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Technical Paper

Numerical modelling of large deformation problems in geotechnical engineering: A state-of-the-art review

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Abstract

Many problems in geotechnical engineering involve large movements or rotations, examples include natural processes such as landslides, and man-made processes such as earthmoving and pile penetration. While the use of numerical modelling, primarily the finite element method (FEM), is now routine in geotechnical design and analysis, the limitations of conventional FEMs soon become apparent when attempting to model large deformation problems. For this reason, the search for alternatives remains a key goal of many geotechnical researchers, both to find accurate methods but also to develop efficient ones. In this review paper, prompted by Technical Committee 103 of the International Society for Soil Mechanics and Geotechnical Engineering (ISSMGE), we survey the current state-of-the-art in numerical modelling techniques aimed at large deformation problems in geotechnics. The review covers continuum and discontinuum methods and provides a clear picture of what is and is not currently possible, which will be of use to both practitioners seeking suitable methods and researchers developing existing or new methods.

Keywords: Large deformation; Numerical modelling; DEM; FEM; Meshless; MPM; SPH; PFEM; DDA

1. Introduction

Geotechnics provides many instances of problems where we can expect large deformations. Examples occur in dealing with very soft geomaterials, such as footings on soft ground, while others involve large structural movement, e.g. piled foundation installation. Further examples are liquefaction-induced lateral spreading, seepage leading to suffusion, landslides, flow slides and debris flow. In some cases, the large deformations are the input to the problem while in other cases they are expected as an output. In either, geotechnical engineers wish to predict the behaviour of the whole system of soil and structure (if present); however there are difficulties in the numerical modelling of these problems precisely because of the presence of large deformations. This paper is an attempt to set out the current state-of-the-art in modelling large deformation problems in geotechnics for a wide range of methods and applications, as compared to previous surveys which focus on subsets, e.g. Soga et al., 2016; Wang et al., 2015. The intention is to provide a narrative survey rather than mathematical or numerical detail, which would in most cases, repeat material in the references cited. In addition, given the space limitations, we cannot cite all the papers we would like, and to those authors whose works we have omitted to mention, we apologise.

Numerical techniques can be split into *continuum* and *discontinuum* approaches. In the first, we assume that the

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particular nature of geomaterials can be represented as a continuous material, without distinguishing individual particles, and variations in properties are dealt with via constitutive models linking stresses to strains at points in the material. In discontinuum methods, the geomaterial is modelled as a collection of explicit particles which may or may not represent a real particle arrangement, and the whole framework is quite different. The most popular approach used in geotechnics is a continuum method, the standard finite element method (FEM), which is based on an assumption about strains (that they are a linear function of displacement) which becomes invalid or inaccurate once deformation or rotation becomes significant with respect to the problem starting geometry. Fundamentally, all calculations during the analysis are done considering the initial, undeformed geometry and the determination of element stiffness matrices, equivalent loading and stress state is done as if the shape, size and location of the elements has not changed during the loading application. This approach provides acceptable results in many geotechnical applications, such as settlement calculations, retaining wall and deep excavation analysis, in which the produced nodal displacements are a relatively small fraction of the typical problem dimensions, but provides inaccurate results for large deformation problems if it works at all. Continuum methods usually solve a weak form of the equilibrium equations (usually equivalent to a virtual work formulation) either quasi-statically or dynamically. Discontinuum methods, such as the discrete element method (DEM), are quite different in that they assume a discretization of a continuum into explicit particles which then interact with each other dynamically. The equilibrium equations are the same in both cases (i.e. Newton's 2nd & 3rd laws) but the issues and applicability of methods are usually different. In what follows we cover continuum methods followed by discontinuum methods.

2. Finite element methods for large deformation problems

Lagrangian finite element methods for large deformations in solid mechanics have been available for decades and remain popular. They work by changing from the classical small-strain/small-deformation Lagrangian analysis, where calculations are based on Cauchy stresses and assume that the original geometry is unchanged, to the *Total Lagrangian* (TL) and *Updated Lagrangian* (UL) approaches (Bathe, 1996). The theoretical formulations of TL and UL consider the second Piola-Kirchhoff stress tensor and the Green-Lagrange strain tensor (strains are no longer treated as infinitesimal and linear functions of displacement). As a result, in both approaches an extra term (compared to the classic small-strain FEM) is introduced in the global force equilibrium equations, stemming from the non-linear terms of the Green-Lagrange strain tensor and accounting for changes in global stiffness as geometry changes (geometrical non-linearity). The basic difference between the two approaches is that TL uses as its frame of reference for the static and kinematic variables, the initial problem configuration (undeformed geometry) throughout the analysis, while UL uses at any given solution increment the geometry calculated in the immediately previous increment. This means that in UL the locations of the nodes are updated in each analysis increment based on the nodal displacements resulting from the previous increment and the terms of the virtual work equation are calculated using the new (deformed) element geometry. The UL has the advantage over TL that the Cauchy stress tensor instead of the 2nd Piola-Kirchhoff stress tensor appears explicitly in the terms of the linearized equations of incremental nodal equilibrium, despite the fact that the latter tensor is present in the virtual work equation. This renders the implementation of UL more straightforward than TL in geotechnical engineering problems, since UL can more easily accommodate existing constitutive models that have been proposed for soils on the basis of Cauchy stresses. However, at the same time, use of UL necessitates the consideration of an objective (frame indifferent) stress rate, e.g. Jaumann or Truesdell stress rates (Crisfield, 1997), unless the multiplicative decomposition of the deformation gradient is considered instead (Simo & Meschke, 1993).

Both TL and UL have seen application in early research works pertaining to large deformations in geotechnics. For example, Carter et al. (1979) used UL for the analysis of elastoplastic large-strain consolidation, while Kiousis et al. (1986, 1988) studied footing loading and CPT cone penetration in clay using TL by expressing the von Mises yield function in terms of the 2nd Piola-Kirchhoff stress tensor. More recently, Rashidi et al. (2005) employed TL for the analysis of footing settlement. The multiplicative decomposition of the deformation gradient has been used in a number of studies related to geotechnics. For example, Simo & Meschke (1993) simulated the penetration of footings and piles using especially developed constitutive models. Borja et al. (1998) studied the large strain consolidation of soft clays using a version of the Modified Cam-Clay constitutive model adapted to the multiplicative decomposition theory. Jeremic et al. (2001) simulated micro-gravity triaxial tests on sand using a hyper-elastoplastic constitutive model. Yuan & Zhong (2017) used TL employing multiplicative decomposition for the analysis of footing penetration.

The UL approach has long been available in popular commercial FE codes used for solving geotechnical engineering problems, such as Abaqus (ABAQUS, 2011) and Plaxis (Brinkgreve et al., 2010), allowing the users to extend the applicability of Lagrangian analysis at a click of a button. However, the range of large deformations that UL can handle is not unlimited. As a UL analysis progresses and the mesh deforms, the elements distort excessively and their geometrical qualities (regularity and aspect ratio) deteriorate. As a consequence, the accuracy of the computations decreases severely, giving rise to numerical instabilities that often lead to premature termination of the analysis. This is particularly true for problems involving plastic deformations and for finite element models with fine meshes.

