Three dimensional numerical manifold method and rock engineering applications

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THREE DIMENSIONAL NUMERICAL MANIFOLD METHOD AND ROCK ENGINEERING APPLICATIONS

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**SCHOOL OF CIVIL AND ENVIRONMENTAL
ENGINEERING
NANYANG TECHNOLOGICAL UNIVERSITY**

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Three Dimensional Numerical Manifold Method and
Rock Engineering Applications

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Summary

Among various numerical methods, the numerical manifold method (NMM) is one of most suitable method to simulate deformations and stabilities of rock masses. The NMM itself can be thought as a bridge connecting two branches of numerical method: continuum methods (e.g. FEM) and discontinuum methods (e.g. DDA). Since it was first proposed in 1991, most of research works on the NMM were carried out within the two-dimensional (2-D) framework. However, it will be more realistic and beneficial to the practicing industry to address the problem with a three-dimensional model and an advanced numerical method is highly demanded in rock engineering.

This thesis extends the numerical manifold method to the 3-D domain based on the 2-D fundamentals. First, the conceptual framework of the 3-D NMM is established, including the definitions of the mathematical cover, physical cover, manifold pattern and manifold element in the 3-D domain. A new general 3-D contact algorithm is subsequently developed for the 3-D NMM. The proposed contact treatment procedure consists of distinct features, including: three operation phases for the checking process, NMM hierarchical contact system, contact warning based on mathematical patterns (*MPs*), transformation of two essential entrance modes, transferring contact information, penalty treatment for contact constraints, open-closed iteration process, and lagged verification on contact state. These features equip 3-D NMM with an efficient and accurate strategy of contact treatment.

A total of ten numerical examples are analyzed in the present thesis, including verification of the 3-D NMM formula, analysis of a discrete blocky system, verification of the contact algorithm, and two scenarios in rock engineering, i.e., stability analysis of rock slopes and tunnels. The proposed 3-D NMM is proved to be a robust, efficient and stable tool with both static and dynamic analysis ability. It has great potential to be further developed and applied in practical rock engineering.

Keywords: 3-D Numerical Manifold Method (NMM), 3-D contact algorithm, 3-D manifold patterns, discontinuous deformation, dynamic analysis, rock slope & tunnel.

List of Symbols

A_0	Required force to stabilize the wedge in the simulation example of roof wedge falling
A_c	Contact area in tangential contact condition
A_i	Area of the face of wedge in the simulation example of roof wedge falling
$A, B, \dots$	Contact bodies of Contact situation in 3-D NMM; or a also denote Area of a face of the wedge in the simulation example of tetrahedral wedge sliding
$\vec{a}$	Unit vector in the direction of the normal to plane 1 with components (a_x, a_y, a_z) in the simulation example of tetrahedral wedge sliding
$\vec{b}$	Unit vector in the direction of the normal to plane 2 with components (b_x, b_y, b_z) in the simulation example of tetrahedral wedge sliding
$\mathbf{b}$	The body force per unit volume in weak form of governing equation
$\mathbf{B}$	Strain matrix in NMM interpolations
C_{ij}	Algebraic complement of determinant matrix in normal contact matrix in Eq.(5-11)
c	Cohesion modulus in the simulation example of tetrahedral wedge sliding
D_α, D_β	Cover displacement on different Manifold Pattern (MP)
$\mathbf{d}_i$	Displacement vector
d_N	Normal gap in non-penetration condition and contact contribution
d_T	Tangential gap function in formulation for contact contribution

E	Young's Modulus
e_i	Unit vector of edge i in contact facet
F	Factor of safety
$\mathbf{f}$	Friction force based on Coulomb's friction law
$\vec{f}$	Unit vector in the direction of the normal to plane 4 with components (f_x, f_y, f_z) in the simulation example of tetrahedral wedge sliding
g	Acceleration of gravity
$\vec{g}$	Vector in the direction of the line of intersection of plane 1 and 4 with components (g_x, g_y, g_z) in the simulation example of tetrahedral wedge sliding
H	The height of the crest of the slope above the intersection in the simulation example of tetrahedral wedge sliding
i	Index denoting the face of the block
$\vec{i}$	Vector in the direction of the line of intersection of plane 1 and 2 with components (i_x, i_y, i_z) in the simulation example of Tetrahedral wedge sliding
i_i	Roughness angle of the i^{th} joint in the simulation example of roof wedge falling
k_N	Penalty parameters in normal direction in formulation for contact contribution
k_T	Penalty parameters in tangential direction in formulation for contact contribution
$k_{s,i}$	Shear stiffness of the i^{th} joint in the simulation example of roof wedge falling
$k_{n,i}$	Normal stiffness of the i^{th} joint in the simulation example of roof wedge falling
$\mathbf{L}$	The differential operator matrix in NMM interpolations
M_I	Mathematic covers;

n	Total edge sum of the facet in contact facet
N	Effective normal reaction on a plane in the simulation example of tetrahedral wedge sliding
$\tilde{\mathbf{N}}$	Average normal of reference entrance facet
P	Penalty spring stiffness in simulation examples
P_I^j	Physical Covers, where I and j is the number index of the physical covers.
P_i	Positions of vertexes in contact description
$\mathbf{P}_T$	Tangential contact traction or friction force in tangential contact condition
$\mathbf{P}_N$	Normal force in smooth transition
q	Component of $\vec{g}$ in the direction of $\vec{b}$ in the simulation example of Tetrahedral wedge sliding
r	Component of $\vec{a}$ in the direction of $\vec{b}$ in the simulation example of Tetrahedral wedge sliding
S	Actuating shear force on a plane in the simulation example of tetrahedral wedge sliding
S_c	Contact face in contact configurations
s	Mathematical cover size in simulation examples
t	Time step in 3-D NMM calculation
$\bar{\mathbf{t}}$	Traction prescribed on the corresponding boundary in weak form of governing equation
$\mathbf{U}_i$	Manifold displacement vector
u	Average water pressure in the simulation example of tetrahedral wedge sliding
$\bar{u}_i$	Displacement function of each math cover in the illustration of manifold pattern
$u(x, y, z)$	Displacement function
$\ddot{\mathbf{u}}$	Acceleration vector in weak form of governing equation
ν	Poisson ratio

$v(x, y, z)$	Displacement function
$\mathbf{v}_T$	Relative velocity in a tangential direction
$\mathbf{v}_n$	Relative velocity in a normal direction
W	Weight of the wedge in the simulation example of roof wedge falling
$w(x, y, z)$	Displacement function
x_c	Contact point or one particle in the contact pair in contact configuration
x_i, y_i, z_i	The coordinates in three directions
α	The slope of plane or angle in simulation examples (e.g., Cube sliding example); or dip direction in the simulation example of Tetrahedral wedge sliding
α_i	Complement of the dip angle of the joint which creates the face in the simulation example of roof wedge falling
μ_s	Static Friction Coefficient in friction law
μ_D	Dynamic Friction coefficient
ε	Strain tensor in weak form of governing equation
ε_s	The numeral mite in contact checking procedure
ω_i	The weight function of match cover in manifold pattern
γ	The parameter in Crossing-lines model in Eq. (5-5) or the unit weight of rock mass in the simulation example of Tetrahedral wedge sliding
σ	Stress tensor in weak form of governing equation, or the In-situ horizontal principle stress in the simulation example of roof wedge falling
$\sigma_{n,i}$	Normal stress acting on the i^{th} face of the wedge in the simulation example of roof wedge falling
ϕ	The friction angles in simulation examples (e.g., cube sliding, roof wedge falling)

$\varphi_I(\mathbf{x}), \varphi_I(x, y, z)$	Weight function on manifold covers
ψ	The dip in the simulation example of Tetrahedral wedge sliding
ρ	The density in weak form of governing equation or the density of materials in simulation example
μ	Friction coefficient
$\lambda, \lambda_N, \lambda_T$	Lagrange multipliers, N is for normal direction and T is for tangential direction.
Ω_c	Contact critical state configuration in contact configuration
Γ_c	Set of particles in contact pair in contact configuration
Π_u	Total energy without contact constraint in numerical modified energy function
Π_c	Energy caused by contact constraints.

List of Abbreviations

3-D:	Three dimensional
2-D:	Two Dimensional
BFSA:	Brute Force Searching Algorithm
BPM:	Bonded-Particle Model
CFD:	Computational Fluid Dynamics
CP:	Contact Pair
CPM:	Common Plane Method
DDA:	Discontinuous Deformation Analysis
DEM:	Discrete/ Distinct Element Method
DOF:	Degree of Freedom
FDM:	Finite Difference Method
FEM:	Finite Element Method
HTA:	Hierarchy Territory Algorithm
IOA:	Inside-Outside Algorithm
ISM:	Inscribed Sphere Method
NMM:	Numerical Manifold Method
MC:	Manifold Cover (Mathematical Cover)
ME:	Manifold Element
MP:	Manifold Pattern
MSC:	Master-Slave Contact method
PC:	Physical Cover.
PEM:	Penetrated Edge Method
PFC:	Particle Flow Code
SPH:	Smoothed-Particle Hydrodynamics
SPM:	Splitting Pinball Method
SSA:	Single Surface Contact Algorithm
TPO:	Target physical objects
XFEM:	Extend Finite Element Method

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Chapter 1 Introduction

1.1 Background

Frequent and prevalent geologic hazards have caused various catastrophic damage and fatality to the advance global infrastructure development. It is important for engineers to understand the hazard mechanism prior their design, which increases the consciousness regarding safety and economic feasibility in the civil and specially the underground engineering field. The drive for the engineers to seek for more rational and reliable solutions to the geotechnical problems becomes urgent and necessary in order to reduce the disastrous damage.

Among those geologic hazards, several of them are very hard to predict and prevent due to the uncertainties and limited understanding of the geological conditions and behavior of rock masses. The up-to-date knowledge in the rock mechanics are apparently thus far too limited for the present infrastructure development, they are not sufficient for us to understand the causes and seasonal behind even after hazard occur. It is worth noting that the rock mechanics analyzing methodologies are developing at a much slower pace comparing to the demand on rock engineering in practices. One of apparent reasons is that it is always a challenge to have an accurate strategy or methodology to measure and model the geological properties of rock masses.

Rock masses, generated in the natural environment, are complex with stochastic uncertainties in different extent of imperfection. These imperfections appear as bedding planes, joints, shear zones and faults, which make the rock mass to be a combined solid of continuum and discontinuum. The distinct feature of the rock masses creates tremendous difficulties in the analysis procedure. In the early stage, geotechnical engineering problems are usually analyzed through differential equations with specified boundary conditions. Crediting to past effort, there are few simple geometrical and material deformation models are available in the closed-form

theoretical solutions. However, those developed solutions nominally over-simplify the actual problem found in reality, the estimated setup scenario usually caused the analysis result varies against the real situation. The limitations from the theoretical solutions motivated the rapid development of numerical methods in the past a few decades. Although, being one of the pioneer numerical methods investigated, the finite element method (FEM) and finite difference method (FDM) are very well developed and have been widely applied in various engineering analysis, but in the rock engineering discipline, both methods extended the short coming on over-simplifying the effect on localize and global influence of the joint network in rock masses. They inherit the assumption of small displacement/deformation from the theoretical method, also, the complex mathematical troubles encountered in meshing and re-meshing processes reduce the efficiency and accuracy of the analysis. A variety of mesh-free and node-based analysis methods have recently been proposed attempting to overcome problems such as “meshing trouble”. The application of these methods is still limited by boundary treatments especially for contact and multi-physical problems with intensive computational cost.

On the other hand, FEM and FDM are initially brought up in the framework of continuum mechanics. In order to extend their applicability for analysis to multi-body, heterogeneous structure and jointed solids, the interface elements or “slide lines” [Goodman *et al.* (1968)] have been put forward, which enables them to model a discontinuous material. However, their application are restricted in many aspects, e.g. multi-intersecting interface cases, new contact detection in complex media or larger displacement between. A better solution related to problems with discontinuous jointed rock mass is by the distinct element method [Cundall (1971)] or the discontinuous deformation analysis (DDA) [Shi (1988)], with handicap in their description of block deformation is relatively inflexible and the stress field descriptions are not sufficiently accurate.

Since the numerical manifold method (NMM) was proposed [Shi (1991)], researchers have paid a lot of attentions to improve and extend it for different purposes. It has been incorporated into other methods and developed as enriched meshless NMM [Li *et al.* (2005)], breakable NMM [Zhang *et al.* (1997)], and

Eulerian NMM [Terada et al. (2007)], etc. In general, the NMM was treated as a combination of the finite element method (FEM) and the discontinuous deformation analysis (DDA) method.

The bridging between the FEM and the DDA is achieved through a fundamental concept of covers (including mathematical and physical covers) under the NMM framework. The terminology “manifold” comes from the topological manifold and differential manifold, which is the main subject of differential geometry, algebraic topology, differential topology and modern algebra of mathematics [Shi (1996)]. Manifold is mathematically defined when a function is continuous and differentiable at each cover in the description domain and all covers are independent. The overlapping mathematical covers create various manifold elements through intersection with the physical domain which generates the continuous and differentiable function description in the whole domain. They are the advantages that make NMM applicable to a blocky system or a cracked system with dense discontinuities in the domain since the NMM inherits the merits of the DDA. As the preparation of mathematical cover is independent of physical domain, the geometrical shape can be user-defined freely. Each mathematical cover does not require conforming to the boundaries of its structure. It is also able to remarkably reduce the workload in processing the meshes. Furthermore, it prompts a new idea for multi-physical modeling by introducing more layers of mathematical meshes.

Although the 2-D NMM has already been widely proven by abundant examples, the real problems in practice are always in the three dimensional space. Due to the complexity in geometry description and the absence of a reliable 3-D contact algorithm, it has been a long time challenge to raise the NMM for three dimensional analysis. However, the increasing underground construction and geotechnical works strongly demand for a 3-D discontinuous deformation analysis tool, especially in rock engineering analysis. Cheng and Zhang (2008) have derived basic theoretical formulation of 3-D NMM, although the solution is far from engineering practical application.

It is necessary to develop a general contact algorithm to the 3-D numerical manifold method. The research on the 3-D contact algorithm is the most critical development to extend the NMM to the 3-D domain. Though various efforts have been contributed under the FEM framework, mathematical descriptions of the 3-D contact algorithm including contact boundary treatment, transferring and automatic contact searching are far from maturely developed.

The present thesis focuses on three main directions: 1) 3-D NMM theory and basic configuration for its algorithm; 2) Development of a general contact algorithm to suit for various contact scenarios. It is mainly to describe the implementation process of the 3-D NMM and to introduce an effective contact treatment logic to handle blocky rock systems; 3) application of the developed 3-D NMM in rock engineering problems, such as rock slope and rock tunnel stabilities.

1.2 Objectives

The primary objective of the present study is to extend the numerical manifold method to the 3-D domain and to develop a numerical tool which is able to simulate rock mass strength and stability in the practically more realistic 3-D space. The scope of work includes,

- 1) Design a general framework for the 3-D NMM, extending from the existing fundamental 2-D NMM theory.
- 2) Develop a general contact algorithm and implement it into the 3-D NMM formulations.
- 3) Apply the developed program for rock engineering problems, such as analysis of rock slope and rock tunnel stabilities.

1.3 Thesis Organization

This thesis is organized into 9 chapters. The background and objective of the research are introduced in Chapter 1.

In Chapter 2, a detailed literature review of the previous studies on the numerical manifold method (NMM) is presented with review and comparison against other numerical methods.

The author's understanding and the 3-D extension of the NMM method is presented with a systemic manner in Chapter 3. A detailed nomenclature explanation provides an efficient way to understand the NMM definitions in both 2-D and 3-D. It includes building-up the geometric configuration of the manifold pattern in a 3-D view, and introduction on fundamental concept of the 3-D NMM. Detailed formulations of the 3-D NMM based on a tetrahedron manifold pattern are also proposed.

Chapter 4 presents the general computational contact mechanics. It mainly contains a systematic summary on all aspects of the contact algorithm: The classic contact mechanism, detailed contact constraint equations and updating history of contact checking.

Chapter 5 further extends to discuss on the contact logic especially for the 3D-NMM. Beside the specific contact equations based on a penalty method, this chapter gives the whole procedure of the contact treatment in the 3-D NMM.

