to guide adaptive refinement. For example, the multiresolution reproducing kernel particle method [75, 76] enables the scale decomposition of the numerical solution by using the meshfree approximation as a filter. The high-scale solution has also been used as the error indicator for adaptive h-refinement [11].

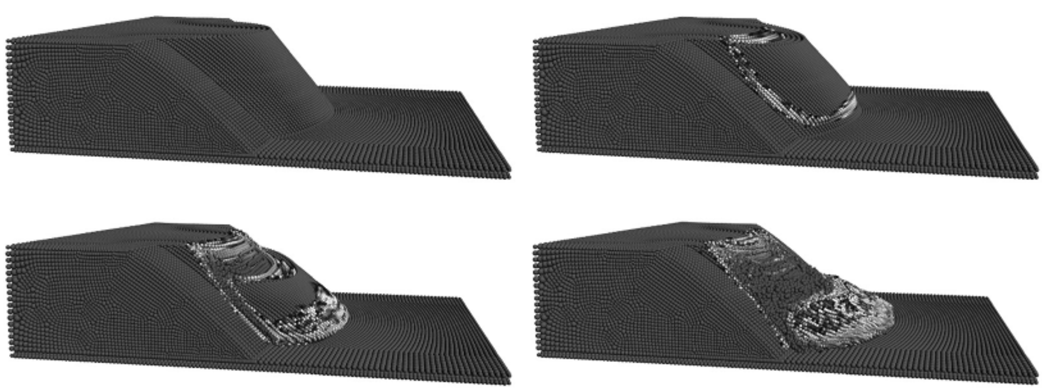


Figure 1.4 Simulation of a landslide triggered by the 1989 Loma Prieta earthquake using meshfree methods. *Source:* Chen et al. [67], figure 26, p. 29 / With permission of ASCE.