Given that the limitations of the UL approach stem from the distortion of the elements, researchers, e.g. Benson (1989), Ghosh & Kikuchi (1991), proposed the substitution of an excessively deformed mesh by another with regularly-shaped elements, a procedure commonly termed *remeshing*, with transfer of the state variables from the old mesh to the new, a procedure termed *remapping* (Fig. 1).

This approach has been called decoupled (operator-split) Arbitrary Lagrangian-Eulerian (ALE) because the computational procedure of the transfer of the material state from one mesh to another is perceived as a convection process similar to that in a classical Eulerian analysis, as for instance in fluid mechanics. Fig. 2 shows a flow chart of the ALE approach.

2.1. Remeshing methods

The mesh substitution can happen at every analysis increment or at regular or irregular intervals (e.g. depending on the analysis outcome). The available remeshing strategies can be divided into two basic categories: i) those that preserve the mesh connectivity and the total number of elements and nodes, relying on simply relocating the nodes in a way that reduces element distortion, and ii) those that rely on generating a completely new mesh each time. The advantage of the first category is that the position of the elements changes only a little between successive remeshing increments, provided that remeshing is performed frequently during the analysis. This way the remapping that follows has no difficulty to interpolate accurately the material states from the old to the new mesh.

There are several methods proposed for the relocation of the inner nodes of the analysis domain (nodes not lying on the boundaries). Among the oldest are smoothing techniques, e.g. equipotential (Winslow, 1963) or volume smoothing (Chang & Kikuchi, 1994). Fig. 3 shows an example of large deformation analysis of pile base penetration in a Tresca material (undrained clay) performed using Abaqus. If no remeshing is employed, i.e. the analysis is

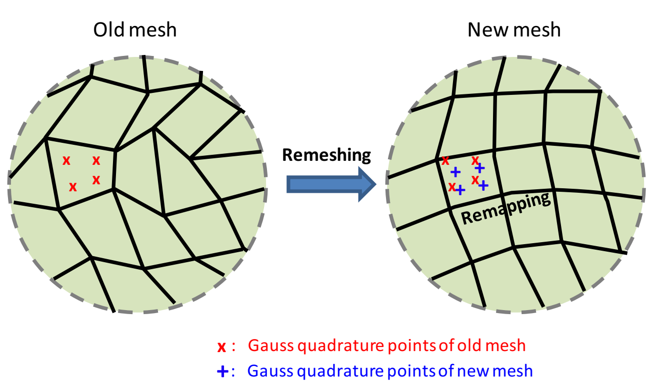

Fig. 1. Schematic of ALE concepts of remeshing and remapping.

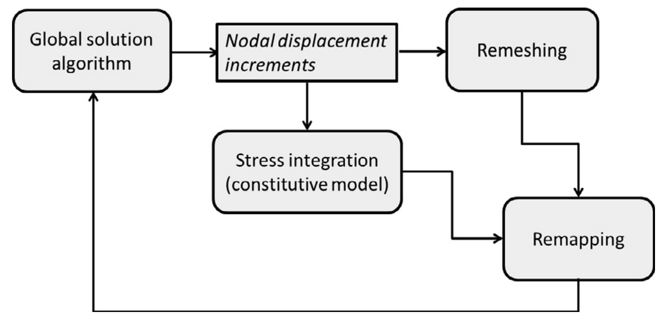

Fig. 2. Flow chart of the Arbitrary Lagrangian-Eulerian approach.

done purely as UL (Fig. 3b), the elements get severely distorted at certain regions of the domain, especially under the base. The ALE analysis (Fig. 3c), performed using the default smoothing scheme available in Abaqus (original configuration projection) manages to retain the quality of the original mesh even at a penetration 2.5 times the pile radius. Interpolation schemes, such as those using radial basis functions (RBF) (Wendland, 1999), can also be used for producing a node motion that will result in more evenly spread nodes inside the analysis domain (De Boer et al., 2007; Vavourakis et al., 2013a). Smoothing and interpolation-type remeshing schemes relocate the nodes based on their current relative position (e.g. densely packed nodes are spread apart) and the element connectivity does not play a role in the outcome. As such, they are relatively simple and easy to implement. However, these schemes do not aim at producing meshes with elements that have the best possible characteristics (aspect ratios close to unity, right angle in quadrilateral elements or 60° angles in triangular elements).

Another node relocation strategy is the spring analogy method (SAM) (Farhat et al., 1998), in which the node relocation is done considering the elastic deformation of a virtual truss generated by substituting the old mesh with linear springs interconnecting the nodes. Rotational springs are also attached to the nodes in order to improve the performance of the method. To produce relocation motion of the nodes, the virtual truss is loaded by prescribed displacements at the boundary that are equal to the incremental displacements of the boundary (outer) nodes produced by the Lagrangian step. The stiffness of the springs is calculated such that the resulting elements are as much regular shaped as possible. The SAM has been shown to perform particularly well in large deformation analysis of geotechnical problems (Vavourakis et al., 2013a). A similar remeshing strategy is the elastic rebound method (ERM) (Nazem et al., 2008; Nazem et al., 2009), in which the old (distorted) mesh is replaced by a new mesh generated by allowing the initial mesh of continuum elements (instead of a virtual truss) to deform purely elastically. The ERM has been applied to dynamic problems (Nazem et al., 2009) and used successfully for simulating the penetration of free-falling penetrometers (Nazem

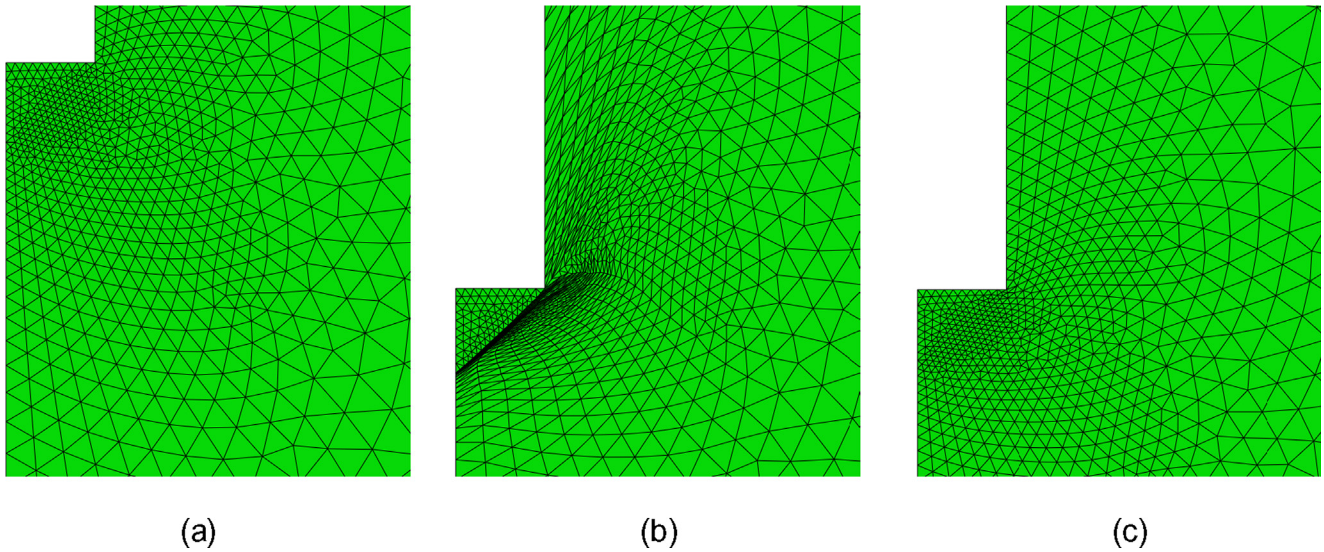

Fig. 3. Mesh quality in an example of pile base penetration: a) initial (undeformed) mesh, b) deformed mesh using UL, c) deformed mesh using ALE.

et al., 2012) and dynamically penetrating anchors (Sabetamal et al., 2016).