A total of 8 examples are demonstrated in Chapter 6 to verify the proposed 3-D NMM formulations and the implemented contact treatment algorithm from both continuous and discontinuous aspects.

The rock slope stability analysis and rock tunnel stability analysis are two classic applications in practical rock engineering. These two case studies are discussed on Chapter 7 and Chapter 8 respectively.

Conclusions of the present study and some recommendations for further research are given in the Chapter 9.

Chapter 2 Literature Review

2.1 Introduction

Conventional numerical methods such as the FEM face technical problems when a solid under simulation is changing from a continuous to a discontinuous state. The numerical manifold method (NMM) [Shi (1991, 1995)] provided a natural bridging to represent the physical change during numerical simulations. It was also advantageous over the conventional numerical methods in analyzing both continuous and discontinuous problems. The NMM links the continuum-based FEM and the discontinuum-based DDA method through defining two separate cover systems, i.e., the mathematical cover and the physical cover. It was mentioned in Shi (1991) that

“Both the finite element method (FEM) for continua and the discontinuous deformation analysis (DDA) for block systems are special cases of this numerical manifold method”.

Crack initiation and propagation in material failure involve in contact evolving and updating, such mechanism sometime will cause a continuum split into a discontinuum. It is strongly recommended to develop an appropriate numerical method to solve such problems. The NMM is considered to be one of the most suitable numerical methods in rock engineering. Its basic theory and recent development are reviewed with comparisons to other numerical methods in this chapter.

2.2 Fundament of 2-D NMM

The fundamental theory of the NMM has been established since Shi's initial effort in 1991. Its basic concepts consist of three major parts, namely, finite cover system, simplex integration and block kinematics [Li *et al.* (2005a)].

2.2.1 Finite cover system

The *finite cover system* divided a problem into two independent cover systems, i.e., a physical cover system in the physical/material domain and a mathematical cover system in the manifold/mathematical domain. The physical covers consisted of a blocky system which provided physical information, such as boundaries of the blocks, joints, and the interfaces of different material zones, etc. The mathematical covers would control the precision level of approximation to the unknown functions. The covers in the mathematical domain were defined according to the geometry of the concerned problem, accuracy requirement and physical zones. At the first stage of preprocessing, the mathematical covers rebuilt the physical block system with sub-blocks. In the second stage, the sub-block system brought back the geometric information to the mathematical covers to construct the manifold element system.

In manifold computation, the mathematical cover system and physical cover system were independent. Therefore, mathematical covers were free to be defined and their size and shape were free to be changed. The mathematical covers could be deformed, split and even removed. Large deformations and moving boundaries could be computed through allocating the mathematical covers. The joints and block boundaries could divide a cover into two or more independent covers together with the dedicated displacement functions, thus the general discontinuous materials could be modeled.

Based on the above concepts, Shi (1991) had derived 19 specific formulas for a 2-D version NMM program.

2.2.2 Simplex integration method

The “Simplex integration method” was adopted in the NMM computation. As shown in Fig. 2-1, an arbitrary 2-D domain of integration to a function was converted into many triangles. Integration was done based on these triangles, which helped to ensure high precision analytically [Li *et al.* (2005a)].

Figure 2- 1 Illustration of simplex integration [Li *et al.* (2005a)]

2.2.3 Block kinematics

2-D NMM inherited contact detection techniques and the block kinematics from the DDA contact algorithm. For example, no-tension and no-penetration criteria between two contact faces must be satisfied, when dealing a problem with the movements of discontinuous boundaries. The contact detection algorithm was described by inequalities [Shi (1988)]. The kinematics for material was based on the contact theory. The discontinuous displacements were computed via searching the contacts in each time step and applying stiff springs on detected contact zones. The contact algorithm had been verified and improved through a few case studies. It had been realized that the contact algorithm migrated into the 2-D NMM is effective and accurate.

2.3 Historical Development of 2-D NMM

2.3.1 State of art

Based on the above mentioned fundamentals, the particular dual-cover algorithm allowed the NMM to model the pre-existing discontinuities in a convenient way. The original version of the 2-D NMM by Shi (1991) lacked the criteria for the evaluation

of crack initiation and propagation. In addition, Shi (1991) adopted a *Constant cover function* and the simplest *triangular manifold element* in the original version of the NMM.

Various developments and applications had been achieved during the last two decades. Most of the publications were included in the series of proceeding of the International Conference on Analysis of Discontinuous Deformation (ICADD) (eg. [Li *et al.* (1995)]; [Salami and Banks (1996)]; [Ohnishi (1997)]; [Amadei (1999)]; [Bicanic (2001)]; [Hatzor (2002)]; [Lu (2003)]; [Maclaughlin and Sitar (2005)]; [Ju *et al.* (2007)] and [Ma and Zhou (2009)]). The main developments and applications of the NMM were summarized below by categorizing them into several groups, including accuracy improvement by higher order cover functions, application in strong and weak discontinuity problems, and so on.

2.3.2 Higher order cover functions

The original version of the NMM was developed based on triangular manifold elements. Some researchers attempted to improve the accuracy through using more complex geometric elements. Shyu and Salami (1995) implemented quadrilateral isoparametric elements (Q4) into the NMM. Generally speaking, the Q4 element was more efficient than the triangular element. However, for bending problems, the precision and efficiency of the Q4 element was not adequate. Cheng *et al.* (2002) incorporated Wilson non-conforming elements into the NMM, which derived the matrices of equilibrium equations and verified its efficiency and precision for a cantilever slab bending problem.

Chen *et al.* (1998) derived detailed formulations on the high-order NMM with high-order cover functions, which verified the necessity for the complicated deformation problems. At the same time, high-order NMM might induce difficulties in finding its explicit solutions. In order to overcome these difficulties, “adoptable high-order solution” (named by the thesis author) was proposed by Su *et al.* (2003) to automatically produce the expressions and the subroutines were written with the commercial software Mathematica.

2.3.3 NMM for discontinuity modeling

The NMM described the discontinuities by splitting mathematical covers into physical covers attached with independent cover functions, enforcing the interface compatibility conditions of a medium using Lagrange multiplier method, penalty method, or augmented Lagrange multiplier method. Lagrange multiplier vector could be identified to be the traction vector on the material interface, so that it could be used to judge the debonding of the material interfaces based on a failure criterion. In order to obtain the accurate Lagrange multipliers and to avoid the instability imposed contact constraints in numerical computation, instead of the traditional Lagrange multiplier method and the penalty method, the augmented Lagrange multiplier method with an iterative procedure is usually adopted.

The NMM could be used to explore the discontinuous problems such as crack initiation, propagation and shear failures models. Lin (2003) examined the NMM from the partition of unity's perspective and demonstrated that the framework of the NMM was similar to the mesh-less methods. The most significant differences of the NMM came from its unique way of modeling discontinuities and its adoption of analytical integration scheme. In the NMM, the mathematical covers adopted could be completely independent and isolated from the geometry of the problem domain during the preprocessing stage, which greatly simplifies the meshing task for crack problems and avoids the re-meshing for crack growth. The mathematical covers were completely cut by the crack surfaces into several physical covers and enriching the singular physical covers which contained the crack tips inside with the asymptotic crack tip functions. The NMM was conceptually applicable for arbitrary crack problems and could treat a complex crack problem easily as a single crack problem, unlike the XFEM restrained by the enrichment functions.

Valuable researches were performed in the past decade for discontinuous implementation specialized in the crack propagation domain. Tsay *et al.* (1999) applied the NMM together with a local mesh refinement and auto-remeshing schemes to predict the crack growth in homogeneous medium. The crack opening

displacement was adopted to evaluate the stress intensity factors. Zhang *et al.* (1999) coupled the NMM with the boundary element method (BEM) to simulate the initiation and crack propagation problems in dam foundation with weak zone such as faults and joints. Zhou *et al.* (1999) coupled the NMM with the element free method for crack propagation. Chiou *et al.* (2002) fused the NMM with the virtual crack extension method to study the mixed-mode fracture propagation.

Wang *et al.* (2003) extended the NMM to model the strong discontinuities resulting from shear failure. Materials under consideration were assumed to be elastic-brittle. In his model, local shear failure was induced when the shear stress in the material reaches the shear strength. Interface elements were incorporated along the discontinuities on which the Mohr-Coulomb law was applied. Zhang *et al.* (2003) utilized the NMM to model cracking of the Wuqianxi ship lock.

Li *et al.* (2005b) and Gao and Cheng (2009) developed enriched mesh-less manifold method for two-dimensional crack modeling. In their models, the mathematical covers were formed by influenced domains of the nodes. The weight functions for each mathematical cover were formed by the partition of unity functions. The physical covers were formed by the subdivisions of mathematical covers in the problem domain. Their enriched mesh-less manifold method was proved to be more efficient than the traditional mesh-less methods.

Ma *et al.* (2009) exhibited the advantageous features of the NMM for multiple branched and intersecting cracks, in which singular physical covers were enriched with asymptotic crack tip functions, the stress intensity factors were evaluated by virtue of domain form of interaction integral. Zhang *et al.* (2009) extended it to simulate the growth of complex cracks, adopting the maximum circumferential stress criterion to determine the crack growth.

Both Ma *et al.* (2009) and Zhang *et al.* (2009) demonstrated the efficiency and robustness of the NMM in modeling complex cracks and their growth. For illustration purpose, a problem with a tree-shaped crack under bi-axial tension in a

finite plate was shown in Fig. 2-2 (a). The detailed description of the parameters used in the computation can refer to [Ma *et al.* (2009)]. The regular mathematical covers for the central part of the problem were depicted in Fig. 2-2 (b). The convergence of the stress intensity factor at crack tip D could be easily observed when the mathematical covers were gradually refined (Fig. 2-2 (c)).

(a) tree-shaped crack

(b) part of the mathematical covers

(c) SIF at crack tip D

Figure 2- 2 Modeling a tree-shaped crack with the NMM [Ma *et al.* (2009)]

In the concern of the heterogeneity of rock mass, Terada *et al.* (2003) suggested the finite cover method (FCM), an alias of the NMM, and presented the formulation for the static equilibrium of a structure with arbitrary physical boundaries including material interfaces. They extended the FCM technique based on the concept and mechanism of NMM to analyze heterogeneous properties and solving problems with

discontinuities evolving in structures involving the discontinuities in strains and displacement caused by debonding or ruptures of material interfaces. The displacement compatibility conditions on the material interface were enforced by Lagrange multiplier method. The FCM might result in generalized elements that were partially within physical domains. Terada and Kurumatani (2004) assessed the performance of such generalized elements and concluded that the performance of generalized elements in the FCM was equivalent to and at least was not inferior to that of the FEM.

Kurumatani and Terada (2005) extended the FCM to elasto-plasticity problems, in which the interface elements (or mortar elements) were introduced to impose the essential boundary conditions, displacement compatibility conditions on material interfaces. It involves modeling of evolving discontinuities in heterogeneous media. For example, Terada *et al.* (2007b) extended the FCM for progressive failure processes with cohesive zone fracture. It started from an interface debonding and evolves toward one of the constituents of heterogeneous solids and structures, in which constituents fail according to the maximum principal stress. In the process, debonding was judged by multipliers of interface elements. Kurumatani and Terada (2009) furthered the FCM to crack simulations for quasi-brittle heterogeneous solids by introducing “*multi-cover-layer*” modeling, in order to capture both weak and strong discontinuities.

2.3.4 Development of Eulerian NMM.

Su and Xie (2005) proposed a NMM with fixed mathematical covers to compute large displacements of structures. After each time step, the deformed boundaries intersected with the fixed mathematical covers to generate new physical covers and new manifold elements prior remapping of the model mechanical properties.

Several approaches were presented to compute initial stresses. Terada *et al.* (2007a) proposed an Eulerian FCM to perform Eulerian numerical analyses of hyperelastic bodies that undergo large deformation. In order to realize the implicit solution scheme for quasi-static equilibrium problems, they proposed a numerical algorithm

to use the Lagrangian and the Eulerian mathematical meshes simultaneously to repeatedly perform re-covering and mapping over generalized elements. Okazawa *et al.* (2009) developed an Eulerian FCM for solid dynamics, which incorporated the approximation strategy of the FCM into the existing Eulerian explicit FEM framework under kinematic and dynamic boundary conditions.

2.3.5 Other developments and applications of 2-D NMM

Li *et al.* (2005b) derived the governing equations of the NMM from weighted residual, which enriched the mathematical foundation of the NMM and extended it to solve problems such as heat conduction and potential flow, where the governing equations cannot be obtained from the minimum potential energy principle or other variational principles.

The NMM had been applied to simulate various problems, such as saturated/unsaturated unsteady groundwater flow analysis [Ohnishi *et al.* (1999)], rock masses containing joints of two different scales [Lin *et al.* (1999)], data compression [Fang *et al.* (2005)], dynamic non-linear analysis of saturated porous media [Zhang and Zhou (2006)], the shear response of heterogeneous rock joints [Ma *et al.* (2007a)], dynamic friction mechanism of blocky rock system [Ma *et al.* (2007b)], fluid-solid interaction analysis [Su and Huang (2007)], plane micropolar elasticity study [Zhao *et al.* (2009)].

NMM was able to deal with the well-known example of multiple discrete blocks well. For example in [Ma *et al.* (2010)], it present a toppling run process in a typical dominos' problem and mineral separation process using the vibrating screen with a set of coal blocks, a vibrating screen and a container (shown in Fig.2-3), which were numerically modeled by the NMM and the results are consistent with the experimentally observed phenomenon.

Figure 2- 3 Mineral separation process with the vibrating screen modeled by the NMM [Ma *et al.* (2010)]

2.4 Development of 3-D Numerical Methods in Rock Engineering

Up till now, there are very few studies performed on the 3-D NMM. Only few literatures found focused on the concept extension and equation derivation, however, they seemed lack convictive application examples to complete their arguments. The main difficulty appeared in the preprocessing tools and development of a contact algorithm that is suitable for the 3-D NMM. These two technical difficulties had to be solved before making any step forward to the 3-D NMM.

This section will systematically review the 3D versions of some mainstreams methods currently used in rock engineering. This section mainly focuses on the review of recent development of discrete element methods, including 3-D DDA, 3-D NMM and 3-D DEM, and PFC 3-D.

A more complete classification and summary on contact algorithm for these methods will be presented in Chapter 4.

2.4.1 Current development of 3-D DDA

Researchers had been working mainly on its basic theory development and simulation to its contact algorithm in 3-D DDA. Shi (2002) (2005) published two articles on basic theory of 3-D discontinuous deformation, the joints mesh generation, block cutting and block searching problem in 3-D DDA. Yeung *et al.* (2003) combined a wedge model with block theory and 3-D DDA to test the wedge structure stability, which demonstrated the efficiency and accuracy of the proposed 3-D DDA. Zhao (2000) develops 3-D DDA based on spherical particle element to calculate the spherical particle materials.

Jiang (2000) derived some of the basic formula of 3-D DDA; Liu (2001) has studied the basic theory of 3-D DDA and derived its corresponding formula. At the same time, he has also discussed the coupling between 3-D DDA and FEM. Moosavi *et al.* (2005) utilized theoretical analysis to verify the results from the dynamic version of 3-D DDA. Wang (2007) had preliminarily calibrated contact searching algorithm among blocky rock masses.

2.4.2 Current development of 3-D NMM

Lin *et al.* (2005) developed the formulations of 3-D NMM with high-order cover functions and proposed a fast simplex integration method based on special matrix operations. Similar to other partition-of-unity based methods, the NMM shape functions were linear dependent and thus the system equations were ill-conditioned when both weight functions and cover functions were chosen as polynomial

functions. However, the linear dependence problem had not been considered in their studies.

Terada and Kurumatani (2005) introduced an integrated procedure for three-dimensional structural analysis utilizing the FCM. They provided the formulations of the FCM with interface elements for the static equilibrium of a structure. They also suggested detailed procedure of the 3-D finite cover modeling, including the geometry modeling with 3-D CAD and the identification of the geometry covered by a regular patterned unit of mathematical covers for numerical integration. Cheng and Zhang (2008) proposed the 3-D NMM on tetrahedron and hexahedron elements and derived the basic matrices of corresponding equilibrium equations based on the minimum potential energy principle.