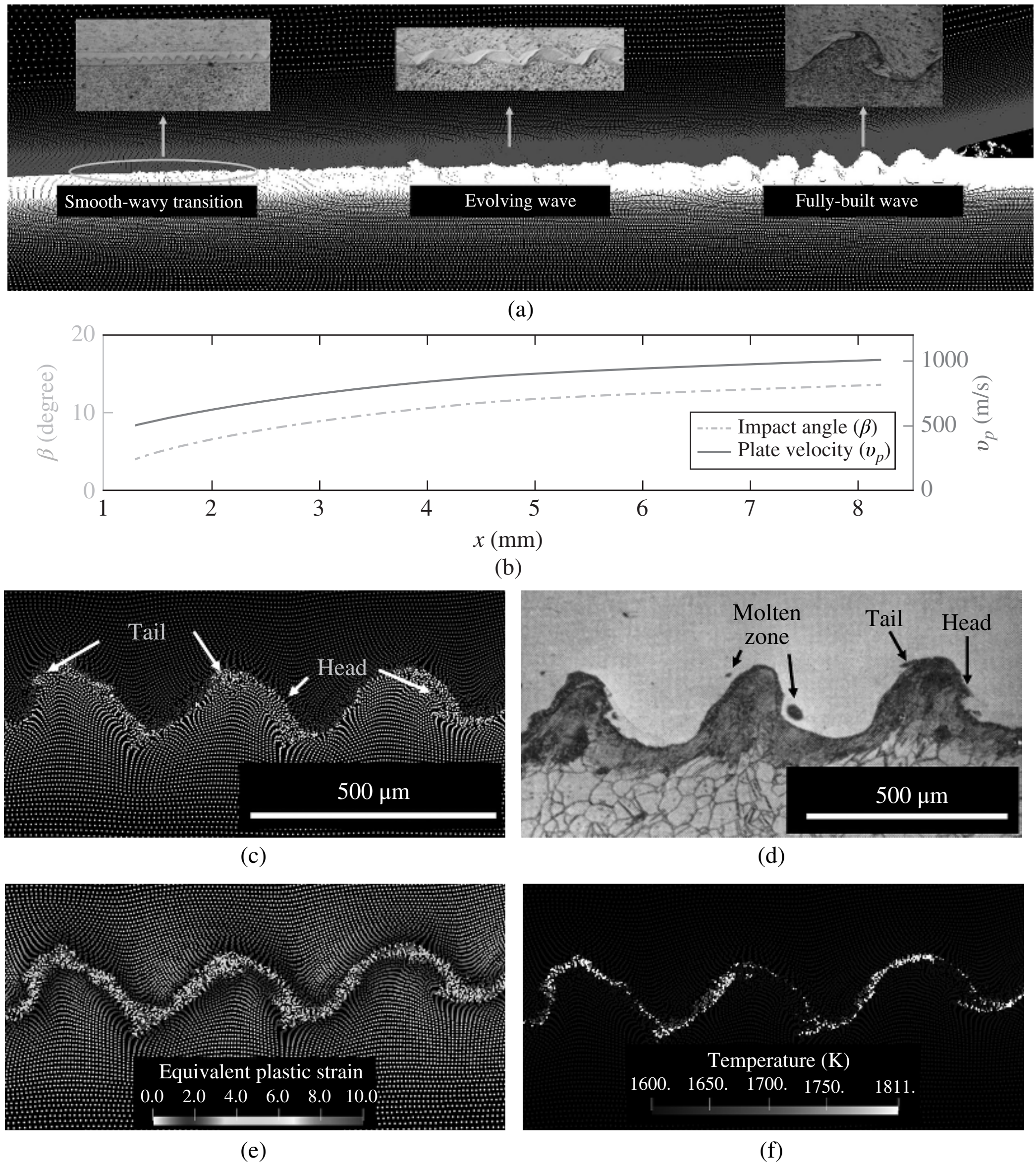


Figure 1.5 Explosive welding: (a) gradually-built interfacial wave compared to the pattern observed in experimental work, (b) the gradually increasing impact angle and vertical plate velocity, (c) numerical wave at steady state, (d) experimental wave at steady state, (e) equivalent plastic strain distribution, and (f) temperature distribution. *Source:* Baek et al. [65], Springer Nature, CC BY 4.0.

While p-adaptivity is not so straightforward, h-p clouds allow the bases to vary throughout the domain such that higher order accuracy can be obtained where needed [40].

Researchers have employed the flexibility of meshfree methods for regularization in localization problems [77–79] to circumvent ambiguous boundary conditions in gradient methods. Methods have also been developed and applied successfully to localization problems difficult for FEM [80, 81].

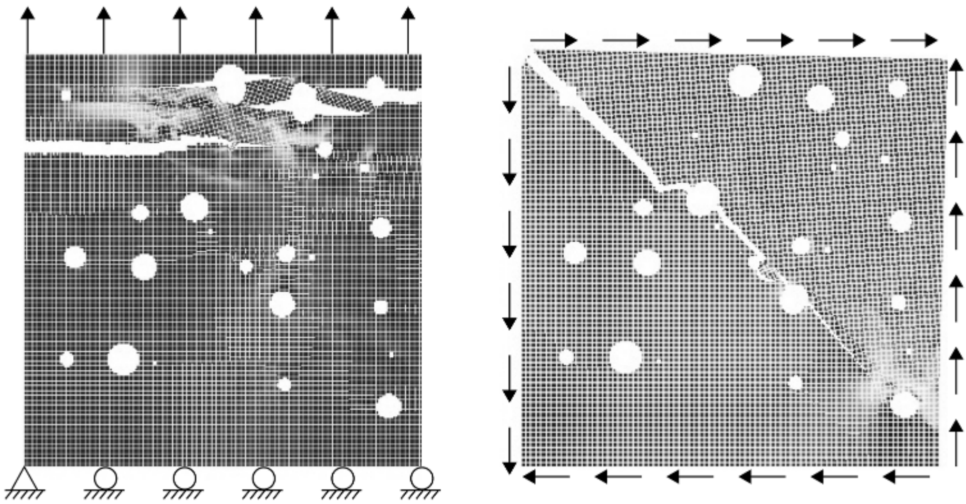


Figure 1.6 Fractures developed in a concrete unit-cell specimen subjected to tension and shear. *Source:* Adapted from Liang et al. [74], figure 11, p 10, and figure 12, p. 10 / With permission of Springer Nature.

By employing the arbitrary smoothness in meshfree approximation functions, a smooth contact algorithm has been proposed that allows continuum-based contact formulations with the full tangent [62]. This, in turn, allows optimal convergence in contact iterations in contrast to finite element-based contact with low continuity and enables robust analysis in applications such as deep drawing of sheet metal with large sliding contact, as shown in Figure 1.7, where C^0 contact fails to converge.

In modeling biomaterials, meshfree methods are well suited for image-based modeling by using pixels as discretization nodes without the tedious procedures in three-dimensional geometry reconstruction from the images with mesh generation [83]. Meshfree methods can also represent the