When solving geotechnical problems, the success of a remeshing method relies on the scheme used for the relocation of the boundary nodes, especially those at the free surface. This relocation must be done before the relocation (using for example SAM or ERM) of the inner nodes and its purpose is to avoid congestion or overspreading of the boundary nodes, while retaining adequate mesh density close to the loaded region. Boundary node relocation schemes for use in geotechnical problems have been proposed by Nazem et al. (2008) and Vavourakis et al. (2013b), in which the nodes are moved along curvilinear free boundaries approximated by chains of quadratic polynomial functions passing (via interpolation) through the locations the boundary nodes occupy at the end of a given Updated Lagrangian step.

In the late 1990s, Hu & Randolph developed a variation of the ALE approach called RITSS (Remeshing and Interpolation Technique with Small Strain), (Hu and Randolph, 1998a). In this method, the virtual work equation of the Lagrangian step is the same as in a classical small strain analysis. This is not a major shortcoming, as the remeshing is performed frequently (e.g. about every 10 increments), with the increments being already of small size due to the material nonlinearities that characterize geotechnical problems, and as a result the geometrical non-linearity terms are practically negligible. In RITSS, the mesh is composed of triangular elements (first- or second-order) and remeshing involves complete substitution of the old mesh by an new one formed from scratch using Delaunay triangulation. As such, the element connectivity or the total number of elements is not necessarily preserved, allowing easy use of h-type mesh refinement, e.g. the use of smaller elements in regions of shear band development as the analysis progresses (Hu & Randolph, 1998b; Hu et al., 1999) in order to increase the numerical accuracy in ultimate limit state problems or problems involving strain localization. In addition, the use of h-adaptivity automatically addresses the issue of appropriate node spacing at the deformed free boundary. The RITSS method, despite its simplicity, has proven robust and has been used for solving several geotechnical problems, especially in the field of offshore geotechnics: cone penetration in clay, spudcan penetration in sands and clays, pile installation in sand, plate anchor pullout, and pipeline-soil interaction (e.g., Lu et al., 2004; Hossain et al., 2005; Wang et al., 2010; Chatterjee et al., 2012; Yu et al., 2012; Tian et al., 2014; Ma et al., 2014a; Ragni et al., 2016). Zhang et al. (2020) employed an efficient and accurate mesh tracking of the free ground surface that allowed the realistic 3D simulation of the extreme deformation and fold-over of the free surface during reinstallation of spudcan foundation in clay. Closely related to ALE and especially RITSS is the Particle Finite Element Method (PFEM), originally developed in the early 2000s (Oñate et al., 2004) for fluid mechanics problems and more widely employed for geotechnics recently, (e.g. Monforte et al. 2017a; Monforte et al., 2019; Yuan et al., 2019) including coupled problems (e.g. Monforte et al., 2017b).

2.2. Remapping methods

Several interpolation schemes have been proposed for remapping the state variables to a new mesh. State variables are a collection of internal variables that include the stresses and any material-level variables that play a role in the mechanical behaviour (e.g. strain hardening/softening variables, porosity, soil fabric, temperature). During the Lagrangian step, the new material state is obtained at the Gauss points of the elements through the integration of the rate form of the constitutive equations using as input the strain rates calculated from the displacement increments produced by the solution of the global equilibrium equations (Figure 2). This material state needs to be projected through some form of interpolation to the Gauss points of the new mesh produced by the remeshing (Figure 1). This can be achieved using the material state of either just the element of the old mesh that contains the Gauss point of the new mesh (parent element) or a patch of elements in the proximity of the new Gauss point (e.g. the parent element plus all the neighbouring elements with which it shares nodes). Among the methods that have been used in solving geotechnical engineering problems are the Inverse Distance Algorithm (IDA) (Shepard, 1968), the Superconvergent Patch Recovery method (Zienkiewicz & Zhu, 1992), the Unique Element Divisional technique (Hu & Randolph, 1998a) and the Radial Basis Point Interpolation Functions (RBPIF) method (Wang & Liu, 2002). Vavourakis et al. (2013a) found that IDA and RBPIF perform much better when considering just the parent element than using a patch of elements in the analysis of penetration in elastoplastic materials. This is because shear bands have a thickness that usually does not extend beyond the width of one element, especially in the cases of non-associated flow rule or softening, and consideration of patches of elements in the remapping process tends to smear the localized state.

2.3. Coupled Eulerian Lagrangian method or multi-material ALE

More recently, a method very similar to ALE, called the Coupled Eulerian Lagrangian (CEL) method, has gained popularity in geotechnical analysis, especially due to its presence in the commercial codes Abaqus/Explicit and LS-DYNA (Hallquist, 2006). The method is also often referred to as the Multi-Material Arbitrary Lagrangian-Eulerian method (MMALE). The basis of CEL is that there are two domains, one Eulerian and one purely Lagrangian, that interact with each other via a suitable contact formulation. The Eulerian domain usually represents a volume of softer material which is expected to deform intensively due to the actions applied by a stiffer domain modelled using the Updated Lagrangian approach. In the context of geotechnical analysis, the Eulerian domain is reserved for modelling the soil and the Lagrangian domain is a structure (e.g. spudcan, mudmat, pipeline) or a penetrator (e.g. pile, anchor).

The origins of the CEL method can be found in Noh (1963), and later in Benson (1992) who proposed a simpler variation which has been adopted in commercial codes. The geometry of the mesh of the Eulerian domain does not change during the analysis (fixed mesh) and, in order to accommodate the large motions of the soft material boundaries (e.g. the free surface of ground or a seafloor), the size of the Eulerian domain is set by the user to be larger than the initial extent of the soft material. The CEL or MMALE method can account for the distortion of the free and inner boundaries by taking into consideration, through special formulations (Benson, 1992; Benson & Okazawa, 2004), that an “element” of the Eulerian domain can be partially filled with material or filled with two different materials. At regular analysis intervals, the state of a material that has moved with respect to the fixed Eulerian mesh is remapped back to it (“advection”). As such, the simplified CEL method is very similar to a form of the ALE approach in which the new mesh is always the original undeformed mesh. Yet, the key difference from the classical ALE is that the Eulerian mesh is oversized and takes into account partially filled elements or elements filled with two or more materials. More recently, Aubram et al. (2016) proposed an extension of the multi-material method in which the Eulerian mesh is allowed to deform. The CEL has been used to analyse several geotechnical problems, such as pile, CPT or spudcan penetration, pipeline-seabed interaction, submarine landslides and soil cutting by tool (Qiu et al., 2011; Pucker et al., 2013; Hu et al.,2014; Dutta et al., 2015; Dey et al., 2016; Bakroon et al., 2020).