He and Ma (2010) also proposed a 3-D NMM based on tetrahedron elements. Generation of mathematical covers, formulation of discrete equations, generating discrete blocks from a given fracture pattern were discussed in details.

2.4.3 Current development of 3-D DEM

Cundall (1971) introduced the Discrete/Distinct Element Method in 1971. It was regarded as a suitable numerical method for jointed blocks, which was originally designed to simulate rock slope failure process. This purpose was in line with the DDA and NMM in the aspect of practical application. It became one of recommended methods in this field recently.

It has gained a lot of valuable fruits in 2-D development of DEM, but being of little interest in this thesis. Here, only its 3-D development is shortly reviewed. In 1988, Cundall (1988) and Hart *et al.* (1988) proposed the 3-D Rigid Discrete Element Method to analyze rock mechanics with detailed illustration including common plane contact searching algorithm, basic kinematics and kinetics equations for this method. Each individual block in the DEM had modeled as a rigid body, which could only translate and rotate in a small range.

Cundall and Lemos (1990) utilized continuous yielding model for structure interface to simulate the interface non-linear behavior during loading/unloading process; Jiao *et al.* (1999) utilized the 3-D rigid discrete element method to check the groundwater influence and bolt stabilization to blocky system. He also gave his algorithm and formulations correspondingly; As actual 3-D block motion involves in large rotation, Kremmer and Favier (2000) studied the specific problem of finite rotation in space. They indicated that the block rotation equation should be calculated through transferring to block inertia under local coordinate system, such that block rotation equation could be simplified sufficiently; Munjiza *et al.* (2003) derived a direct integration scheme based on the 4th-order Runge-Kutta method, which were used to study the rotation problem for irregular rigid blocks; Li and Wang (2004) further studied into the parameter settings in the 3-D discrete element method and discussed about the setting rules among rigidness, time-step and damping in the 3-D DEM code. Zhang (2004) compiled “3MDEM” code based on 3-D DEM theory and undertook the analysis to a “Arch Dam-Foundation stability”.

Similar to 2-D discrete element method, Cundall further implemented 3-D deformable discrete element method by building up the tetrahedral sub-element system inside each 3-D block. Based on this, the software 3DEC [Itasca Consulting Group Inc. (2003)] finally commercialized. Psycharis *et al.* (2003) employed 3DEC to understand the dynamic behavior of a historic building, and design reinforcement measure to strengthen the dynamic safety of the structure.

2.4.4 Current development of PFC 3-D

There was another branch of DEM, called the granular discrete element method. Cundall and Stack (1978) (1979a) (1979b) developed this method especially suitable for soil mechanics and subsequently converted it to a 2-D program “Ball” and a 3-D program “Trunbal”. These two programs were further improved by the efforts of Itasca company, which generated the two commercial software (PFC^{2D} [Itasca Consulting Group Inc. (2004)] and PFC^{3D} [Itasca Consulting Group Inc. (2005)]) based on the discrete sphere element. It was a simplification of 3-D DEM and it was actually a compromise to the difficulties of contact algorithm to a general 3-D block

system. In essence, its fundamental idea was consistent with the rigid DEM. The only difference between the 3-D rigid DEM and the PFC^{3D} was the object shapes. It was 3-D concave blocks in the rigid DEM, while it is represented as a spheres in the PFC^{3D}. Since basic object was a sphere in the PFC^{3D}, it became much easier for contact relationship searching and treatment. With the rapid development of computer technology, the ability to deal with a large number of spheres in numerical simulations had become possible.

Unexpectedly, this simplification step extended DEM into another main stream computational field, namely, Computational Fluid Dynamics (CFD). It had achieved splendid performance in simulating fluid and viscoelastic large deformation body through interactively combining granular DEM and Smoothed-Particle Hydrodynamics (SPH) under similar framework [Hodjigeorgiou *et al.* (2009)] [Venugopal and Rajamani (2001)] [Thiago Costa (2010)].

Before 2004, the small sphere in PFC^{3D} was normally shown as independent and contactable only in spherical surface in applications, presenting as “sand” status. Potynody and Cundall (2004) extended the existent PEC^{3D} and build a “bonded” connection among small spheres. A “Bonded-Particle Model (BPM)” for a piece of rock mass was represented by a dense packing of non-uniform-sized spherical particles that were bonded together at their contact points. Damage was represented explicitly as broken bonds, which formed and coalesced into macroscopic fractures when load was applied. Through reasonably designed broken criteria for those bonds in micro-level, the BPM reproduced many macro-features of rock mass behavior. This could be seen as a technical overfly of the PFC.

In general, the PFC particle was not associated with an elementary constituent of the physical material, because the size of PFC particle and micro-level entities of physical material were not in the same order of magnitude. It was also often difficult to choose appropriate input parameters that to make the behavior of the virtual material similar to that of the physical material. In order to calibrate the PFC^{3D} code for application purpose, Oreskes et al. (1994), Mishra and Murty (2001), Di Renzo

and Di Maio (2004), Tripodi et al. (1992), and Landry et al. (2006) had done series of parameter studies for PFC modeling to warrant the predications of PFC code agreeing with observation and measured data on the real physical laboratory and field-scale events.

2.5 Comparison with other Numerical Methods

2.5.1 Relation with the FEM

In the FEM, the problem domain was divided into a collection of elements with smaller sizes and standard shapes having fixed number of nodes at vertices and/or on the sides. Trial functions, usually polynomial, were used to approximate the unknown field at the element level with nodes serving as interpolation points for unknown variables and generate local algebraic equations. The elemental equations were then assembled into a global system of equations whose solution then produced unknowns at the nodes, after imposing the properly defined initial and boundary conditions.

On the other hand, the approximation in the NMM is established based on physical covers attached with independent cover functions containing unknowns to be determined. As mentioned in the introduction section of this chapter, FEM could be seen as one special case of NMM with general understanding to NMM.

If the cover function of each physical cover is chosen as a constant (equivalent to the unknowns of each node in the FEM), the weight functions are chosen as the nodal shape functions in the FEM, and physical features including internal discontinuities (e.g. cracks and material interfaces) and external boundaries do not intersect the manifold elements, the NMM will exactly reduce to the standard FEM. In other words, the FEM is a special case of the NMM.

2.5.2 Relation with the DDA

The Discontinuous Deformation Analysis (DDA) was originally developed to solve problems in which a rock mass is delimited into blocks by joints. Thus, in addition to the contact detection and frictional contact modeling, the DDA also presents algorithm to form blocks from joints. Since rock blocks generally undergo small deformation, the DDA simulates each discrete body as a simple deformable block with only six degrees of freedom (DOFs) in a two-dimensional setting. The NMM is developed based on the DDA. It preserves all the characteristics of the discrete element modeling such as the kinematics constraints, contact detection and modeling from the DDA. However, the NMM employs a number of covers to raise the DOFs to describe the displacement field and stress field in each block more accurately. Hence, the NMM could be said to be the DDA with each block discretized into finite covers. In other words, if one discrete block is one manifold element with linear displacement field, the NMM will be exactly the DDA.

Some researches try to take advantage of these two methods, through a coupled discontinuous deformation analysis and numerical manifold method (NMM-DDA) (e.g., [Miki *et al.* (2009)]).

2.5.3 Relation with the DEM

The Distinct Element Method (DEM) is an explicit version of discrete element method, while the DDA is an implicit version of the discrete element method. Compared with the distinct element method (DEM), the NMM and the DDA have the following four basic advantages [Jing (2003)]:

- (1) The equilibrium condition is automatically satisfied for quasi-static problems without using excessive iteration cycles;
- (2) The length of the time step can be larger without introducing numerical instability;
- (3) Closed-form integrations can be performed without the need of Gaussian quadrature techniques;
- (4) It is easy to convert an existing FEM code into DDA/NMM code and to include

many mature FEM techniques without inheriting the limitations of the FEM, such as small deformation, continuous material geometry, and reduced efficiency for dynamic analysis. However, matrix equations are produced and need to be solved in the NMM/DDA. The DEM used the explicit solver.

2.6 Significance of 3-D NMM

2.6.1 Purpose of 3-D NMM development

Undeniable, 2-D numerical method has already been able to provide reasonable solution to some practical engineering problems. Most of them are modeling approaches limited to plane strain, plane stress, and sometimes even symmetric to an axis, which are far away from the realistic 3-D world. 2-D algorithm analysis is suitable to compare with simple experimental results, hence to verify the fundamental of the algorithms. However, 2-D is only a sub-sample to the real case of 3-D in practice, and it is important to apply 3-D techniques to find solutions to engineering problems.

For example in the case of the crack propagation in a dam, crack here is no longer presented as “2-D curved line”, but as “3-D curved surface”, because of complex real boundary conditions. In such case, 2-D tools are not sufficient.

Besides, rock engineering problems, such as rock slope and tunnel stability analyses are all in 3-D domain. With the introduction of rock faults and joint planes, the geological condition of a rock mass can only be represented by a 3-D model.

In summary, it is of significance to further develop NMM to 3-D version for more practical applications.

2.6.2 Preparation for 3-D NMM

The development from 2-D NMM to 3-D NMM is not the simple one more

dimensional expansion, but a step to overcome the limitations to the 2-D analysis that required in practical engineering.

Some preliminary work has been done on the 3-D NMM in the literature, but the previous works did not have a unified and consistent acknowledgement to the NMM concepts and terminology. The first task in the extension is to clarify the concepts to build a unified 3-D NMM platform.

The second task is to derive its basic equations for a continuous version, and to do proper verifications.

Further studies on the 3-D NMM, especially generation of discrete blocks from realistic fracture patterns, 3-D contact detection and modeling are essential to simulate the real engineering problems in a reasonable manner.

2.7 Summary

Since the origination of NMM, it has attracted many researchers to devote their effort. Especially, it has shown sound development momentum in recent years. In practice, this method has demonstrated its versatile ability in simulating multi-field physics, crack propagation, blocky system and so on. These applications have constrained themselves within two dimension.

The difficulties to 3-D are mainly on the bellowing three aspects:

- As mentioned, it lacks unified understanding to NMM, especially for 3-D situation. Different from 2-D, the geometric configuration of 3-D manifold pattern is not intuitive.
- It also lacks proper modeling tools. Current modeling tools could not fulfill the interaction between the physical domain and mathematic domain. No pre-process tool is available at hand.
- Referable 3-D contact algorithm is also not available.

This thesis attempts to overcome these difficulties.

Chapter 3 Theory of the 3-D Numerical Manifold Method

3.1 Understanding of Numerical Manifold Method

Since the introduction of NMM, its proposed concepts and perspectives are distinct from the definitions of traditional numerical method. It makes relatively hard to understand at the beginning, which also inhibits its developments at a certain level. Several versions of NMM's nomenclature could be found in literatures (refer to Chapter 2), some of them were only based on limited understanding, although most have been conceived as a specific self-system. Under these conditions, they seem to have satisfied the requirement of NMM development, but on the other hand, it is impossible to establish researchers a unique platform to discuss further. It is necessary to re-clarify and re-interpret some relevant concepts with indispensable complementary, before we further go forward development towards 3-D extension.

This is the main purpose of the chapter. Firstly for convenience of understanding, the nomenclature has been re-explained. 2-D cases are briefly illustrated in *Section 3.2*. Further discussion on 3-D relevance is given in *Section 3.3* and *Section 3.4*.

3.1.1 Nomenclature

“Manifold” – means “multiple purposes” or “multiple functions”. The term comes from the topological manifold and differential manifold, which is the main subject of differential geometry, algebraic topology, differential topology and modern algebra of mathematics.

“Numerical Manifold Method” -- NMM was firstly proposed by Shi in 1991 and it is one of the newest numerical methods in recent years. It merges the “FEM” and “DDA” nicely and thus it reconciles the “*Continuum-based methods*” with “*Discontinuum-based methods*”. The discretization involves two domains: “*Physical domain*” is used to describe geometry property and “*Mathematical domain*” is used

to build global displacement function. The mathematical treatment to these two domains is relatively independent, but these two domains interact with each other according to special integration and interpolation scheme. Because its geometrical model can be prepared independently without considering the meshing issue, NMM becomes very suitable for the numerical simulations of crushing-like material (rock mass) or relevant complex engineering application.

“Physical domain” -- other term for “Modeling domain”, as one of the NMM domains, it consists of block systems which includes all physical information, such as the boundaries of the material volume, joints, and the interfaces of different material zones etc. “Physical domain” in the NMM procedure is defined as two stages if the crack initiation and propagation issue are not considered: 1)The first stage -- it defines “Target physical objects”(TPOs) which includes geometrical and mechanical information; 2)The second stage -- TPOs are rebuilt by “initial mathematical mesh” in mathematical domain, then bring in the “Manifold element (ME)” system with mechanical conditions back; These two stages interact with other two stages in the “Mathematical domain”.

“Mathematical domain” -- is the other domain in NMM. In the mathematical domain, it defines the spatial approximation of unknown functions, which is used to build the global equilibrium equation. Similarly to “Physical domain”, in the NMM definition, mathematical domain undergoes two stages without crack simulation function: 1) The first stage -- according to accuracy requirement, the “Initial mathematical mesh” is chosen by users; 2) The second stage -- due to combination of the geometry and physical information, “Initial mathematical mesh” is split into series of “Manifold covers (MC)”. Adjacent “MCs” overlap, thus the “Manifold pattern (MP)” system is established.

“Target physical objects” -- “TPOs” are created according to the setting of the considered physical problem. The block is one of fundamental entities for analysis. It also represents loading conditions, discontinuities information (crack, joint and fault), initial conditions and temperature condition, etc. Each block is an independent entity

that may be isolated from other blocks or may contact with others via contact forces. The boundary of each block has been defined as a “*Loop (2D) or Contact surface (3D)*”, which is employed for contact kinematic analysis. Another term for “*TPOs*” is “physical model” which will be rebuilt by “*Initial mathematical mesh*” to detached “*Manifold element (ME)*” further.

“Initial mathematical mesh” -- the initial mesh of mathematical domain is chosen by the users according to the size of problem, solution accuracy requirement, and the physical property zoning. It is applied to split the “*TPOs*” system into “*Manifold Element (ME)*” system in the stage 2 of physical domain. The basic component of mesh is “*Manifold pattern (MP)*”.

“Mathematical cover (MC)” -- the essential component in mathematical domain. Each MC has separate “*Cover function*” and the static/dynamic response of the MC has been reflected on its nominal centroid---“*Manifold star*”. These “*MCs*” overlap and the common part constitutes as a “*Manifold pattern(MP)*”. “*Manifold stars*” are connected by “weight function” in a mathematical sense to describe the “*MP*” displacement function. As a result, the global displacement function is generated by the weighted average of local independent cover functions on the common part of corresponding *MCs*.

“Physical cover (PC)” -- generated as an intermediate product in the physical domain: stage 2. In fact, it is the pre-stage of “*Manifold element*”. Each *PC* will have one “*Manifold cover*” correspondingly. The *PCs* are overlapping to each other to form *ME*.

“Manifold star” -- normally in the nominal centroid of “*Manifold cover*” and is the node of “*Manifold pattern*”. It is to represent the corresponding “*Manifold cover*” completely. The number of variables on each star is determined by the order of the “*Cover function*”. For example, under the first order: the variables u_0, v_0 the displacements along the X and Y axes respectively; r_0 the rigid-body rotation in radian around the point (x_0, y_0) ; $\varepsilon_x, \varepsilon_y, \gamma_{xy}$ strains of the block. (which are same

to 2-D DDA variables)

“Manifold element (ME)” -- the entity product in the second stage of the “Physical domain”. It is created by “cutting” a “TPO” with “Initial mathematical mesh”. It also includes the geometrical information which is mapped back to the corresponding “Manifold pattern”. In a sense, it is equivalent to the integration field of element in FEM.

“Manifold pattern (MP)” -- corresponding with “Manifold element”, the basic cell of manifold mesh and the entity product in the second stage of “Mathematical domain”. MEs with geometrical and mechanical information re-mapped back “Mathematical domain” to discretized the original mathematical mesh, and then the “Manifold pattern” system has been generated by “Manifold covers” overlapping. “Manifold pattern” system is the foundation of numerical calculations. In some sense, it is equivalent to the interpolation field of element in FEM.