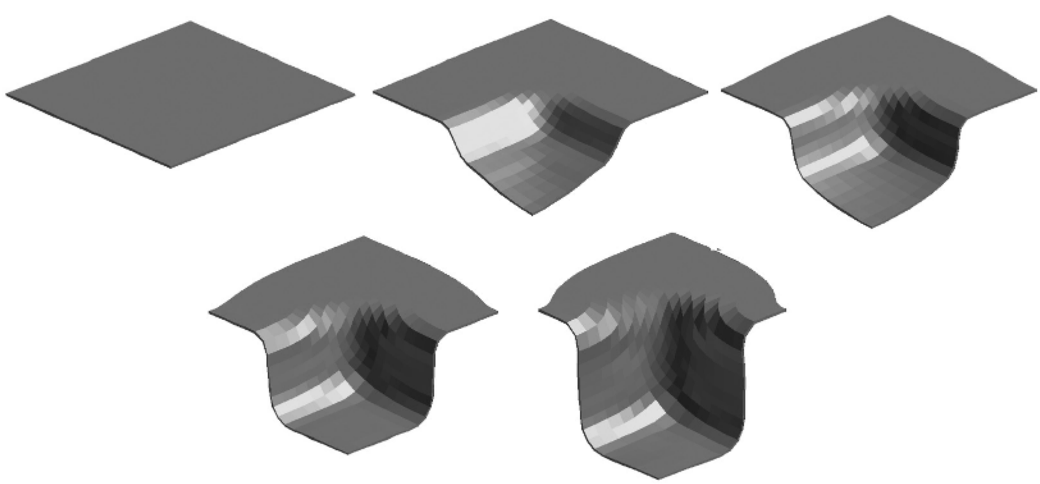


Figure 1.7 Progressive deformation in deep drawing of metal. *Source:* Adapted from Chen et al. [82], Figure 23, p. 38.

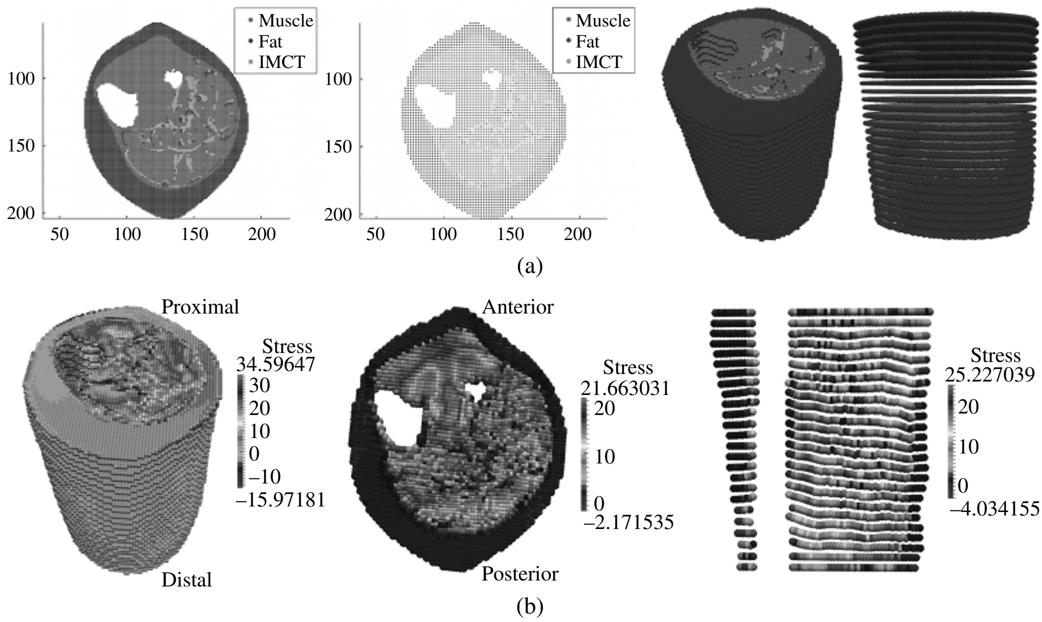


Figure 1.8 Image-based meshfree modeling of a skeletal muscle (a) pixel points as the meshfree discrete points (with muscle, fat, and intramuscular connective tissue (IMCT); fine and course models), perspective views, and (b) maximum principal Cauchy stress (N/cm^2) distribution at pixel points. *Source:* Chen et al. [83], figures 9 and 13, p. 9 and 12 / With permission of Taylor & Francis (https://www.tandfonline.com/).

smooth transition of material properties across material interfaces in biomaterials. Figure 1.8 shows how a skeletal muscle is modeled by meshfree methods. Image pixel points can be used directly as the discretization. The associated stress distribution is computed using material properties and fiber orientations defined at the pixel points.

Another good application of meshfree methods is for problems that involve higher-order differentiation in the PDE, such as thin plate and shell problems [84–86], where meshfree approximation functions with higher-order continuity can be employed with virtually no additional effort. For shape optimization, meshfree methods can avoid mesh distortion in the iterative process [87, 88]. Finally, the smooth meshfree approximation functions are well-suited for optimal employment of Petrov–Galerkin stabilization techniques in convection-dominated problems [89].

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