3. Material point methods

The second group of continuum methods to be covered come under the heading of the *Material Point Method* (MPM) which has attracted much interest from the geotechnical community in the past five years with major conferences being devoted to the MPM in geotechnics in 2017 (Delft) and 2019 (Cambridge), a recent textbook (Fern et al., 2019) and even an appearance in the 2017 Rankine Lecture (Alonso, 2021).

In truth, the MPM is closely related to standard finite element methods and, contrary to some authors’ opinions, is not a meshless method (these are discussed briefly below). The basic idea of the MPM is that information on a material (e.g. deformation gradient, stress and strain) is held at points scattered through the problem domain, as is the case for the Gauss points in a FEM. This information is mapped to the nodes of a finite element mesh that overlays the problem domain and then a calculation is carried out. The resulting nodal displacements (and in the case of coupled problems, pore pressures) are then mapped back to the material points and the cycle begins again. Fig. 4 shows the process at an element level in 2D. The key feature that makes the MPM attractive is the fact that the background mesh can be reused in its original undistorted form in each cycle; it is effectively a calculation device, and there is no need for the mesh to respect the problem domain geometry (it just has to contain it). All the deformation is recorded in the material points and therefore one is never working with a distorted mesh, so large deformations can be accommodated.

The MPM for solids was developed from methods aimed at fluids (particle-in-cell methods) with the first key publication on the MPM for solids being by a US mathematician, Deborah Sulsky (Sulsky et al., 1994; Sulsky et al., 1995). Most initial development of the MPM used an explicit approach, with an implicit approach first pub-

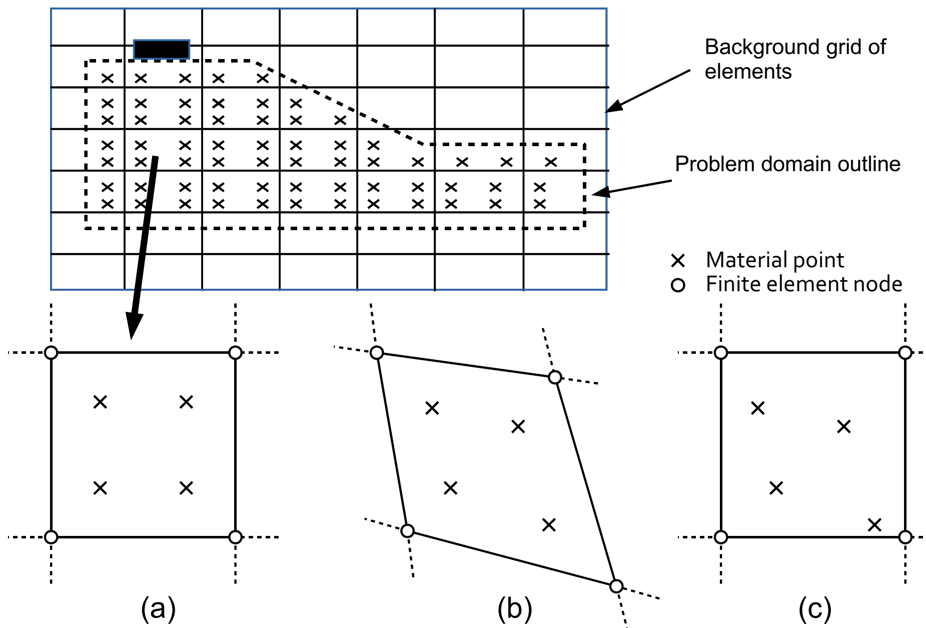

Fig. 4. The MPM in 2D with four-noded quad elements for a slope problem. (a) Prior to calculation; (b) calculated deformations applied to nodes and MPs; (c) mesh reset to original ready for next calculation. Deformation preserved in the MPs.

lished in 2003 (Guilkey & Weiss, 2003). Subsequent developments of the MPM have sought to deal with issues such as *cell crossing* where a material point moves in one analysis step into a new element and in doing so radically transfers a contribution to stiffness from one element to another, causing errors in the stress field predicted. Cell crossing errors have been tackled by moving away from material points representing single points within a continuum to them modelling small regions (Bardenhagen & Kober, 2004; Buzzi et al. 2008), which can also change shape (Sadeghirad et al., 2011; Sadeghirad et al., 2013). Once again, these have been for the explicit MPM but have been followed by similar developments for implicit (Charlton et al., 2017; Wang et al. 2016b).

Other significant problems with the MPM are associated with essential boundary conditions, locking and the mapping from material points to nodes and back. While easier to impose than is the case with some other methods, e.g. SPH, see below, essential boundary conditions can present problems if their location does not coincide with the edges of the calculation mesh and while this condition can be met for some geotechnical problems such as slope stability, it is a major restriction on the modelling of soil-structure interaction, so recent advances have focussed on solutions drawn from immersed boundary methods found elsewhere in computational mechanics (e.g. Cortis et al., 2018; Remmerswaal, 2017). Locking is the phenomenon whereby excessive non-physical stiffness is generated in a numerical model, leading to useless results, and once again recourse has been made to previous solutions for FEMs which have been adapted for the MPM, e.g. (Mast et al., 2012; Coombs et al., 2018). The mapping issue results from mismatches between the numbers of nodes in an element and the, often much larger, number of material points within and various solutions have been tried from the computational mechanics community (Steffen et al. 2008) and more recently geotechnics (Tran & Solowski, 2019). It is clear that there is still much interesting research to be done on the basics of the MPM for solids.

The first publications linking the MPM to geotechnics appear to be those from Vermeer and co-workers (Beuth et al., 2007, Vermeer at al., 2008) with inspiration apparently from the earlier work on granular flow problems such as Wieckowski (2004). Prior to this, however, Konagai and Johansson (2001), presented the Lagrangian Particle Finite Difference Method (LPFDM), which has strong similarities to MPM, but where the background calculations are carried out using finite differences. They demonstrate the use of the LPFDM on its use on Mohr-Coulomb soils. Early geotechnical adopters of the MPM were mostly focussed on slope stability and run-out problems with examples for slope modelling in general (Søren Mikkel and Lars Vabbersgaard, 2009; Andersen & Andersen, 2010), and later works providing surveys and examples in 3D, e.g. Soga et al. (2016) and Wang et al. (2016a) respectively. Coincidentally and since there have been a sizable number of papers on application of the MPM to real slope failures, including the Aznalcóllar Dam in Spain (Zabal & Alonso, 2011), landslides in China (Li et al., 2016; Xu et al., 2018), the USA (Yerro et al., 2019) and Italy (Conte et al., 2019). The impacts of landslides on existing structures have also been of interest, e.g. in Ceccato et al. (2018b) which also compares the MPM to the DEM, and in Dong et al. (2017) for submarine pipelines. Seismic triggering of landslides is modelled using the LPFDM (Konagai & Johansson, 2001) in a surprisingly early paper by Numada et al. (2003) and later with the MPM in Bhandari et al. (2016). Considerable scope exists for more ambitious modelling here, based on earlier non-geotechnical studies of explosions and rapid impacts, e.g. Ma & Zhang (2007) and Ma et al. (2009), and for fluid–structure interaction such as dam-break problems (Zhao et al., 2017b) and others (Hamad et al., 2017). In terms of soil-structure interaction problems, where the input is a large deformation, the MPM has seen most use in pile installation and penetration such as for jacked piles (Tehrani et al., 2016; Phuong et al., 2016; Lorenzo et al., 2018), screw piles (Wang et al., 2017), general penetration and footing problems (e.g. Woo and Salgado, 2018; Sołowski and Sloan, 2015) and anchors (e.g. Coetzee et al., 2005). The MPM has also been used to model ground improvement techniques such as dynamic compaction (Zhang et al., 2019) and soils testing, e.g. cones and piezocones (Ceccato et al., 2016; Francesca et al., 2020). In these types of problems, modelling the contact between soil and structure accurately is vital and there have been a number of contributions leading to improved contact models specifically for geotechnics, (e.g. Ma et al., 2014; Zhang et al., 2009). A key contribution to MPM by geotechnical researchers has been in coupled problems to allow the modelling of the transition from undrained to drained. Naturally, the MPM has been developed starting from the much earlier development of the FEM for coupled problems, e.g. Lewis and Schrefler (1998) where formulations are based on classical poroelasticity and other components such as plasticity or the ability to model two fluid phases for unsaturated problems are added. A key issue is which basic field variables to choose to solve: usually either displacement-pore pressure $(u - p)$ or solid velocity-fluid velocity $(v - w)$ and various MPM approaches have been proposed. Some model with material points carrying information on both the solid matrix and the fluid (e.g. Zhang et al., 2009; Jassim et al., 2013; Ceccato et al., 2016); others have two or three sets of material points which carry separated information (Abe et al., 2014; Bandara & Soga, 2015). Ceccato et al. (2018b) compares these approaches. The constitutive modelling of unsaturated soils is itself a major current research challenge on its own, and a few researchers are already venturing into using the MPM to tackle these difficult problems (e.g. Yerro Colom et al., 2015; Bandara et al., 2016).