“Loop/Contact surface” -- used to represent the periphery or internal boundaries (i.e., holes within the model) of the NMM model (physical entities). It is the prerequisite of “contact algorithm”.

“Cover function” -- for the manifold method, the “cover functions” are independently defined on every individual MC. It can be a constant, linear, high order polynomials or locally defined functional series. Original NMM uses a constant as the “Cover function”, which means the stress/strain keeps same within a manifold cover. All the interacting response of one “Manifold cover” is represented by the “Manifold star”.

“Weight function” -- is actually weighted average, which is to take a percentage from each cover function to form a global displacement function on the whole material volume. It is used to connect all the response of the “Manifold star”.

“Simplex integration” – a more efficient integration algebras scheme than “Gauss

integration” which is widely used in FEM codes. This scheme is specially designed for the complex polygon (2-D) and polyhedron (3-D). It transforms the integration process into polynomials calculation. The integration formula is represented by a polynomial using the coordinates of boundary vertices. The convergence and accuracy of numerical manifold method algorithms mainly rest upon the high-accurate simplex integrations on complex shapes, no matter it is a convex or concave shape.

“Discontinuity” -- A discontinuity is an existing geologic feature that separates a physical mass into distinct parts or partial connected bodies. Discontinuities, for example, include joints, faults and fractures and other discontinuous features in a rock mass.

3.1.2 Finite Cover System in 2-D

The finite cover system is defined by Shi (1991) as a combination of the mathematical domain and physical domain. The TPOs in physical domain includes the boundaries of the material volume, joints, and the interfaces of different material zones. The constantly changed underground water surfaces are also part of the physical domain. The TPOs represents material conditions which cannot be chosen artificially. The mathematical mesh defines the fine or rough approximation of unknown functions. It can be a mesh of some regular manifold patterns (*MPs*), or a combination of some arbitrary figures. This mesh is chosen by the user according to the problem geometry, solution accuracy requirement, and the physical property zoning.

The mathematical mesh is used to build mathematical covers that present small regions of the whole field and can be any of shape and size. They can overlap each other and do not need to coincide with the physical cover as long as they are large enough to cover the physical blocks.

With reference to the schematic plot in Fig. 3-1, the definitions of three basic components in the NMM, namely the mathematical cover, the physical cover and the manifold element, are presented. All the physical features such as the internal discontinuities (e.g. cracks, joints, material interfaces, holes, etc.) and the external

geometries on which boundary conditions are prescribed in a physical domain (Fig. 3-1(a)), whereas a domain which is independent but completely cover the physical domain is called the mathematical domain (Fig. 3-1(b)).

The mathematical domain can be constructed as a union of a finite number of small patches, which can overlap each other either partially or totally. Each patch is called a mathematical cover. The mathematical covers are consecutively denoted as M_I ($I=1 \sim n_M$). See the example in Fig. 3-1, there are two mathematical covers in total, i.e. M_1 and M_2 (Fig. 3-1(c)).

The physical covers are the intersection of mathematical covers and the physical domain. If completely cut by the physical features, a mathematical cover, such as M_I , will be partitioned into several physical covers, denoted as P_I^j ($j=1 \sim m_I$) ($P_I^j \subset \Omega$), the indices indicating that it is the j th physical cover generated from the mathematical cover M_I , where m_I is the total number of physical covers generated from M_I . Therefore, physical covers are in fact the subdivision of mathematical covers by the physical domain. See the example in Fig. 3-1, mathematical cover M_1 is completely cut into three isolated regions by the physical features and two of them are within the problem domain, so two physical covers, i.e. P_1^1 and P_1^2 are formed (Fig. 3-1(d)). Similarly, mathematical cover M_2 also forms two physical covers, i.e. P_2^1 and P_2^2 (Fig. 3-1(d)).

Here, each physical cover has two indices, i.e. I and j . To simplify an implementation, we reallocate a single index to each physical cover, expressed as $P_i \triangleq P_I^j$ with i calculated by

$$i(I, j) = \sum_{l=1}^{I-1} m_l + j \quad (3-1)$$

Using the algorithm given in Eq. (3-1), each of the four physical covers in Fig. 3-1(d) is reallocated a single index, i.e. $P_1 \triangleq P_1^1$, $P_2 \triangleq P_1^2$, $P_3 \triangleq P_2^1$, and $P_4 \triangleq P_2^2$, in sequence of the two mathematical covers.

The manifold element is defined as the common region shared by several physical covers. The four physical covers in Fig. 3-1(d) finally form five manifold elements, i.e. $E(P_1^1, P_2^1)$, $E(P_2^1)$, $E(P_1^2)$, $E(P_1^2, P_2^2)$, and $E(P_2^2)$, shown in Fig. 3-1(e).

Figure 3- 1 NMM components

For NMM, the cover displacement functions are independently defined on individual physical covers. Local displacement functions can be connected together to form a global displacement function on the whole material volume by weight functions. Details will be discussed in the following section.

3.1.3 Procedure of NMM

After clarifying the nomenclature of NMM, the procedure of NMM is illustrated in Fig. 3-2.

Figure 3- 2 General procedure of NMM

More clearly, Fig. 3-3 illustrates the interaction process of stage 1 and stage 2 in Fig. 3-2. A manifold pattern system and a discrete material domain (MEs) are generated.

Figure 3- 3 Illustration of NMM procedure

Therein the material attributes on the physical domain, including geometric condition and properties of the crack curve (fault, joints, etc.) are all loaded on the mathematical system. All these information are mapped into every relevant manifold

pattern. Therefore, the pre-process of NMM can be simply understood as two simultaneous process, as in Fig. 3-2 and 3-3.

In the stage of mathematical domain, these “*Manifold covers*” overlap and the common part constitutes as “*Manifold pattern (MP)*”. Fig. 3-4 gives the illustration for “*Manifold pattern*” generating procedure.

Figure 3- 4 Illustration of manifold pattern construction

3.2 Geometric Configuration of 3-D Mathematical Cover

3.2.1 Fundamentals of the 3-D NMM

Similarly, the NMM is based on three important concepts: mathematical cover (*MC*), physical cover (*PC*) and manifold element (*ME*). Inherited from 2-D version, one significant advantage is that arbitrary geometric shapes (e.g. polyhedron in 3-D) can be the basic *MC* of the mathematical domain. Each different shaped *MC* has its own mathematical description inside. These polyhedrons are overlapping in space, and the only requirement is to guarantee that those *MCs* can fulfill the whole space

completely.

Physical domain is used to represent the portrait of target physical objects (*TPO*) in a general sense. *TPOs* include all the physical features such as internal discontinuities (e.g. joints, material interfaces and cracks) and external geometries on which boundary conditions are prescribed.

Then, *MCs* intersect and paste seamlessly to re-divide the *TPOs*, during which *PCs* are generated. Further, elements (*MEs*) in the NMM framework can be considered as the common part of overlapping *PCs*. In this way, the NMM can be easily understood and extended to the three dimensional case.

Fig. 3-5 (a) illustrates the three basic concepts of the NMM in a 3-D view. There are two *MCs* in total, a sphere *MC1* and a hexahedron *MC2*. A pyramid represents the physical domain in this instance. A discontinuity inserts into the pyramid body. Interactions with the physical domain, four *PCs*, as shown in Fig. 3-5 (c), are generated. These *PCs* finally form five manifold elements as shown in Fig. 3-5 (e).

(a) Physical domain and mathematical covers

(b) Pyramid with discontinuity (TPOs) in physical domain

(c) Physical Covers (PCs) with Manifold Covers(MCs)

(d) Representation of Manifold Pattern (MP)

(e) Manifold Elements (MEs)

Figure 3- 5 Illustration of finite cover system in the 3-D NMM

On a MC denoted as M_I , a weight function is defined, which satisfies

$$\begin{aligned} \varphi_I(\mathbf{x}) &\in C^0(M_I) \\ \varphi_I(\mathbf{x}) &= 0, \mathbf{x} \notin M_I \end{aligned} \tag{3-2a}$$

with

$$\sum_{\substack{I \\ \text{if } \mathbf{x} \in M_I}} \varphi_I(\mathbf{x}) = 1 \quad (3-2b)$$

Eq. (3-2a) indicates that the weight function has non-zero value only on its corresponding MC, but zero otherwise, whereas Eq. (3-2b) is just the partition of unity property to assure a conforming approximation. The weight function $\varphi_I(\mathbf{x})$ associated with M_I will be accordingly transferred to any of the PCs in M_I . With these concepts, the interpolation approximation can be constructed. First, a cover function $\mathbf{u}_i(\mathbf{x})$ is defined individually as a local approximation on the PC (P_i) for the displacement field, which can be a constant, linear, high order polynomials or other functions with unknowns (also termed DOFs) to be determined. Then, the global displacement $\mathbf{u}(\mathbf{x})$ on a certain ME (e) is approximated to be

$$\mathbf{u}^h(\mathbf{x}) = \sum_{\substack{i \\ \text{if } e \subset P_i}} \varphi_i(\mathbf{x}) \cdot \mathbf{u}_i(\mathbf{x}) \quad (3-3)$$

3.2.2 Manifold Patterns (MP) in 3-D

A geometrical pattern is a type of theme of the recurring objects, sometimes referred to as elements of a set, to generate space or parts of an object [Nooshin *et al.* (1997)]. The first step to extend the NMM to 3-D is to select a basic MP to fill the entire space, which is the same as required in the 2-D NMM. In most cases, MP geometry is based on platonic solids (see Fig. 3-6). Except the first three basic polyhedrons, other polyhedrons given in Fig. 3-6 are seldom used to form up the space in other fields. The NMM creates a possible platform to extend the applications of different platonic solids. However, for computational convenience, simple and regular manifold patterns are suggested. The equilateral triangle and rectangle are excellent choice for the 2-D NMM, as their high identification and uniformity. Unfortunately, regular tetrahedron is not able to fill the entire 3-D space. Hexahedron seems to be the best choice geometrically because it has relatively a simple topological structure and equally sized hexahedrons can fill the space completely. The generalized octahedron is another wise choice. It is worth noting that MCs can be any shapes in Fig. 3-6 and even some other possible irregular solids, if proper weight functions are implemented.

Tetrahedron	Hexahedron Or Cube	Octahedron	Dodecahedron	Icosahedron

Figure 3- 6 Five convex regular polyhedral (Platonic solids) [Atiyah *et al.* (2003)]

In addition, the NMM is based on the incremental method, suitable for large deformation and large displacement analysis. The simplex integration method can gain the accurate integration for any arbitrary shape [Li *et al.* (2005a)]. If the interpolation function in a global Cartesian system for any arbitrary shape is able to be built, the governing equation with the NMM incremental step is viable. In other words, the hexahedron/octahedron is not the best MC choice in the 3-D NMM. Returning back to the integration accuracy, the general tetrahedron can be considered as an ideal unit cell to form the manifold element in 3-D.

Similar to the 2-D NMM, one background node is a star of one MC, which can be any geometry significance points of the cover (e.g. center of gravity). By considering a tetrahedron manifold element, four MCs are required to overlap to create one manifold element. On the other hand, it is well known that any shaped convex polygon can be decomposed into several triangles. Similarly, any convex polyhedron in the 3-D space can also be decomposed into several tetrahedrons. The decomposition plans are innumerable (e.g. choosing different block size). The division plan determines the shape of the MCs. It can be seen in Fig. 3-7 that a hexahedron can be decomposed into 6 Tetrahedrons (Fig. 3-7 (a)), 5 Tetrahedrons (Fig. 3-7 (b) and 3-7 (c)) or 24 Tetrahedrons (Fig. 3-7 (d)).

Figure 3- 7 Decomposition plan from hexahedron to tetrahedron

As a matter of fact, it is not the only kind of 6 Tetrahedrons plan (as shown in Fig.3-7(a)). The advantage is that the cube has the property of center-symmetry, and it can build up the entire 3D space without rotation. The two schemes of 5 Tetra-plan (Fig. 3-7(b) and 3-7(c)) are usually coupled and applied as a mixed-discretization (M-D) zone [Itasca Consulting Group, Inc (2003)]. As these two kinds of mesh are symmetric to each other, they can overlap at the same position to decrease “the strain instability induced by choosing mesh direction”. One cubic domain and cover is generated by two “anisotropy” mathematical covers, which is another extension of the manifold concept. When using the centers of cube and 6 faces as auxiliary points, a cube can be decomposed into 24 different tetrahedrons. The mathematical mesh has

extremely symmetrical property by this 24-tetrahedron decomposition scheme.

3.2.3 MC and its formulation

The corresponding MC belongs to the field of geometrical topology. When the decomposition in Fig. 3-7(b) is applied, their geometry structure is shown in Fig.3-8[Bronstein *et al.* (2007)]. Similarly, other decompositions can also be found to gain a cover structure.

Figure 3- 8 Configuration of MC in 3-D view

a) Weight Function:

Here, four overlapping MCs (one type-I and three type-II covers) have a common area E (complete tetrahedron Manifold Pattern), the displacement functions $u(x, y, z)$, $v(x, y, z)$ and $w(x, y, z)$ in this common area E can be obtained by taking the weighted average of the four cover functions, which satisfy Eq. (3-2b). In a tetrahedral common area (tetrahedron cornered by four stars $i j k l$), there are the four weight functions of the four covers:

$$\begin{Bmatrix} \varphi_i(x, y, z) \\ \varphi_j(x, y, z) \\ \varphi_k(x, y, z) \\ \varphi_l(x, y, z) \end{Bmatrix} = \begin{bmatrix} f_{11} & f_{12} & f_{13} & f_{14} \\ f_{21} & f_{22} & f_{23} & f_{24} \\ f_{31} & f_{32} & f_{33} & f_{34} \\ f_{41} & f_{42} & f_{43} & f_{44} \end{bmatrix} \begin{Bmatrix} 1 \\ x \\ y \\ z \end{Bmatrix} = \mathbf{W}_a \mathbf{l}(\mathbf{x}, \mathbf{y}, \mathbf{z}), \quad a = i, j, k, l \quad (3-4)$$

where

$$W_a = \begin{bmatrix} f_{11} & f_{12} & f_{13} & f_{14} \\ f_{21} & f_{22} & f_{23} & f_{24} \\ f_{31} & f_{32} & f_{33} & f_{34} \\ f_{41} & f_{42} & f_{43} & f_{44} \end{bmatrix} = \frac{1}{\Delta} \begin{bmatrix} A_{11} & -A_{12} & A_{13} & -A_{14} \\ -A_{21} & A_{22} & -A_{23} & A_{24} \\ A_{31} & -A_{32} & A_{33} & -A_{34} \\ -A_{41} & A_{42} & -A_{43} & A_{44} \end{bmatrix},$$

$$\Delta = \begin{vmatrix} 1 & x_i & y_i & z_i \\ 1 & x_j & y_j & z_j \\ 1 & x_k & y_k & z_k \\ 1 & x_l & y_l & z_l \end{vmatrix}, \quad l(x, y, z) = \begin{bmatrix} 1 \\ x \\ y \\ z \end{bmatrix}$$

A_{ij} is a_{ij} 's algebraic complement of Δ .

b) Cover Function:

The manifold cover displacement functions can be constant, linear, and even higher order polynomials or locally defined series. The cover function is expressed as

$$U_i = \sum_{j=1}^m \begin{bmatrix} f_{ij}(x, y, z) \\ f_{ij}(x, y, z) \\ f_{ij}(x, y, z) \end{bmatrix} \begin{Bmatrix} d_{i,3j-2} \\ d_{i,3j-1} \\ d_{i,3j} \end{Bmatrix} = F_i d_i \quad (3-5)$$

Normally, there are $3m$ unknowns to describe the i th manifold cover. The value of m depends on the order of cover function chosen.

Then the displacement for the common area is written as:

$$U = \sum_{i=1}^q \varphi_i(x, y, z) U_i \quad (3-6)$$

where q is the sum of the mathematical covers for an element(ME).

By substituting Eq. (3-5) into Eq. (3-6), the following displacement function is obtained:

$$U = \varphi F d = N d \quad (3-7)$$

c) Constant Cover Function

A constant cover function can be written as

$$U_i = \begin{Bmatrix} u(x, y, z) \\ v(x, y, z) \\ w(x, y, z) \end{Bmatrix} = \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix} \begin{Bmatrix} d_{i1} \\ d_{i2} \\ d_{i3} \end{Bmatrix} = F_i d_i \quad (3-8)$$

The $m=1$ for constant cover function and then,

$$\mathbf{N}_i = \begin{bmatrix} \varphi_i & & \\ & \varphi_i & \\ & & \varphi_i \end{bmatrix} \quad (3-9)$$

It can be seen that the constant cover displacement functions generate linear displacement variation in the complete element, which are the same as that of a tetrahedron element in the FEM.

d) Linear Cover Function

A linear cover displacement function can be written as

$$\mathbf{U}_i = \begin{Bmatrix} u(x, y, z) \\ v(x, y, z) \\ w(x, y, z) \end{Bmatrix} = \begin{bmatrix} 1 & x & y & z & & \\ & 1 & x & y & z & \\ & & 1 & x & y & z \end{bmatrix} \begin{Bmatrix} d_{i1} \\ d_{i2} \\ d_{i3} \\ d_{i4} \\ d_{i5} \\ d_{i6} \\ d_{i7} \\ d_{i8} \\ d_{i9} \\ d_{i10} \\ d_{i11} \\ d_{i12} \end{Bmatrix} = \mathbf{F} \mathbf{d}_i \quad (3-10)$$

$m=4$ for linear cover function and then,

$$\mathbf{N}_i = \begin{bmatrix} \varphi_i & 0 & 0 \\ 0 & \varphi_i & 0 \\ 0 & 0 & \varphi_i \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 & x & 0 & 0 & y & 0 & 0 & z & 0 & 0 \\ 0 & 1 & 0 & 0 & x & 0 & 0 & y & 0 & 0 & z & 0 \\ 0 & 0 & 1 & 0 & 0 & x & 0 & 0 & y & 0 & 0 & z \end{bmatrix}, \quad i=1 \sim q \quad (3-11)$$

e) Second-order Cover Function

The second-order cover displacement function can be written as

$$\begin{aligned}
\mathbf{U}_i &= \begin{Bmatrix} u(x, y, z) \\ v(x, y, z) \\ w(x, y, z) \end{Bmatrix} \\
&= \begin{bmatrix} 1 \cdot \mathbf{E} & x \cdot \mathbf{E} & y \cdot \mathbf{E} & z \cdot \mathbf{E} & x^2 \cdot \mathbf{E} & y^2 \cdot \mathbf{E} & z^2 \cdot \mathbf{E} & xy \cdot \mathbf{E} & yz \cdot \mathbf{E} & xz \cdot \mathbf{E} \end{bmatrix} \begin{Bmatrix} d_{i1} \\ \vdots \\ d_{i30} \end{Bmatrix} = \mathbf{F} \mathbf{d}_i
\end{aligned} \tag{3-12}$$

$m=10$ for second-order cover function and then,

$$\mathbf{N}_i = \begin{bmatrix} \varphi_i & 0 & 0 \\ 0 & \varphi_i & 0 \\ 0 & 0 & \varphi_i \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 & x & 0 & 0 & y & 0 & 0 & z & 0 & 0 & & & xz & 0 & 0 \\ 0 & 1 & 0 & 0 & x & 0 & 0 & y & 0 & 0 & z & 0 & \cdots & & 0 & xz & 0 \\ 0 & 0 & 1 & 0 & 0 & x & 0 & 0 & y & 0 & 0 & z & & & 0 & 0 & xz \end{bmatrix}, \tag{3-13}$$

From the format of above formula, the NMM will exactly reduce to the standard FEM if the following conditions are satisfied [Terada *et al.* (2003)]:

- Cover functions of physical covers are constant (equivalent to the unknowns of the nodes in the FEM, Eq. (3-8)) and the weight functions are constructed based on the (bi-)linear shape functions of the FEM;
- Physical features including internal discontinuities such as cracks and material interfaces, and external boundaries do not intersect the manifold elements.

On another hand, if one discrete block is exactly one manifold element with a linear cover function Eq. (3-11), the NMM will become the DDA.

3.3 General Formulations of NMM approximation

3.3.1 Weak form of governing equations

The widely known principle of virtual work is used to derive the weak form of the governing equation. The virtual work done by external forces is equal to the virtual strain energy of the system, which leads to the corresponding weak form

$$\int_{\Omega} \delta \boldsymbol{\varepsilon}^T \boldsymbol{\sigma} dV = \int_{\Omega} \delta \mathbf{u}^T \mathbf{b} dV + \int_{\Gamma_t} \delta \mathbf{u}^T \bar{\mathbf{t}} d\Gamma - \int_{\Omega} \delta \mathbf{u}^T \rho \ddot{\mathbf{u}} dV \tag{3-14}$$

where $\boldsymbol{\varepsilon}$ is the strain tensor; $\boldsymbol{\sigma}$ is the stress tensor; $\boldsymbol{u}$ is the displacement vector; $\boldsymbol{b}$ is the body force per unit volume; $\bar{\boldsymbol{t}}$ is the traction prescribed on the corresponding boundary; ρ is the density; $\ddot{\boldsymbol{u}}$ is the acceleration vector.

An increment approach is often adopted in the dynamic analysis. The total-time is divided into a finite number of time steps. Variables such as displacement, velocity and acceleration are known at the beginning time t_n of the current step, and the increments of several variables during the current time step $t_n \sim t_{n+1}$ are as unknowns to be determined. Therefore, the incremental form of the principle of virtual work is required. Energy status at time t_n and t_{n+1} are both satisfied under Eq. (3-14). The increment form of the principle is obtained by subtracting two energy equations at time t_n and t_{n+1} , and ignoring the higher order terms.

$$\int_V \delta \Delta \boldsymbol{\varepsilon}^T \Delta \boldsymbol{\sigma} dV - \int_{\Omega} \delta \Delta \boldsymbol{u}^T \Delta \boldsymbol{b} dV - \int_{\Gamma_t} \delta \Delta \boldsymbol{u}^T \Delta \bar{\boldsymbol{t}} d\Gamma + \int_{\Omega} \delta \Delta \boldsymbol{u}^T \rho \Delta \ddot{\boldsymbol{u}} dV = 0 \quad (3-15)$$

3.3.2 NMM interpolations

In a manifold element, the NMM interpolation follows Eq. (3-7). The strain is expressed as

$$\boldsymbol{\varepsilon} = \boldsymbol{L} \boldsymbol{N} \boldsymbol{d} = \boldsymbol{B} \boldsymbol{d} \quad (3-16)$$

where $\boldsymbol{B} = \boldsymbol{L} \boldsymbol{N}$ is the strain matrix; $\boldsymbol{L}$ is the differential operator matrix.

The constitutive relation is

$$\boldsymbol{\sigma} = \boldsymbol{E} \boldsymbol{L} \boldsymbol{N} \boldsymbol{d} = \boldsymbol{S} \boldsymbol{d} \quad (3-17)$$

where $\boldsymbol{E}$ is the elastic matrix; $\boldsymbol{S} = \boldsymbol{E} \boldsymbol{L} \boldsymbol{N}$ is the stress matrix.

Eq. (3-7) can be rewritten in an incremental form

$$\Delta \boldsymbol{u} = \boldsymbol{N} \Delta \boldsymbol{d} \quad (3-18)$$

Hence, the incremental strain is

$$\Delta \boldsymbol{\varepsilon} = \boldsymbol{L} \boldsymbol{N} \Delta \boldsymbol{d} = \boldsymbol{B} \Delta \boldsymbol{d} \quad (3-19)$$

The constitutive relation in the incremental form is

$$\Delta \boldsymbol{\sigma} = \boldsymbol{E} \boldsymbol{L} \boldsymbol{N} \Delta \boldsymbol{d} = \boldsymbol{S} \Delta \boldsymbol{d} \quad (3-20)$$

3.3.3 Discrete equations

Discrete equations for the dynamic analysis are derived from Eq. (3-15) at the element level and the arbitrariness of variation $\delta\{\Delta\mathbf{d}\}$.

$$\mathbf{K}\Delta\mathbf{d} + \mathbf{M}\Delta\ddot{\mathbf{d}} = \Delta\mathbf{F} \quad (3-21)$$

where the stiffness matrix $\mathbf{K}$, mass matrix $\mathbf{M}$ and the incremental load $\Delta\mathbf{F}$ at the current time step are

$$\mathbf{K} = \int_{\Omega} \mathbf{B}^T \mathbf{E} \mathbf{B} dV \quad (3-22)$$

$$\mathbf{M} = \int_{\Omega} \rho \mathbf{N}^T \mathbf{N} dV \quad (3-23)$$

$$\Delta\mathbf{F} = \int_{\Omega} \mathbf{N}^T \Delta\mathbf{b} dV + \int_{\Gamma_t} \mathbf{N}^T \Delta\bar{\mathbf{t}} d\Gamma \quad (3-24)$$

The stiffness and mass matrices are symmetric from Eq. (3-22) and Eq. (3-23). In fact, they are also banded and sparse because of the local property of the MC weight functions. These properties are inherited from the FEM, due to the usage of the element.

In the dynamic analysis, the acceleration and the velocity (if any) can also be expressed by using the Newmark scheme,

$$\begin{aligned} \mathbf{d}_{n+1} &= \mathbf{d}_n + \Delta t \dot{\mathbf{d}}_n + \frac{(\Delta t)^2}{2} ((1-2\beta)\ddot{\mathbf{d}}_n + 2\beta\ddot{\mathbf{d}}_{n+1}) \\ \dot{\mathbf{d}}_{n+1} &= \dot{\mathbf{d}}_n + \Delta t ((1-\gamma)\ddot{\mathbf{d}}_n + \gamma\ddot{\mathbf{d}}_{n+1}) \end{aligned} \quad (3-25)$$

where γ and β are two constants.

Then,

$$\Delta\ddot{\mathbf{d}} = \frac{1}{\beta(\Delta t)^2} \left(\Delta\mathbf{d} - \Delta t \dot{\mathbf{d}}_n - \frac{(\Delta t)^2}{2} \ddot{\mathbf{d}}_n \right) \quad (3-26)$$

Applying the scheme of the average acceleration, i.e. $\beta=1/4$ and $\gamma=1/2$, Eq. (3-26) becomes

$$\Delta\ddot{\mathbf{d}} = \frac{4}{(\Delta t)^2} \Delta\mathbf{d} - \frac{4}{\Delta t} \dot{\mathbf{d}}_n - 2\ddot{\mathbf{d}}_n \quad (3-27)$$

Substituting Eq. (3-27) into Eq. (3-21), then

$$\bar{\mathbf{K}}\Delta\mathbf{d} = \Delta\bar{\mathbf{F}} \quad (3-28)$$

where equivalent stiffness matrix $\bar{\mathbf{K}}$ and the equivalent loading vector $\Delta\bar{\mathbf{F}}$ are

$$\bar{\mathbf{K}} = \mathbf{K} + \frac{4}{(\Delta t)^2} \mathbf{M} \quad (3-29)$$

$$\Delta\bar{\mathbf{F}} = \Delta\mathbf{F} + \frac{4}{\Delta t} \mathbf{M}\dot{\mathbf{d}}_n + 2\mathbf{M}\ddot{\mathbf{d}}_n \quad (3-30)$$

The element matrices are assembled together to form the system matrices, then the system equation is solved for the unknowns attached to physical covers.

It is to be noted that the discrete equations are derived in a dynamic analysis. For a static analysis, discrete equations can be derived similarly by removing the inertia term in Eq. (3-15).

3.4 Detailed Formulations for 3-D NMM

3.4.1 Equilibrium equation base on tetrahedral MP

Theoretically any shape of manifold pattern (*MP*) can be used in the 3-D NMM. However, integration of manifold elements (*MEs*) is related to the *MP* shape and a reasonable choice of *MP/MC* shape is very important. Current developed 3-D NMM is built on tetrahedron-based *MP*, hence followed equations are correlated with tetrahedral *MP* configuration without special notification.

For FEM, the integration domains of the stiffness matrices are whole elements with standard boundaries. In numerical manifold method, the integration domains of the stiffness matrices are the *MEs*(could be whole or part of the *MPs*) which depends on the true intersection shape of physical block and mathematical mesh. Integral domain and interpolation domain are separated.

As same as the finite element method, physical equation ---the relationship between stress and strain, is given by

$$\begin{Bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \\ \tau_{xy} \\ \tau_{yz} \\ \tau_{xz} \end{Bmatrix} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1 & \frac{\nu}{1-\nu} & \frac{\nu}{1-\nu} & 0 & 0 & 0 \\ & 1 & \frac{\nu}{1-\nu} & 0 & 0 & 0 \\ & & 1 & 0 & 0 & 0 \\ & & & \frac{1-2\nu}{2(1-\nu)} & 0 & 0 \\ Sym & & & & \frac{1-2\nu}{2(1-\nu)} & 0 \\ & & & & & \frac{1-2\nu}{2(1-\nu)} \end{bmatrix} \begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \gamma_{xy} \\ \gamma_{yz} \\ \gamma_{xz} \end{Bmatrix} \quad (3-31)$$

where E , ν are Young's modulus and Poisson's ratio respectively; and elastic matrix in 3-D is

$$\mathbf{E} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)} \begin{bmatrix} 1 & \frac{\nu}{1-\nu} & \frac{\nu}{1-\nu} & 0 & 0 & 0 \\ & 1 & \frac{\nu}{1-\nu} & 0 & 0 & 0 \\ & & 1 & 0 & 0 & 0 \\ & & & \frac{1-2\nu}{2(1-\nu)} & 0 & 0 \\ Sym & & & & \frac{1-2\nu}{2(1-\nu)} & 0 \\ & & & & & \frac{1-2\nu}{2(1-\nu)} \end{bmatrix}$$

Geometric equation --- the relationship between stress and displacement,

$$\begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \gamma_{xy} \\ \gamma_{yz} \\ \gamma_{xz} \end{Bmatrix} = \mathbf{LU} = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & 0 \\ 0 & \frac{\partial}{\partial y} & 0 \\ 0 & 0 & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & \frac{\partial}{\partial x} \end{bmatrix} \begin{Bmatrix} u \\ v \\ w \end{Bmatrix} \quad (3-32)$$

Generally speaking, assuming that the total number of manifold covers (denoted by stars) in the system is n , and there are $3m$ unknowns in each manifold cover/star

$$\mathbf{d}_i = \begin{Bmatrix} d_{i1} \\ d_{i2} \\ d_{i3} \\ d_{i4} \\ \vdots \\ d_{i3m-1} \\ d_{i3m} \end{Bmatrix}, i = 1, 2, \dots, n \quad (3-33)$$

The total potential energy has the form

$$\begin{aligned} \Pi = & \frac{1}{2} \begin{pmatrix} \mathbf{d}_1^T & \mathbf{d}_2^T & \mathbf{d}_3^T & \cdots & \mathbf{d}_n^T \end{pmatrix} \begin{pmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} & \mathbf{K}_{13} & \cdots & \mathbf{K}_{1n} \\ \mathbf{K}_{21} & \mathbf{K}_{22} & \mathbf{K}_{23} & \cdots & \mathbf{K}_{2n} \\ \mathbf{K}_{31} & \mathbf{K}_{32} & \mathbf{K}_{33} & \cdots & \mathbf{K}_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{K}_{n1} & \mathbf{K}_{n2} & \mathbf{K}_{n3} & \cdots & \mathbf{K}_{nn} \end{pmatrix} \begin{Bmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \\ \mathbf{d}_3 \\ \vdots \\ \mathbf{d}_n \end{Bmatrix} \\ & + \begin{pmatrix} \mathbf{d}_1^T & \mathbf{d}_2^T & \mathbf{d}_3^T & \cdots & \mathbf{d}_n^T \end{pmatrix} \begin{Bmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \mathbf{f}_3 \\ \vdots \\ \mathbf{f}_n \end{Bmatrix} + C \end{aligned} \quad (3-34)$$