In conclusion, the MPM has been of great recent interest to geotechnical modellers and the research area remains a vibrant one, but there remain challenges associated with computational cost and stability. Interestingly, there has been much activity in the computer graphics community in the development of MPM (e.g. Stomakhin et al., 2013) which has yet to cross over to geotechnics and may be a fruitful area in which to work. While no commercial MPM software is currently available for geotechnical modellers, there are a number of open source options for applications, e.g. Anura 3D (Fern et al., 2019), training, e.g. AMPLE (Coombs & Augarde, 2020) and research, e.g. UINTAH.

4. Other continuum methods

We now deal briefly with other continuum methods which have received somewhat less attention than those covered above by geotechnical engineers. Smoothed Particle Hydrodynamics (SPH) is a continuum method based on discretisation by particles alone which was originally developed (and is still in use) for astrophysics problems. SPH particles interact with other particles within a short distance via basis-type functions with local support, a key difference from FE methods being that the strong form of the underlying physical equations is used as opposed to the weak form. SPH has been most successful in modelling fluids problems but less so for solids. Two key difficulties with SPH for solid modelling are the modelling of essential boundary conditions and the so-called tensile instability. Various attempts have been made over the years to address the latter issue, notably Dyka et al. (1997) who showed that this could be partially addressed by calculation of stresses away from particle centroids, Gray et al. (2001) using artificial short-range forces between particle, and more recently Lee et al. (2016), who introduced stabilisation ideas from CFD, and also dealt with imposition of essential boundary conditions. The earliest attempts to model geotechnical problems using SPH date from the mid-2000s, and included modelling soil as a fluid (e.g. Naili et al., 2005) as well as models in which solid constitutive models were used in a coupled formulation (e.g. Blanc & Pastor, 2012). Significant contributions to geotechnical modelling have been led by Bui with co-workers from 2008, e.g. Bui et al.(2008), which presents methods for dealing with the difficulties mentioned above and for modelling simple elasto-plastic soil models and Bui & Nguyen (2017) in which separate particles were used for solid and liquid phases for the first time. Later work has included application to slope stability problems (Bui et al. 2011), large runouts triggered by landslides (Huang et al., 2012; Zhu et al., 2018) and has recently focussed on soil desiccation (e.g. Tran et al., 2019) where SPH has advantages over grid-based methods for modelling crack propagation. SPH is likely to remain of interest to geotechnical modellers as it offers more robust modelling of shear bands than most standard FE methods (Zhao et al., 2017a), and is amenable to parallelisation for very large simulations (Peng et al., 2019). A close relative of SPH is the Moving Particle Semi-Implicit (MPS) Method, originally developed for fluids in Koshizuka & Oka (1996) and more recently employed to model fluidised geomaterials in, for example, flow slides and liquefaction, e.g. Nohara et al. (2018); Zhu & Huang (2016), Zhu et al. (2021).

In the 1990s there was considerable interest in the computational mechanics community in meshless (or meshfree) methods based on weak forms of the equilibrium equations (in contrast to SPH) but again using only nodes. These include the *Element Free Galerkin* Method (Belytschko et al., 1994) and the *Meshless Petrov-Galerkin* method (Atluri and Zhu, 1998). Weak form-based meshless methods really only differ from FEMs in that no elements are used to connect nodes, which are the only discretization of the problem domain. Since a weak form is used to derive the linear system solved for nodal displacements (or pore pressures in coupled problems), integration is necessary. Shape functions are still associated with nodes (as in the FEM), however the domain of influence of a node (i.e. where its shape function is non-zero) is now not defined by the elements to which it is attached, as there are none. Instead meshless methods have to include a means of defining the zone of influence of a node in another way. Despite continuing research interest, some in geotechnics (Heaney et al., 2010; Samimi & Pak, 2012; Kardani et al., 2017), key barriers to wider use of meshless methods in geotechnics have been, that a mesh is still needed for integration for some methods, and the computational cost outweighs standard FEMs for small to medium problems. It seems likely that these methods could be competitive when looking at very large 3D analyses with large deformations, where no remeshing would be needed, thus saving computational cost.

Before moving to discontinuum methods, it is worth noting a major drawback of particle based continuum methods and that is of capture of a free surface. These methods handle this issue by placement of particles or material points along free surfaces and deciding on a suitable interpolation between, e.g. as in the MPM with the use of B-splines in Bing et al. (2019).

5. Discontinuum methods

In contrast to the continuum methods described above, there is a separate set of tools based on modelling a soil continuum as a collection of particles, interacting through their contacts, with other particles and boundaries, the so-called discontinuum approaches. A key difference is that discontinuum methods automatically include large deformations so none of the mathematics set out above is required. Granular material, in general, is characterized by its complex behaviour that is neither completely solid nor fluid due to its particulate nature, and is still poorly understood as there is no universal theory or model to characterize the mechanical behaviour on the wide spectrum of scales (Andrade et al., 2008). The discontinuum-based methods are widely adopted to account for such discrete nature of granular materials in numerical simulation, whereby each particle is explicitly modelled as an individual rigid or deformable element to consider the particle interactions and associated energy dissipations at the particle scale. Therefore, compared to the continuum approaches, the discontinuum-based methods appear to be ideal for modelling the large deformation and post failure problems in geotechnical engineering. However, these methods are computationally demanding since they explicitly model the particle interactions, and key issues that have been dealt with rest on particle size and shape, are discussed in detail below.