Because each cover has $3m$ degrees of freedom (DOFs), each submatrix $\mathbf{K}_{ij}$ in the coefficient matrix given in Eq. (3-34) is a $3m \times 3m$ matrix. $\mathbf{d}_i$ and $\mathbf{f}_i$ are $3m \times 1$

vectors, where $\mathbf{d}_i$ represents the displacement variables $(d_{i1}, d_{i2}, d_{i3}, \dots, d_{i3m})^T$ of manifold cover/star i . For the formulation of Π , the Eq. (3-34) can be written as a symmetric representation

$$\mathbf{K}_{ij} = \mathbf{K}_{ji}^T \quad (3-35)$$

The equilibrium equation is derived by minimizing the total potential energy Π and can be written as

$$\begin{pmatrix} \mathbf{K}_{11} & \mathbf{K}_{12} & \mathbf{K}_{13} & \cdots & \mathbf{K}_{1n} \\ \mathbf{K}_{21} & \mathbf{K}_{22} & \mathbf{K}_{23} & \cdots & \mathbf{K}_{2n} \\ \mathbf{K}_{31} & \mathbf{K}_{32} & \mathbf{K}_{33} & \cdots & \mathbf{K}_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \mathbf{K}_{n1} & \mathbf{K}_{n2} & \mathbf{K}_{n3} & \cdots & \mathbf{K}_{nn} \end{pmatrix} \begin{pmatrix} \mathbf{d}_1 \\ \mathbf{d}_2 \\ \mathbf{d}_3 \\ \vdots \\ \mathbf{d}_n \end{pmatrix} = \begin{pmatrix} \mathbf{f}_1 \\ \mathbf{f}_2 \\ \mathbf{f}_3 \\ \vdots \\ \mathbf{f}_n \end{pmatrix} \quad (3-36)$$

The i -th row of Eq. (3-36) consists of $3m$ linear equations

$$\frac{\partial \Pi}{\partial d_{i(r)}} = 0, \quad r = 1, 2, \dots, 3m \quad (3-37)$$

The element in the r -row, s -column of $\mathbf{K}_{ij}$ is

$$\frac{\partial \Pi}{\partial d_{i(r)} d_{j(s)}}, \quad r, s = 1, 2, \dots, 3m \quad (3-38)$$

The r -row element of $\mathbf{f}_i$ is the derivative of Π at value 0, namely all variables $\mathbf{d}_1, \dots, \mathbf{d}_n$ equal to zero

$$\left. \frac{\partial \Pi(0)}{\partial d_{i(r)}} \right|_{d_1, d_2, \dots, d_n = 0}, \quad r = 1, 2, \dots, 3m \quad (3-39)$$

where d_{ir} is the displacement variable of cover i .

For material analysis, $\mathbf{f}_i$ is the loading on cover i distributed to the $3m$ displacement variables. Submatrices $\mathbf{K}_{ii}$ depend on the material properties of cover i and $\mathbf{K}_{ij}$, where $i \neq j$ is defined by the overlapping or contact between cover i and cover j .

More specifically, recent version of 3-D NMM chooses the tetrahedron as Manifold Pattern e for the mathematical mesh, with a constant cover function. Thus, $m=1$ and it gives

$$\begin{aligned}
\mathbf{U} = \begin{Bmatrix} u \\ v \\ w \end{Bmatrix} &= \boldsymbol{\varphi} \mathbf{F} \mathbf{d} = \mathbf{N} \mathbf{d} = \sum_{i=1}^4 \mathbf{N}_{e(i)} \cdot \mathbf{d}_{e(i)}, \\
&= \begin{bmatrix} \mathbf{N}_{e(1)} & \mathbf{N}_{e(2)} & \mathbf{N}_{e(3)} & \mathbf{N}_{e(4)} \end{bmatrix} \begin{Bmatrix} \mathbf{d}_{e(1)} \\ \mathbf{d}_{e(2)} \\ \mathbf{d}_{e(3)} \\ \mathbf{d}_{e(4)} \end{Bmatrix}
\end{aligned} \tag{3-40}$$

where

$$\mathbf{N}_{e(i)} = \begin{bmatrix} \varphi_{e(i)} & 0 & 0 \\ 0 & \varphi_{e(i)} & 0 \\ 0 & 0 & \varphi_{e(i)} \end{bmatrix}, \quad \mathbf{d}_{e(i)} = \begin{Bmatrix} u_{e(i)} \\ v_{e(i)} \\ w_{e(i)} \end{Bmatrix} \text{ is the displacement of } i\text{th star in a}$$

tetrahedral MP (e) with constant cover function.

As mentioned before, the weight functions are

$$\begin{Bmatrix} \varphi_{e(1)}(x, y, z) \\ \varphi_{e(2)}(x, y, z) \\ \varphi_{e(3)}(x, y, z) \\ \varphi_{e(4)}(x, y, z) \end{Bmatrix} = \begin{bmatrix} f_{11} & f_{12} & f_{13} & f_{14} \\ f_{21} & f_{22} & f_{23} & f_{24} \\ f_{31} & f_{32} & f_{33} & f_{34} \\ f_{41} & f_{42} & f_{43} & f_{44} \end{bmatrix} \begin{Bmatrix} 1 \\ x \\ y \\ z \end{Bmatrix} = \begin{Bmatrix} f_{11} + f_{12}x + f_{13}y + f_{14}z \\ f_{21} + f_{22}x + f_{23}y + f_{24}z \\ f_{31} + f_{32}x + f_{33}y + f_{34}z \\ f_{41} + f_{42}x + f_{43}y + f_{44}z \end{Bmatrix} \tag{3-41}$$

Therefore,

$$\begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \gamma_{xy} \\ \gamma_{yz} \\ \gamma_{xz} \end{Bmatrix} = \mathbf{LU} = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & 0 \\ 0 & \frac{\partial}{\partial y} & 0 \\ 0 & 0 & \frac{\partial}{\partial z} \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \\ 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} \\ \frac{\partial}{\partial z} & 0 & \frac{\partial}{\partial x} \end{bmatrix} \begin{bmatrix} N_{e(1)} & N_{e(2)} & N_{e(3)} & N_{e(4)} \end{bmatrix} \begin{Bmatrix} \mathbf{d}_{e(1)} \\ \mathbf{d}_{e(2)} \\ \mathbf{d}_{e(3)} \\ \mathbf{d}_{e(4)} \end{Bmatrix}$$

$$= \begin{bmatrix} \frac{\partial \varphi_{e(1)}}{\partial x} & 0 & 0 & & & & \frac{\partial \varphi_{e(4)}}{\partial x} & 0 & 0 \\ 0 & \frac{\partial \varphi_{e(1)}}{\partial y} & 0 & & & & 0 & \frac{\partial \varphi_{e(4)}}{\partial y} & 0 \\ 0 & 0 & \frac{\partial \varphi_{e(1)}}{\partial z} & \dots & \dots & & 0 & 0 & \frac{\partial \varphi_{e(4)}}{\partial z} \\ \frac{\partial \varphi_{e(1)}}{\partial y} & \frac{\partial \varphi_{e(1)}}{\partial x} & 0 & & & & \frac{\partial \varphi_{e(4)}}{\partial y} & \frac{\partial \varphi_{e(4)}}{\partial x} & 0 \\ 0 & \frac{\partial \varphi_{e(1)}}{\partial z} & \frac{\partial \varphi_{e(1)}}{\partial y} & & & & 0 & \frac{\partial \varphi_{e(4)}}{\partial z} & \frac{\partial \varphi_{e(4)}}{\partial y} \\ \frac{\partial \varphi_{e(1)}}{\partial z} & 0 & \frac{\partial \varphi_{e(1)}}{\partial x} & & & & \frac{\partial \varphi_{e(4)}}{\partial z} & 0 & \frac{\partial \varphi_{e(4)}}{\partial x} \end{bmatrix} \begin{Bmatrix} u_{e(1)} \\ v_{e(1)} \\ w_{e(1)} \\ u_{e(2)} \\ v_{e(2)} \\ w_{e(2)} \\ u_{e(3)} \\ v_{e(3)} \\ w_{e(3)} \\ u_{e(4)} \\ v_{e(4)} \\ w_{e(4)} \end{Bmatrix}$$

$$= \begin{bmatrix} f_{12} & 0 & 0 & f_{22} & 0 & 0 & f_{32} & 0 & 0 & f_{42} & 0 & 0 \\ 0 & f_{13} & 0 & 0 & f_{23} & 0 & 0 & f_{33} & 0 & 0 & f_{43} & 0 \\ 0 & 0 & f_{14} & 0 & 0 & f_{24} & 0 & 0 & f_{34} & 0 & 0 & f_{44} \\ f_{13} & f_{12} & 0 & f_{23} & f_{22} & 0 & f_{33} & f_{32} & 0 & f_{43} & f_{42} & 0 \\ 0 & f_{14} & f_{13} & 0 & f_{24} & f_{23} & 0 & f_{34} & f_{33} & 0 & f_{44} & f_{43} \\ f_{14} & 0 & f_{12} & f_{24} & 0 & f_{22} & f_{34} & 0 & f_{32} & f_{44} & 0 & f_{42} \end{bmatrix} \begin{Bmatrix} u_{e(1)} \\ v_{e(1)} \\ w_{e(1)} \\ u_{e(2)} \\ v_{e(2)} \\ w_{e(2)} \\ u_{e(3)} \\ v_{e(3)} \\ w_{e(3)} \\ u_{e(4)} \\ v_{e(4)} \\ w_{e(4)} \end{Bmatrix} \quad (3-42)$$

Set

$$\mathbf{B}_e = [\mathbf{B}_{e(1)} \quad \mathbf{B}_{e(2)} \quad \mathbf{B}_{e(3)} \quad \mathbf{B}_{e(4)}],$$

$$\mathbf{B}_{e(i)} = \begin{bmatrix} f_{i2} & 0 & 0 \\ 0 & f_{i3} & 0 \\ 0 & 0 & f_{i4} \\ f_{i3} & f_{i2} & 0 \\ 0 & f_{i4} & f_{i3} \\ f_{i4} & 0 & f_{i2} \end{bmatrix}, \quad i = 1, 2, 3, 4 \quad (3-43)$$

It is worth to notice that terms of $\mathbf{B}_{e(i)}$ here is constant value in each element of matrix. It caused by the constant cover function chosen for current version of 3-D NMM. If we choose one or more order cover function, the terms in $\mathbf{B}_{e(i)}$ will be polynomials containing the terms like x, y, z . It should be taken into account when getting the integration to form the total coefficient matrix later on.

Then,

$$\begin{Bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \\ \gamma_{xy} \\ \gamma_{yz} \\ \gamma_{xz} \end{Bmatrix} = \mathbf{L}\mathbf{U} = \mathbf{B}_e \mathbf{D}_e = [\mathbf{B}_{e(1)} \quad \mathbf{B}_{e(2)} \quad \mathbf{B}_{e(3)} \quad \mathbf{B}_{e(4)}] \begin{Bmatrix} \mathbf{d}_{e(1)} \\ \mathbf{d}_{e(2)} \\ \mathbf{d}_{e(3)} \\ \mathbf{d}_{e(4)} \end{Bmatrix} \quad (3-44)$$

3.4.2 Elastic stiffness matrix

The elastic strain energy Π_e that generated by elastic stresses in a Manifold Pattern (MP) e is

$$\Pi_e = \iiint_v \frac{1}{2} \boldsymbol{\varepsilon}^T \boldsymbol{\sigma} dx dy dz \quad (3-45)$$

where the integral domain v is within “manifold element (ME)” which is Co-represented by this MP.

$$\begin{aligned}
\Pi_e &= \iiint_v \frac{1}{2} \begin{pmatrix} \varepsilon_x & \varepsilon_y & \varepsilon_z & \gamma_{xy} & \gamma_{yz} & \gamma_{xz} \end{pmatrix} \begin{Bmatrix} \sigma_x \\ \sigma_y \\ \sigma_z \\ \tau_{xy} \\ \tau_{yz} \\ \tau_{xz} \end{Bmatrix} dx dy dz \\
&= \frac{1}{2} \iiint_v \mathbf{d}_e^T \cdot \mathbf{B}_e^T \mathbf{E} \mathbf{B}_e \cdot \mathbf{d}_e dx dy dz \\
&= \frac{1}{2} \mathbf{d}_e^T \cdot \iiint_v \mathbf{B}_e^T \mathbf{E} \mathbf{B}_e dx dy dz \cdot \mathbf{d}_e \\
&= \frac{1}{2} \mathbf{d}_e^T \cdot \left(S^1 \cdot \mathbf{B}_e^T \mathbf{E} \mathbf{B}_e \right) \cdot \mathbf{d}_e
\end{aligned} \tag{3-46}$$

where S^1 is the volume for the current element (ME). As explained before, as only the constant term is left in $\mathbf{B}_e$, the volume integral is resulted as S^1 .

Therefore,

$$S^1 \cdot \mathbf{B}_e^T \mathbf{E} \mathbf{B}_e = S^1 \begin{Bmatrix} \mathbf{B}_{e(1)}^T \\ \mathbf{B}_{e(2)}^T \\ \mathbf{B}_{e(3)}^T \\ \mathbf{B}_{e(4)}^T \end{Bmatrix} \mathbf{E} \begin{pmatrix} \mathbf{B}_{e(1)} & \mathbf{B}_{e(2)} & \mathbf{B}_{e(3)} & \mathbf{B}_{e(4)} \end{pmatrix} \tag{3-47}$$

This is the stiffness matrix of MP e .

$$S^1 \cdot \mathbf{B}_{e(r)}^T \mathbf{E} \mathbf{B}_{e(s)} \rightarrow \mathbf{K}_{e(r)e(s)}, \quad r, s = 1, 2, 3, 4 \quad \text{for tetrahedron GP} \tag{3-48}$$

Notice that $\mathbf{K}_{e(r)e(s)}$ is a 3×3 sub-matrix, it will be put into the corresponding position of the coefficient matrix according to the global number $e(r)$, $e(s)$ of star. $\mathbf{E}$ is 6×6 matrix in Eq. (3-31).

3.4.3 Inertia term matrix

Inertia force matrix is equivalent to the mass matrix of FEM. This matrix is the most important matrix of the NMM. Given a small time step, inertia force matrix will control the movements and the stability of all points of the whole material volume. In each time step, the displacements should be small enough to let the result independent from the choice of the specific time step.

Denote $(u(t), v(t), w(t))$ as the time-dependent displacements of any points (x, y, z) in MP i , the force of inertia per unit volume is

$$\begin{Bmatrix} f_x \\ f_y \\ f_z \end{Bmatrix} = -\rho \frac{\partial^2}{\partial t^2} \begin{Bmatrix} u(t) \\ v(t) \\ w(t) \end{Bmatrix} = -\rho \mathbf{N} \frac{\partial^2 \mathbf{d}}{\partial t^2} \quad (3-49)$$

where ρ is the mass per unit volume.

The potential energy of inertia force is

$$\Pi_i = -\iiint_V (u \quad v \quad w) \begin{Bmatrix} f_x \\ f_y \\ f_z \end{Bmatrix} dx dy dz = \iiint_V \rho \mathbf{d}^T \cdot \mathbf{N}^T \mathbf{N} \cdot \frac{\partial^2 \mathbf{d}}{\partial t^2} dx dy dz \quad (3-50)$$

Assume $\mathbf{d}(\mathbf{0}) = \{0\}$ as the star displacement at the beginning of the time step, $\mathbf{d}(\Delta) = \mathbf{d}$ as the displacement at the end of the time step, Δ as the time interval of this time step.