5.1. The discrete element methods for computational granular mechanics

The discrete element method (DEM) was proposed by Cundall and Strack (1979) for use in granular mechanics, and is currently the most popular discontinuum-based numerical method (O'Sullivan, 2011). DEM explicitly considers the microscopic particles' interactions via a spring-damper model. The motion is updated based on explicit time integration of the 2nd order differential equations of motion, in which force and acceleration are the primary variables. When DEM was proposed in 1979, it was originally developed for geotechnical applications, but has been widely adopted in a number of cross-disciplinary applications to model discontinuities in material and structural systems, e.g., analysis of masonry structures (Ghaboussi, 1988; DeJong & Vibert, 2012), material fracture (Tavarez & Plesha, 2007), progressive collapse of building structures (Masoero et al., 2010) and human traffic flow for evacuation (Helbing et al., 2000).

Cundall and Strack (1979) originally named the proposed method as the 'distinct' element method, but now it is commonly referred to as the 'discrete' element method. Cundall and Hart (1992) proposed the numerical techniques be collectively called the 'discrete' element method if it "*(a) allows finite displacements and rotations of discrete bodies, including complete detachment, and (b) recognizes new contacts automatically as the calculation progresses*" and they indicated four classes of 'discrete' element methods which conformed to the definition – (i) distinct element method, (ii) discontinuous deformation analysis (DDA), (iii) modal methods, and (iv) momentum-exchange methods. For clarity, hereinafter DEM refers to the (i) distinct element method by Cundall and Strack (1979).

There are several key differences between (i) DEM and (ii) DDA. In the original formulation and most of its extensions since, DEM treats the element as a rigid body. However, in some subsequent studies, particle deformation was considered using a combined finite element approach such as the discrete finite element method (Barbosa & Ghaboussi, 1990) and the combined finite-discrete element method (Munjiza, 2004). The rigid DEM particles are 'virtually deformable' in that interpenetration (overlap) between particles is allowed during contact. This approach is considered as a 'soft contact' model where the 'virtual deformability' does not refer to the particle deformation but the implication of being deformable (D'Addetta, 2004). The contact force is computed from the interpenetration using a contact model such as the spring-dashpot. The particle motion is then updated using the equation of motion for which an explicit time integration is used such as the central difference scheme. Therefore, this explicit

DEM is conditionally stable, requiring the use of a small time step size.

The DDA has its origin in Shi & Goodman (1985) and Shi (1988). Unlike DEM, DDA considers the particle deformability, i.e., modelling the strains in particle as well as the rigid body translation and rotation. In the original formulation, strain and stress fields were assumed constant in the particle. Later, high-order elements were introduced (Hsiung, 2001), and a sub-division technique was proposed to better represent the deformability (Lin et al., 1996). DDA employs a 'hard contact' model, where no interpenetration is allowed between particles in contact and a set of kinematic constraints is enforced at every time step. Similar to FEM, the governing equations are represented by a set of linear equilibrium equations obtained by minimizing the total potential energy of the particle system. Therefore, DDA has an advantage over DEM in that the FEM code can be easily modified to analyze discontinuities (Jing & Hudson, 2002). DDA obtains the force balance at every time step by solving simultaneous linear equations while the explicit DEM does not completely satisfy the force balance. The equations are solved implicitly, and are therefore numerically stable, and a large time step size can be adopted. However, DDA is inefficient if there are large changes in the contact configuration as the stiffness matrix needs to be updated through many iterations until convergence is reached. Therefore, DDA is mostly popular for rock mechanics problems where a smaller number of geometry changes are involved in jointed rock mass deformations (O'Sullivan, 2011).

The (iii) modal methods and (iv) momentum-exchange methods were used in past studies of granular materials as discussed in Cundall and Hart (1992) but more recently there has been much activity in the computer graphics community. For example, the modal methods were adopted to provide an interactive design capability (Williams and Pentland, 1992) and the momentum-exchange methods have been developed to deliver physical plausibility of animations (Mirtich, 1996) rather than accurate contact force modelling required for geotechnical engineering problems. However, recent developments adapting these methods are gaining popularity again in the granular materials research (Lee, 2014). For example, Lee and Hashash (2015) developed the impulse-based DEM (iDEM) that can be considered as a momentum-exchange method to efficiently simulate large-scale granular flows. Izadi & Bezuijen (2018) and He & Zheng (2020) demonstrated using open-source impulse-based physics engines such as Bullet Physics (Coumans, 2017) and PhysX (NVIDIA, 2019) for simulation of quasi-static geotechnical laboratory tests. And recently, Park et al. (2021) used iDEM to perform unprecedented granular flow simulations with 52 million 3D polyhedral particles.

Non-Smooth Contact Dynamics is another branch of the discrete element method which can be traced back to the work of Lötstedt (1981, 1982) that formulates the frictional contact problem between rigid bodies into a linear complementarity problem (LCP) fashion. This Contact Dynamics method has been developed by Moreau (1994, 1995), Jean (1999) and their collaborators for the study of granular materials, resulting in the development of software, LMGC90 (Dubois et al., 2011; Azéma et al., 2012). However, this method has gained relatively less attention compared to DEM due to the complexity of the mathematical formulation based on the complementarity problem and associated difficulty of the code implementation. Therefore, there are far fewer publications using this method in the research community (Donzé et al., 2009; Krabbenhoft et al., 2012).

5.2. Towards realistic particle shape modelling

In the original DEM, each particle was modelled as a 2D disk. The early DEM formulations were then followed by employing 3D spherical or ellipsoidal particles such as TRUBAL (Strack & Cundall, 1984), ELLIPSE2 (Ng, 1994) and ELLIPSE3D (Lin & Ng, 1997). This became a trend for a while in DEM research, because simulation of such simple shapes was computationally manageable considering the computing power was quite limited then. Such particle geometries could greatly simplify the contact detection procedure and reduce the run-time, but suffered from limited capability in capturing essential aspects of geometric inter-particle interactions and corresponding mechanical behaviour. However, there are limitations to understanding the microscopic fabric of granular materials using spherical particles, in particular the effect of particle shape and the arrangement of particles which can significantly influence mechanical properties (Oda et al., 1985; Thornton, 2000; Ng, 2009; Yimsiri & Soga, 2010; Radjai et al., 2012; Guo & Zhao, 2013; Fu & Dafalias, 2015; Kuhn et al., 2015). It is therefore necessary to present realistic particle shapes. Building upon the early developments, DEM has evolved to consider realistic particle shapes for more accurate interactions, and to enable systematic modelling at the particle scale and quantitative comparisons with experimental data (Cundall, 1988; Ghaboussi & Barbosa, 1990; Sallam, 2004; Zhao et al., 2006; Hogue & Newland, 1994; Williams & O'Connor, 1999; Peña et al., 2007; Latham et al., 2008; Andrade et al., 2012; Kawamoto et al., 2016; Mollon & Zhao, 2013).

By and large, the currently available techniques to model complex particle shape (other than spheres and ellipsoids) for the discrete element simulation can be categorized into the following three classes: (a) clumping spherical particles, (b) polyhedral particle modelling, and (c) other approaches. Clumping spherical particles is the well-known facile technique in the granular materials research community due to its relatively manageable computational cost and the simplicity of modelling non-spherical particles. The relative ease of particle breakage modelling is another incentive. For this reason, the majority of published simulations were performed with DEM software that provides a sphere clumping function such as PFC (Itasca Consulting Group, 2019), LIGGGHTS (DCS Computing Gmbh, 2016), EDEM (DEM Solutions Ltd., 2019), YADE (Kozicki & Donzé, 2008). However, this modelling approach generates particles with ‘knobbly’ surfaces that inherently overestimate the geometric interactions (Munjiza, 2004; Houlsby, 2009). The computational cost is not necessarily inexpensive, as a large number of spheres are required to model realistic particle shapes. Polyhedral particle modelling requires more computational resources than the sphere clumping due to the complexity in the particle modelling and simulation, especially in the expensive geometric contact detection between the polyhedral particles. However, this approach can better model particle geometries and capture the microscopic interactions at the grain scale. A variation of this approach using spheres for rounded corners (dilated polyhedral element) has been reported in Fraige et al. (2008), Wang et al. (2011) and Ji et al. (2015).

Compared to (a) and (b), the other approaches are less popular or may be considered as recent developments in the research community, e.g., polar representation (Hogue & Newland, 1994), voxel-based representation (Druckrey et al., 2016) that may be seen as a variation of the discrete function representation (Williams & O’Connor, 1999), Radon transform-based modelling (Leavers, 2000), super-quadric particles (Hogue, 1998; Delaney & Cleary, 2009; Zhao et al., 2019), Non-Uniform Rational Basis-Splines (NURBS)-based modelling (Andrade et al. 2012), polyarc discrete element (Fu et al., 2012), potential particles (Houlsby, 2009), and level set functions-based modelling (Kawamoto et al., 2016), just to list a few. These techniques utilize a tailored contact detection method to take advantage of the geometric modelling parameters. Fig. 5 illustrates some of the approaches mentioned above.

5.3. Developments in DEM simulations with polyhedral elements

Ghaboussi and Barbosa (1990) pioneered 3D DEM with polyhedral elements to account for realistic geometric interactions between particles. They comprehensively investigated all computational aspects of the method and developed a polyhedral DEM code, BLOCKS3D. A number of efforts have been put into capturing ground truth particle geometry for accurate polyhedral DEM modelling. Early work by Tutumluer et al. (2000) and Masad (2005) introduced an image analysis technology to the granular materials research community and developed UIAIA (University of Illinois Aggregate Image Analyzer) and AIMS (Aggregate Imaging System), and later E-UIAIA, an enhanced version of UIAIA (Moaveni et al., 2013) to characterize the morphological properties of coarse aggregates. With these scanning technologies, the digitized morphological data could be utilized to develop the polyhedral particle shapes for use in DEM modelling. The particle morphology could be also quantified using various morphology indices, e.g., flat and elongated ratio, angularity index, sphericity, roundness. And recently, M−A−V−L (Su et al., 2020) was developed which dramatically enhanced the way 3D particle morphology is characterized. Recent advances in optical geo-characterization, e.g., X-ray computed tomography and photogrammetry (Garboczi, 2002; Paixão et al., 2018) have been used to capture 3D particle geometry. Developments in mobile applications using smartphones makes field application of 3D scanning more affordable and accessible (Zhang et al., 2016). These recent advances that help compile the geometry data will enhance the fidelity of the polyhedral particle modelling.

On the other hand, consideration of realistic particle shapes requires expensive geometric tests for the contact detection; this most time-consuming operation of an entire DEM simulation can take up to 80% of the total computation time (Nezami et al., 2004). In 1988, the Common Plane (CP) method was first introduced for faster contact detection in polyhedral DEM simulations (Cundall, 1988). The CP is defined as the plane that bisects the space between two particles in contact, which made it possible to simplify the complex ’particle-to-particle’ contact detection problem into the much easier ‘particle-to-plane’ contact detection problem. Since then, significant algorithmic developments have been made to enable a faster particle contact detection between polyhedral particles (Gilbert et al., 1988; (Lin & Canny, 1991); Williams & O’Connor, 1999; Liu & Lemos, 2001; Yang et al., 2002; Nezami et al., 2006; Vorobiev, 2012; Boon et al., 2012; Nassauer et al., 2013). For example, the Shortest Link Method developed by Nezami et al. (2006) is a CP-based contact detection method that results in a contact detection up to 17 times faster than the conventional CP method.

With these major algorithmic enhancements and the increase in computing power, it has become possible to conduct relatively large-scale polyhedral DEM simulations, and researchers can get a better insight into the mechanical behaviour of granular materials. However, DEM simulation is still a memory- and processor-intensive task, and significant computational challenges remain to address the needs of the granular materials research community. O’Sullivan (2011) examined the DEM simulations published since 1998 and concluded that simulation of 1 million spherical particles on personal computer was still demanding at the time of that study. While the survey is now a decade old, this result still implies the computational challenges in the polyhedral DEM for geotechnical problems. DEM simulation is relatively practical for analysis of a short-duration problem. To our knowledge, Tutumluer et al. (2013) conducted the longest simulation, which runs for 2000s (~30 min) of simulation time with 13,000 polyhedral particles. Practical time step sizes are also linked to particle size and for this reason, simulations of small-grained granular materials are generally less doable because a smaller time step size is required to capture realistic microscopic interaction between the parti-