Then, applying the scheme of the average acceleration in Eq. (3-27),

$$\mathbf{d} = \mathbf{d}(\Delta) = \mathbf{d}(\mathbf{0}) + \Delta \frac{\partial \mathbf{d}(\mathbf{0})}{\partial t} + \frac{\Delta^2}{2} \frac{\partial^2 \mathbf{d}(\mathbf{0})}{\partial t^2} = \Delta \frac{\partial \mathbf{d}(\mathbf{0})}{\partial t} + \frac{\Delta^2}{2} \frac{\partial^2 \mathbf{d}(\mathbf{0})}{\partial t^2} \quad (3-51)$$

$$\frac{\partial^2 \mathbf{d}(\mathbf{0})}{\partial t^2} = \frac{2}{\Delta^2} \mathbf{d} - \frac{2}{\Delta} \frac{\partial \mathbf{d}(\mathbf{0})}{\partial t} = \frac{2}{\Delta^2} \mathbf{d} - \frac{2}{\Delta} \mathbf{V}(\mathbf{0}) \quad (3-52)$$

where

$$\mathbf{V}(\mathbf{0}) = \frac{\partial \mathbf{d}(\mathbf{0})}{\partial t} \quad (3-53)$$

$$\mathbf{V}(\mathbf{t}) = \frac{\partial}{\partial t} \begin{Bmatrix} d_1(t) \\ d_2(t) \\ d_3(t) \end{Bmatrix} = \begin{Bmatrix} V_1(t) \\ V_2(t) \\ V_3(t) \end{Bmatrix} \quad (3-54)$$

The velocity at the end of this time step $\mathbf{V}(\Delta)$ is

$$\begin{aligned} \mathbf{V}(\Delta) &= \mathbf{V}(\mathbf{0}) + \Delta \frac{\partial \mathbf{V}(\mathbf{0})}{\partial t} \\ &= \mathbf{V}(\mathbf{0}) + \Delta \frac{\partial^2 \mathbf{d}(\mathbf{0})}{\partial t^2} = \frac{2}{\Delta} \mathbf{d} - \mathbf{V}(\mathbf{0}) \end{aligned} \quad (3-55)$$

Then, the potential energy becomes

$$\begin{aligned}
\Pi_i &= \rho \mathbf{d}^T \left[\iiint_V \mathbf{N}_i^T \mathbf{N}_i dx dy dz \right] \left(\frac{2}{\Delta^2} \mathbf{d}(\Delta) - \frac{2}{\Delta} \mathbf{V}(\mathbf{0}) \right) \\
&= \rho \mathbf{d}^T \left[\iiint_V \mathbf{N}_i^T \mathbf{N}_i dx dy dz \right] \left(\frac{2}{\Delta^2} \mathbf{d} - \frac{2}{\Delta} \mathbf{V}(\mathbf{0}) \right)
\end{aligned} \tag{3-56}$$

Then, we have

$$\frac{2\rho}{\Delta^2} \iiint_V \mathbf{N}_{i(r)}^T \mathbf{N}_{i(s)} dx dy dz \rightarrow \mathbf{K}_{i(r)i(s)}, \quad r, s = 1, 2, 3, 4 \tag{3-57}$$

$$\frac{2\rho}{\Delta} \left[\iiint_V \mathbf{N}_{i(r)}^T \mathbf{N}_{i(s)} dx dy dz \right] \mathbf{V}_{i(s)}(\mathbf{0}) \rightarrow \mathbf{f}_{i(r)}, \quad \begin{matrix} r = 1, 2, 3, 4 \\ s = 1, 2, 3, 4 \end{matrix} \tag{3-58}$$

where

$$\mathbf{V}_{i(s)}(\mathbf{0}) = \frac{\partial}{\partial t} \begin{Bmatrix} u_{i(s)}(0) \\ v_{i(s)}(0) \\ w_{i(s)}(0) \end{Bmatrix}$$

The integration can be obtained from

$$\iiint_V \mathbf{N}^T \mathbf{N} dx dy dz = \iiint_V \begin{bmatrix} \varphi_{i(r)} \cdot \varphi_{i(s)} & 0 & 0 \\ 0 & \varphi_{i(r)} \cdot \varphi_{i(s)} & 0 \\ 0 & 0 & \varphi_{i(r)} \cdot \varphi_{i(s)} \end{bmatrix} dx dy dz = \begin{bmatrix} n_{i(r)i(s)} & 0 & 0 \\ 0 & n_{i(r)i(s)} & 0 \\ 0 & 0 & n_{i(r)i(s)} \end{bmatrix} \tag{3-59}$$

where

$$\begin{aligned}
n_{i(r)i(s)} &= \iiint_V (f_{1(r)} + f_{2(r)} \cdot x + f_{3(r)} \cdot y + f_{4(r)} \cdot z)(f_{1(s)} + f_{2(s)} \cdot x + f_{3(s)} \cdot y + f_{4(s)} \cdot z) dx dy dz \\
&= f_{1(r)} f_{1(s)} S^1 + (f_{1(r)} f_{2(s)} + f_{1(s)} f_{2(r)}) S^x + (f_{1(r)} f_{3(s)} + f_{1(s)} f_{3(r)}) S^y + (f_{1(r)} f_{4(s)} + f_{1(s)} f_{4(r)}) S^z \\
&\quad + f_{2(r)} f_{2(s)} S^{xx} + f_{3(r)} f_{3(s)} S^{yy} + f_{4(r)} f_{4(s)} S^{zz} \\
&\quad + (f_{2(r)} f_{3(s)} + f_{2(s)} f_{3(r)}) S^{xy} + (f_{2(r)} f_{4(s)} + f_{2(s)} f_{4(r)}) S^{xz} + (f_{3(r)} f_{4(s)} + f_{3(s)} f_{4(r)}) S^{yz}
\end{aligned} \tag{3-60}$$

$S^1 \sim S^{yz}$ will be given in the 3-D Simplex Integration for 1~yz terms (*Section 3.5*).

3.4.4 Initial stress matrix

The NMM computes step by step. The computed stresses of previous time step will be the initial stresses of the next time step. Therefore, initial stress matrix is essential for NMM.

Assume the initial stresses for MP s is

$$\boldsymbol{\sigma}_s^0 = \begin{pmatrix} \sigma_x^0 & \sigma_y^0 & \sigma_z^0 & \tau_{xy}^0 & \tau_{yz}^0 & \tau_{zx}^0 \end{pmatrix}^T \quad (3-61)$$

The strain energy Π done by the initial stresses is:

$$\Pi_\sigma = \iiint_V \boldsymbol{\varepsilon}_s^T \boldsymbol{\sigma}_s^0 dx dy dz = \mathbf{d}_s^T \cdot \iiint_V \mathbf{B}_s^T dx dy dz \cdot \boldsymbol{\sigma}_s^0 \quad (3-62)$$

Therefore, the initial stress matrix belongs to the load matrix, we have

$$-\iiint_V \mathbf{B}_s^T dx dy dz \cdot \boldsymbol{\sigma}_s^0 \rightarrow \mathbf{f}_{s(r)}, \quad r = 1, 2, 3, 4 \quad (3-63)$$

The integration can be obtained from

$$\iiint_V \mathbf{B}_{s(r)}^T dx dy dz = \mathbf{B}_{s(r)}^T \cdot \iiint_V 1 dx dy dz = S^1 \cdot \mathbf{B}_{s(r)}^T \quad (3-64)$$

3.4.5 Point loading matrix

Assuming the point loading of point (x_0, y_0, z_0) is

$$\mathbf{p}^0(x_0, y_0, z_0) = \begin{Bmatrix} f_x^0 \\ f_y^0 \\ f_z^0 \end{Bmatrix} \quad (3-65)$$

The potential energy done by the point loading is

$$\begin{aligned} \Pi_p &= -\left(f_x u(x_0, y_0, z_0) + f_y v(x_0, y_0, z_0) + f_z w(x_0, y_0, z_0)\right) \\ &= -\begin{pmatrix} u_p(x_0, y_0, z_0) & v_p(x_0, y_0, z_0) & w_p(x_0, y_0, z_0) \end{pmatrix} \begin{Bmatrix} f_x^0 \\ f_y^0 \\ f_z^0 \end{Bmatrix} = -\mathbf{d}_p^T \cdot \mathbf{N}_p(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)^T \begin{Bmatrix} f_x^0 \\ f_y^0 \\ f_z^0 \end{Bmatrix} \end{aligned} \quad (3-66)$$

Therefore, the point loading matrix is

$$\mathbf{N}_{p(r)}(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)^T \begin{Bmatrix} f_x^0 \\ f_y^0 \\ f_z^0 \end{Bmatrix} \rightarrow \mathbf{f}_{p(r)}(x_0, y_0, z_0), \quad r = 1, 2, \dots, p_n \quad (3-67)$$

where p_n is the total number of fixed point.

3.4.6 Body force matrix

When constant body force (g_x, g_y, g_z) acts on the material volume of MP b , the corresponding potential energy is

$$\Pi_g = -\iiint_V (u \quad v \quad w) \begin{Bmatrix} g_x \\ g_y \\ g_z \end{Bmatrix} dx dy dz = -\mathbf{d}_b^T \left[\iiint_V \mathbf{N}_b^T dx dy dz \right] \begin{Bmatrix} g_x \\ g_y \\ g_z \end{Bmatrix} \quad (3-68)$$

Therefore, we have the body loading matrix as

$$\iiint_V \mathbf{N}_{b(r)}^T dx dy dz \cdot \begin{Bmatrix} g_x \\ g_y \\ g_z \end{Bmatrix} \rightarrow \mathbf{f}_{b(r)}, \quad r = 1, 2, \dots, b_n \quad (3-69)$$

where b_n is the total number of MP on which body force is imposed.

The integration can be obtained from

$$\iiint_V \mathbf{N}_{b(r)}^T dx dy dz = \iiint_V \begin{bmatrix} \varphi_{b(r)} & 0 & 0 \\ 0 & \varphi_{b(r)} & 0 \\ 0 & 0 & \varphi_{b(r)} \end{bmatrix} dx dy dz = \begin{bmatrix} h_{b(r)} & 0 & 0 \\ 0 & h_{b(r)} & 0 \\ 0 & 0 & h_{b(r)} \end{bmatrix} \quad (3-70)$$

where

$$\begin{aligned} h_{b(r)} &= \iiint_V \varphi_{b(r)} dx dy dz = \iiint_V (f_{1(r)} + f_{2(r)} \cdot x + f_{3(r)} \cdot y + f_{4(r)} \cdot z) dx dy dz \\ &= f_{1(r)} \cdot S^1 + f_{2(r)} \cdot S^x + f_{3(r)} \cdot S^y + f_{4(r)} \cdot S^z \end{aligned}$$

Similarly, $S^l \sim S^z$ will be given in the 3-D Simplex Integration for $l \sim z$ terms in Section 3.5.

3.4.7 Matrix for displacement boundary point & fixed point

Penalty method is utilized to impose fixed point or displacement boundary in NMM.

As boundary condition, displacements (u_m, v_m, w_m) are sometimes fixed or pre-determined in prescribed points in MPs. In three dimension, the penalty method applies three relative stiff springs to restrict or move them. The stiffness of the springs is normally set under the order of magnitude around $10 \sim 100E_0L_0$, to ensure that the whole coefficient matrix will not become ill-condition as the introduction of these springs. E_0 is the Young's modulus of the blocks and L_0 is the average block "diameter". The penalty spring forces work and system internal energy increases.

Setting a point $a(x_0, y_0, z_0)$ in MP f at current time step to have a displacement of (u_m, v_m, w_m) . So the displacement of the fixed point is

$$\mathbf{d}_m = \begin{Bmatrix} u_m(x_0, y_0, z_0) \\ v_m(x_0, y_0, z_0) \\ w_m(x_0, y_0, z_0) \end{Bmatrix} = \begin{Bmatrix} 0 \\ 0 \\ 0 \end{Bmatrix} \quad (3-71)$$

Assuming that the virtual displacement of a is (u, v, w) , it imposes three stiff springs to force its displacement (u, v, w) to (u_m, v_m, w_m) . The springs are exactly along global x, y and z direction with stiffness k , and the spring force is

$$\begin{Bmatrix} f_x \\ f_y \\ f_z \end{Bmatrix} = \begin{Bmatrix} -k_x(u - u_m) \\ -k_y(v - v_m) \\ -k_z(w - w_m) \end{Bmatrix}, \quad \text{normally, } k_x = k_y = k_z = k \quad (3-72)$$

The total strain energy for the springs is

$$\begin{aligned} \Pi_f &= \frac{k}{2} \left((u(x_0, y_0, z_0) - u_m)^2 + (v(x_0, y_0, z_0) - v_m)^2 + (w(x_0, y_0, z_0) - w_m)^2 \right) \\ &= \frac{k}{2} \begin{pmatrix} u(x_0, y_0, z_0) - u_m & v(x_0, y_0, z_0) - v_m & w(x_0, y_0, z_0) - w_m \end{pmatrix} \begin{Bmatrix} u(x_0, y_0, z_0) - u_m \\ v(x_0, y_0, z_0) - v_m \\ w(x_0, y_0, z_0) - w_m \end{Bmatrix} \\ &= \frac{k}{2} \begin{pmatrix} u(x_0, y_0, z_0) & v(x_0, y_0, z_0) & w(x_0, y_0, z_0) \end{pmatrix} \begin{Bmatrix} u(x_0, y_0, z_0) \\ v(x_0, y_0, z_0) \\ w(x_0, y_0, z_0) \end{Bmatrix} \\ &\quad - k \begin{pmatrix} u(x_0, y_0, z_0) & v(x_0, y_0, z_0) & w(x_0, y_0, z_0) \end{pmatrix} \begin{Bmatrix} u_m \\ v_m \\ w_m \end{Bmatrix} + \frac{k}{2} \begin{pmatrix} u_m & v_m & w_m \end{pmatrix} \begin{Bmatrix} u_m \\ v_m \\ w_m \end{Bmatrix} \\ &= \frac{k}{2} \mathbf{d}_f^T \mathbf{N}_f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)^T \mathbf{N}_f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) \mathbf{d}_f - k \mathbf{d}_f^T \mathbf{N}_f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)^T \mathbf{d}_m + C \end{aligned} \quad (3-73)$$

If the prescribed point is fixed, $\mathbf{d}_m = \mathbf{0}$ the above equation is only left with its first term. Differentiating it to get the minimum value of Π_f

$$\begin{aligned} \mathbf{K}_f &= \frac{\partial^2 \Pi_f}{\partial d_r \partial d_s} \\ &= \frac{\partial^2}{\partial d_r \partial d_s} \left[\frac{k}{2} \mathbf{d}_f^T \cdot \mathbf{N}_f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)^T \mathbf{N}_f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) \cdot \mathbf{d}_f \right] \end{aligned} \quad (3-74)$$

Hence,

$$\begin{aligned} &k \cdot \mathbf{N}_f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)^T \mathbf{N}_f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) \\ &= k \begin{Bmatrix} \mathbf{N}_{f(1)}(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)^T \\ \mathbf{N}_{f(2)}(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)^T \\ \mathbf{N}_{f(3)}(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)^T \\ \mathbf{N}_{f(4)}(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)^T \end{Bmatrix} \left\{ \mathbf{N}_{f(1)}(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) \quad \mathbf{N}_{f(2)}(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) \quad \mathbf{N}_{f(3)}(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) \quad \mathbf{N}_{f(4)}(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) \right\} \end{aligned} \quad (3-75)$$

Then,

$$k \cdot \varphi_{f(r)}(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) \cdot \varphi_{f(s)}(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0) \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \rightarrow \mathbf{K}_{f(r)f(s)}, \quad r, s = 1, 2, 3, 4 \quad (3-76)$$

No matter it is fixed point or displacement boundary, Eq. (3-76) always satisfies the principle of minimum total potential energy, hence the contribution to total coefficient matrix are as same as in Eq. (3-76).