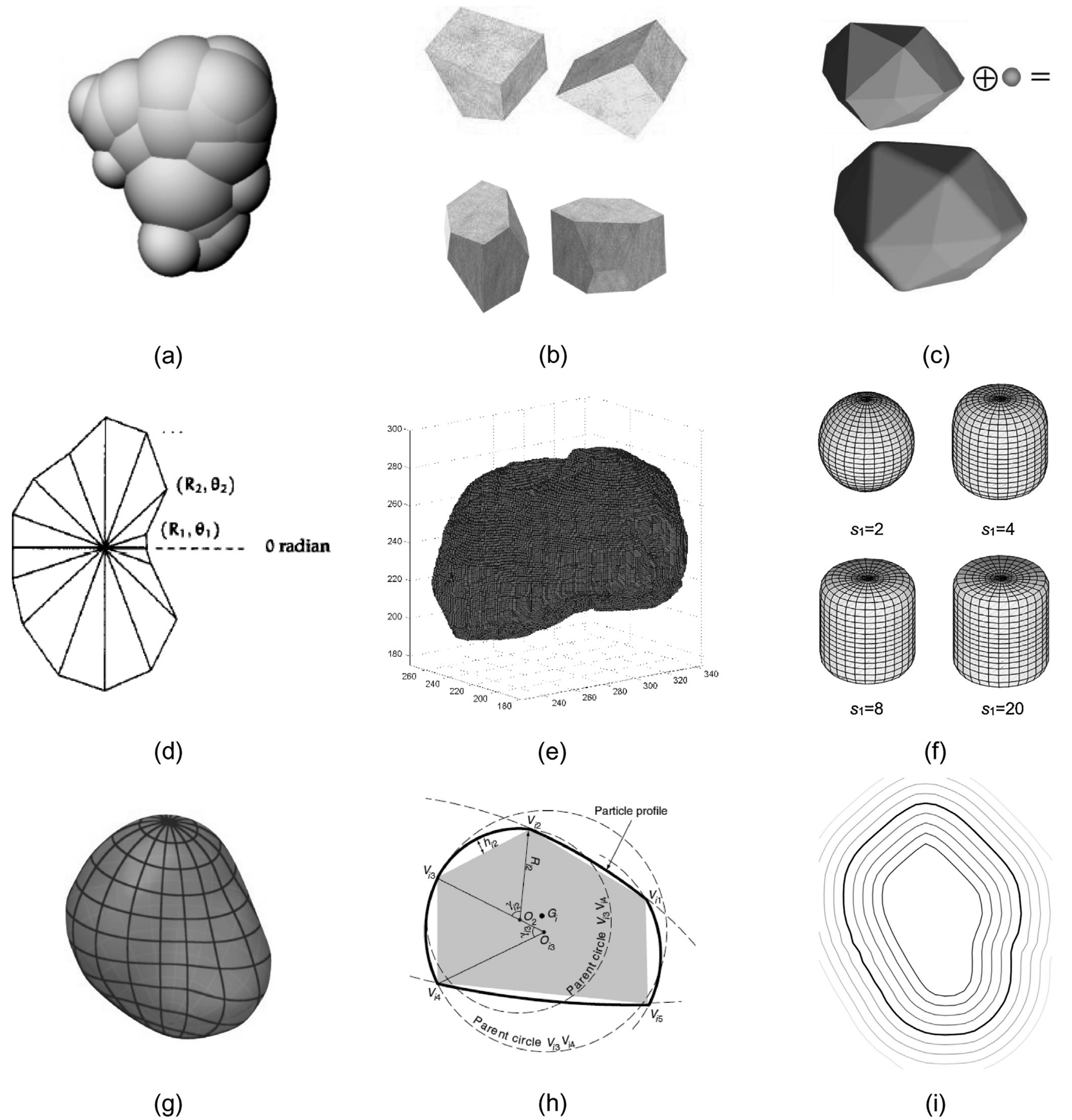

Fig. 5. Non-spherical particle modelling techniques for DEM; (a) Sphere-clumps (EDEM, 2020), (b) Polyhedral particle (Lee et al., 2012), (c) Dilated polyhedral element after Minkowski sums also known as spheropolyhedron (Ji et al., 2015) (d) Polar representation (Hogue and Newland, 1994), (e) Voxel-based representation (Druckrey et al., 2016), (f) Super-quadrics (Zhao et al., 2019), (g) NURBS-based modeling (Andrade et al., 2012; Lim, 2015), (h) Polyarc discrete element (Fu et al., 2012), (i) Level set-based representation (Kawamoto et al., 2016); All figures reused with written permissions from the copyright owners.

cles. Linear scaling of particle size is, therefore, often used in DEM studies to decrease the number of particles in the simulation and to increase the particle size and the time step size. However, this particle size scaling is generally applicable to a uniformly graded granular material only, as opposed to a well-graded granular material. Therefore, DEM studies of a well-graded granular material are sparse to date (Matsushima, 2003; Evans et al., 2009; Huang et al., 2013). Recent research efforts have also focussed on using hardware acceleration techniques such as high-performance computing machines to perform large scale DEM simulations (Horner et al., 2001; Owen & Feng, 2001; Walther & Sbalzarini, 2009; Iglberger & Rüde, 2011). High-performance clusters with graphics processing units (GPU) are getting more affordable and accessible (Govender et al., 2016), which will therefore help researchers to perform large scale DEM simulations. These tools will become more powerful and useful in understanding the underlying mechanisms of complex granular materials behaviour at various time and length scales.

5.4. Application of DEM for field scale large deformation problems

As discussed above, the discontinuum-based methods are inherently suitable to simulate large deformation phenomena, and have been extensively used in academia to study the fundamental mechanisms at the particle scale that are associated with the large deformation. However, considering a large number of particles needed to model a large-scale problem, the use of DEM for field or industrial scale applications has been less common in the geotechnical engineering practice due to the high computational cost to achieve the required simulation fidelity.

With the recent advances of computing power, increasing numbers of studies adopt DEM to simulate the large deformation phenomena. These efforts have been actively made in the industry using commercial codes including PFC (Itasca Consulting Group, 2019), 3DEC , UDEC , EDEM (2020), Rocky DEM and others. A good number of examples regarding the field scale DEM applications for large deformation problems were presented in the five international symposia hosted by the Itasca Consulting Group since Itasca Consulting Group, 2008. These applications adopted a suite of Itasca's DEM codes along with the discrete fracture network (DFN) approaches to describe natural joint sets and fracture patterns present in the field. Field scale DEM simulations have now been conducted for various large deformation problems in geotechnical engineering including mining and underground construction (e.g. Sainsbury & Grubb, 2011; Bhusan et al., 2020), slope stability analysis (e.g. Utili & Nova, 2008; Najarro & Vargas, 2016) and hydraulic fracturing (e.g. Alfonsi & Grelaud, 2008; Moghadam et al., 2020). The spatial scale of published simulations now varies from less than a metre to several hundred kilometres.

Penetration problems such as pile driving and cone penetration testing involving large deformation of soils have been also of great interest to DEM modellers in geotechnical engineering (O'Sullivan, 2011). In addition, geotechnical engineers have adopted DEM to better understand the large deformation phenomena associated with natural hazards such as sinkholes, earthquake fault rupture, and liquefaction. Examples can be found in Noury et al. (2018), Abe et al. (2016), Kuhn et al. (2014), respectively. Moreover, with enhanced computing power, earthworks processes involving large deformation (e.g., earth moving, ploughing, trenching) have become more feasible, e.g. Knuth et al. (2012), Tutumuler et al. (2013) and Mahmoud et al. (2016).

6. Conclusions

Reviewing the current methods, it is clear that for routine calculations and analysis the FEM will remain the tool of choice (certainly in 2D), due to inefficiencies in other continuum methods that have yet to be addressed properly. FEMs adapted for large deformations (such as the ALE and CEL methods) are now mature and have been implemented in commercial software, so it is likely these will see much activity in general use. The Material Point Method has rightly attracted much attention in the geotechnical community as it (a) appears to provide a tool that can model very large deformation problems including coupled problems and (b) makes use of many standard components of the FEM, making implementation somewhat more straightforward than other continuum meshless methods. The DEM is also experiencing considerable popularity in geotechnical research communities, but it is still nearly impossible to model boundary value problems of entire geotechnical constructions with the DEM due to computational costs. The key role of the DEM in the coming years may lie in improving understanding of the link between the real particle scale and macro observed behaviour. In recent years, hierarchical multiscale frameworks have been developed using a combined DEM-FEM method to link the particle-scale microscopic properties with the macroscopic behaviour of granular materials (Andrade et al., 2011; Guo & Zhao, 2014; Liu et al., 2016). These studies commonly showed that DEM microanalysis can play an important role in eliminating the phenomenological assumptions required by the conventional continuum-based macro-analysis methods. There is also some interesting activity from researchers combining the DEM with continuum methods, such as MPM with DEM in Ceccato et al. (2018a) and SPH with DEM in Trujillo-Vela et al. (2020), which is another way forward, as are the possibilities offered by other combinations, e.g. MPM and finite differences in Higo et al. (2010) and Nøst (2019). It is worth remembering, however, none of these methods can avoid the fact that large problems will require large computing resources (time and memory) to obtain high simulations fidelity and that approaches adapted for use with high performance computing are the only current solution.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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