When $(u_m, v_m, w_m) \neq 0$,

$$\begin{aligned} \mathbf{f}_f &= -\frac{\partial \Pi_f(0)}{\partial d_r} \\ &= \frac{\partial}{\partial d_r} \left[k \cdot \mathbf{d}_f^T \cdot \mathbf{N}_f(\mathbf{x}_0, \mathbf{y}_0, \mathbf{z}_0)^T \cdot \mathbf{d}_m \right] \end{aligned} \quad (3-77)$$

Hence ,

$$\begin{aligned}
& k \cdot N_f(x_0, y_0, z_0)^T d_m \\
& = k \begin{Bmatrix} N_{f(1)}(x_0, y_0, z_0)^T \\ N_{f(2)}(x_0, y_0, z_0)^T \\ N_{f(3)}(x_0, y_0, z_0)^T \\ N_{f(4)}(x_0, y_0, z_0)^T \end{Bmatrix} \begin{Bmatrix} u_m \\ v_m \\ w_m \end{Bmatrix} \quad (3-78)
\end{aligned}$$

$$k \cdot N_{f(r)}(x_0, y_0, z_0)^T \begin{Bmatrix} u_m \\ v_m \\ w_m \end{Bmatrix} \rightarrow f_{f(r)}, \quad r = 1, 2, 3, 4 \quad (3-79)$$

It should be noted that $\begin{Bmatrix} u_m \\ v_m \\ w_m \end{Bmatrix}$ has two parts:

- 1) The rigid displacement to force point a , induced by the predetermined (u_m, v_m, w_m) ;
- 2) During the calculation, it is not enough to lock the fixed point (or force the point a to the prescribe position) only through terms of strong stiffness springs (Eq. (3-76)) in total coefficient matrix $\mathbf{K}$. It could not increase the spring stiffness infinitely to lock the fixed point too, as it might induce ill-conditioned matrix $\mathbf{K}$. Since it could not prevent such cases, it still can be diverted. We permit the residual displacement at the fixed/displacement points induced by improper strong stiffness springs in the previous time step. It is not difficult to get the cumulative error displacement in the system actually. Therefore, we impose an equivalent negative force in the current time step to draw back the residual displacement. In the aspect of energy, it is the negative force to apply negative work, which consumes the unnecessarily residual potential position energy at the fixed points. In reality, it is quite hard to determine the precise value of the equivalent negative force, as improper force could leave new residual cumulative displacement to the latter time steps. In such case, it has to repeatedly impose the so-called “correction forces” in each time step. Such correction forces might induce the whole system to small vibration surrounding the fixed point. To

control the vibration amplitude, it has to apply proper stiffness spring again. One has to balance-off during these two contradicting processes.

3.5 Simplex Integration for 3-D arbitrary polyhedron

For any arbitrary shaped polyhedron, we need its precise volume, center of gravity and other integration within the polyhedral domain. It is not hard to gain such integration by using the geometrical information and topological structure.

In addition, simplex integration is precise integration within the polyhedral body. It will help to increase the precision of 3-D NMM.

Assuming the vertex list of i -th plane loop is [Shi (1996a)]

$$P_1^{[i]} P_2^{[i]} P_3^{[i]} \dots P_{n(i)}^{[i]} \quad (3-80)$$

where $n(i)$ is the sum of vertex on i -th plane.

To complete the definition of i -th polygon loops by repeating the first vertex on plane.

$$P_1^{[i]} = P_{n(i)+1}^{[i]} \quad (3-81)$$

The coordinate of each vertex can be expressed as:

$$P_j^{[i]} = (x_j^{[i]}, y_j^{[i]}, z_j^{[i]}) \quad j = 1, 2, \dots, n(i) \quad (3-82)$$

Then, s polygon loops in total are assumed to compose the current block and set $P_0 = (0, 0, 0)$. The volume of this block is given by Eq. (3-83). Computed by simplex integrations, integrals for I , x , y , z , x^2 , y^2 , z^2 , xy , yz , xz are represented by the coordinates of the boundary vertices only [Ma and He (2008)].

$$\begin{aligned}
S^1 &= \iiint_V 1 dx dy dz = \sum_{i=1}^s \sum_{k=1}^{n(i)} \int_{P_0 P_1^{[i]} P_k^{[i]} P_{k+1}^{[i]}} 1 D(x, y, z) \\
&= \frac{1}{6} \sum_{i=1}^s \sum_{k=1}^{n(i)} \begin{vmatrix} x_1^{[i]} & y_1^{[i]} & z_1^{[i]} \\ x_k^{[i]} & y_k^{[i]} & z_k^{[i]} \\ x_{k+1}^{[i]} & y_{k+1}^{[i]} & z_{k+1}^{[i]} \end{vmatrix}
\end{aligned} \tag{3-83}$$

Integration for x, y, z within corresponding domain:

$$\begin{aligned}
S^x &= \iiint_V x dx dy dz = \sum_{i=1}^s \sum_{k=1}^{n(i)} \int_{P_0 P_1^{[i]} P_k^{[i]} P_{k+1}^{[i]}} x D(x, y, z) \\
&= \frac{1}{24} \sum_{i=1}^s \sum_{k=1}^{n(i)} \begin{vmatrix} x_1^{[i]} & y_1^{[i]} & z_1^{[i]} \\ x_k^{[i]} & y_k^{[i]} & z_k^{[i]} \\ x_{k+1}^{[i]} & y_{k+1}^{[i]} & z_{k+1}^{[i]} \end{vmatrix} \cdot (x_1 + x_k + x_{k+1})
\end{aligned} \tag{3-84}$$

$$\begin{aligned}
S^y &= \iiint_V y dx dy dz = \sum_{i=1}^s \sum_{k=1}^{n(i)} \int_{P_0 P_1^{[i]} P_k^{[i]} P_{k+1}^{[i]}} y D(x, y, z) \\
&= \frac{1}{24} \sum_{i=1}^s \sum_{k=1}^{n(i)} \begin{vmatrix} x_1^{[i]} & y_1^{[i]} & z_1^{[i]} \\ x_k^{[i]} & y_k^{[i]} & z_k^{[i]} \\ x_{k+1}^{[i]} & y_{k+1}^{[i]} & z_{k+1}^{[i]} \end{vmatrix} \cdot (y_1 + y_k + y_{k+1})
\end{aligned} \tag{3-85}$$

$$\begin{aligned}
S^z &= \iiint_V z dx dy dz = \sum_{i=1}^s \sum_{k=1}^{n(i)} \int_{P_0 P_1^{[i]} P_k^{[i]} P_{k+1}^{[i]}} z D(x, y, z) \\
&= \frac{1}{24} \sum_{i=1}^s \sum_{k=1}^{n(i)} \begin{vmatrix} x_1^{[i]} & y_1^{[i]} & z_1^{[i]} \\ x_k^{[i]} & y_k^{[i]} & z_k^{[i]} \\ x_{k+1}^{[i]} & y_{k+1}^{[i]} & z_{k+1}^{[i]} \end{vmatrix} \cdot (z_1 + z_k + z_{k+1})
\end{aligned} \tag{3-86}$$

Integration for x^2, y^2, z^2 within domain:

$$\begin{aligned}
S^{x^2} &= \iiint_V x^2 dx dy dz = \sum_{i=1}^s \sum_{k=1}^{n(i)} \int_{P_0 P_1^{[i]} P_k^{[i]} P_{k+1}^{[i]}} x^2 D(x, y, z) \\
&= \frac{1}{60} \sum_{i=1}^s \sum_{k=1}^{n(i)} \begin{vmatrix} x_1^{[i]} & y_1^{[i]} & z_1^{[i]} \\ x_k^{[i]} & y_k^{[i]} & z_k^{[i]} \\ x_{k+1}^{[i]} & y_{k+1}^{[i]} & z_{k+1}^{[i]} \end{vmatrix} \\
&\quad \times (x_1 x_1 + x_1 x_k + x_1 x_{k+1} + x_k x_k + x_k x_{k+1} + x_{k+1} x_{k+1})
\end{aligned} \tag{3-87}$$

$$\begin{aligned}
S^{y^2} &= \iiint_V y^2 dx dy dz = \sum_{i=1}^s \sum_{k=1}^{n(i)} \int_{P_0 P_1^{[i]} P_k^{[i]} P_{k+1}^{[i]}} y^2 D(x, y, z) \\
&= \frac{1}{60} \sum_{i=1}^s \sum_{k=1}^{n(i)} \begin{vmatrix} x_1^{[i]} & y_1^{[i]} & z_1^{[i]} \\ x_k^{[i]} & y_k^{[i]} & z_k^{[i]} \\ x_{k+1}^{[i]} & y_{k+1}^{[i]} & z_{k+1}^{[i]} \end{vmatrix} \\
&\quad \times (y_1 y_1 + y_1 y_k + y_1 y_{k+1} + y_k y_k + y_k y_{k+1} + y_{k+1} y_{k+1})
\end{aligned} \tag{3-88}$$

$$\begin{aligned}
S^{z^2} &= \iiint_V z^2 dx dy dz = \sum_{i=1}^s \sum_{k=1}^{n(i)} \int_{P_0 P_1^{[i]} P_k^{[i]} P_{k+1}^{[i]}} z^2 D(x, y, z) \\
&= \frac{1}{60} \sum_{i=1}^s \sum_{k=1}^{n(i)} \begin{vmatrix} x_1^{[i]} & y_1^{[i]} & z_1^{[i]} \\ x_k^{[i]} & y_k^{[i]} & z_k^{[i]} \\ x_{k+1}^{[i]} & y_{k+1}^{[i]} & z_{k+1}^{[i]} \end{vmatrix} \\
&\quad \times (z_1 z_1 + z_1 z_k + z_1 z_{k+1} + z_k z_k + z_k z_{k+1} + z_{k+1} z_{k+1})
\end{aligned} \tag{3-89}$$

Integration for xy , xz , yz within domain:

$$\begin{aligned}
S^{xy} &= \iiint_V xy dx dy dz = \sum_{i=1}^s \sum_{k=1}^{n(i)} \int_{P_0 P_1^{[i]} P_k^{[i]} P_{k+1}^{[i]}} xy D(x, y, z) \\
&= \frac{1}{120} \sum_{i=1}^s \sum_{k=1}^{n(i)} \begin{vmatrix} x_1^{[i]} & y_1^{[i]} & z_1^{[i]} \\ x_k^{[i]} & y_k^{[i]} & z_k^{[i]} \\ x_{k+1}^{[i]} & y_{k+1}^{[i]} & z_k^{[i]} \end{vmatrix} \\
&\quad \times (2x_1 y_1 + x_1 y_k + x_1 y_{k+1} + x_k y_1 + 2x_k y_k + x_k y_{k+1} + x_{k+1} y_1 + x_{k+1} y_k + 2x_{k+1} y_{k+1})
\end{aligned} \tag{3-90}$$

$$\begin{aligned}
S^{xz} &= \iiint_V xz dx dy dz = \sum_{i=1}^s \sum_{k=1}^{n(i)} \int_{P_0 P_1^{[i]} P_k^{[i]} P_{k+1}^{[i]}} xz D(x, y, z) \\
&= \frac{1}{120} \sum_{i=1}^s \sum_{k=1}^{n(i)} \begin{vmatrix} x_1^{[i]} & y_1^{[i]} & z_1^{[i]} \\ x_k^{[i]} & y_k^{[i]} & z_k^{[i]} \\ x_{k+1}^{[i]} & y_{k+1}^{[i]} & z_k^{[i]} \end{vmatrix} \\
&\quad \times (2x_1 z_1 + x_1 z_k + x_1 z_{k+1} + x_k z_1 + 2x_k z_k + x_k z_{k+1} + x_{k+1} z_1 + x_{k+1} z_k + 2x_{k+1} z_{k+1})
\end{aligned} \tag{3-91}$$

$$\begin{aligned}
S^{yz} &= \iiint_V yz dx dy dz = \sum_{i=1}^s \sum_{k=1}^{n(i)} \int_{p_0 p_1^{[i]} p_k^{[i]} p_{k+1}^{[i]}} yz D(x, y, z) \\
&= \frac{1}{120} \sum_{i=1}^s \sum_{k=1}^{n(i)} \begin{vmatrix} x_1^{[i]} & y_1^{[i]} & z_1^{[i]} \\ x_k^{[i]} & y_k^{[i]} & z_k^{[i]} \\ x_{k+1}^{[i]} & y_{k+1}^{[i]} & z_k^{[i]} \end{vmatrix} \\
&\quad \times (2y_1 z_1 + y_1 z_k + y_1 z_{k+1} + y_k z_1 + 2y_k z_k + y_k z_{k+1} + y_{k+1} z_1 + y_{k+1} z_k + 2y_{k+1} z_{k+1}) \\
&\hspace{15em} (3-92)
\end{aligned}$$

Chapter 4 Contact Mechanics -- General

Contact Algorithm

4.1 Overview

Contact algorithm is a key for further developing the numerical simulation technique. For example, the further development on popular topics including complex crack propagation and fluid-solid coupling problem are highly dependent on a reliable contact algorithm. Indeed, contact algorithm in computational mechanics is not a new topic, which has been discussed as a hot topic in FEM during 90s in last century. Diverse contact treatments and concepts are raised through time. Simultaneously, some famous commercial software (e.g., LSDYNA, AUTODYN) stands out due to embedding in some good contact algorithms.

It is pity that the current discussion on contact algorithm is much rare. It is not because the algorithm has been already developed completely, but contact algorithm has been sealed into commercial software as a “*black box*”. Undeniably, those commercial giants have made their efforts on continuing development of FEM and gained fruitful improvement. However, such “*black box*” treatment blocks necessary competition, which impedes the enrichment of other numerical methods.

The difficulty of contact is not just only on its mechanical parts, but also on its logic and organization. In this chapter, it starts with basic introduction of contact mechanics. Then, it follows with detailed discussion on corresponding aspects of contact treatment, meanwhile, sorts and summarizes the previous scholars’ work. Finally, a general framework of 3-D contact treatment is proposed.

This chapter includes:

- General contact problem and contact boundary description (classic contact mechanics)

- Mechanical properties of contact boundary (classical contact mechanics)
- Contact checking algorithm (computational contact mechanics)
- Numerical treatment of contact constraints to complement/revise the transient energy functional. This is the implement procedure of equivalent contact force. (classical contact mechanics)

4.2 General Statement of Contact Problem

A contact system engages one or more contact bodies. Contact may occur within a single body or between two or more bodies, and the contact interaction for each body is a typical boundary value problem. Contact interaction itself is nothing but one special kind of boundary with trigger condition, also called “*contact constraint*”, except widely known loading boundary and displacement boundary in continuum mechanics. In other words, we are only required to put additional terms, triggered by contact, into local balance equations based on continuum mechanics. These equations, which describe the behavior of bodies whether coming into contact or not, have not made essential difference.

Therefore, boundary conditions can be classified into two groups: 1) *prescribed boundary conditions* and 2) *uncertain boundary conditions*. Obviously, the prescribed boundary conditions are motion-deformation independent, while the uncertain one is motion-deformation dependent. The contact constraint is an important branch of uncertain boundary conditions.

More specifically, the uncertainties of contact constraints are originated from two main sources: i) the contact zone size between the contact interface, relative positions, and contact status (intensity), are unknown prior to solution, and also changing all the time. ii) Three criteria are necessary during whole contact process: no penetration among contact objects, only normal compressive pressure between contact interfaces, and frictional constitutive condition in tangential direction. Because of these, contact problem has become typical nonlinear one. It also brings the third kind of nonlinearity into solid mechanics: contact interface nonlinearity, except for material

nonlinearity and geometric nonlinearity.

Furthermore, it becomes another major topics on “how to properly apply or release such equivalent-reversed contact constraint at the right time and position”. We postpone our discussion on “contact detection & tracking” and “treatment of contact constraint” to later sections. In this section, the contact position is assumed to be determinate, and we pay more attention on how to describe this physical phenomenon with systematical and mathematical manner.

4.2.1 Formal descriptions of the problem

Consider a homogeneous, isotropic elastic body Ω as shown in Fig. 4-1.

Figure 4- 1 Configuration of general contact problem

The local balance of momentum with respect to a volume element in current configuration Ω can be expressed as

$$\nabla \cdot \boldsymbol{\sigma} + \mathbf{b} = \rho \ddot{\mathbf{x}} \quad (4-1)$$

where ∇ is the gradient operator with respect to the current position $\mathbf{x}$, and $\boldsymbol{\sigma}$ denotes the **CAUCHY** stress tensor. $\ddot{\mathbf{x}}$ is the acceleration, ρ is the density of mass. Hence, $\rho \ddot{\mathbf{x}}$ defines the inertia force term, which can be neglected in the case of static analysis. $\mathbf{b}$ is the volumn or body force per unit mass.

Assuming the following conditions hold on the boundary (see Fig. 4-1)

- 1) Displacement boundary conditions, also called DIRICHLET conditions:

$$\mathbf{u} = \bar{\mathbf{u}} \quad \text{on } \Gamma_u \quad (4-2)$$

It is worth to notice that the velocity and acceleration on Γ_u can be also defined with the displacement on the corresponding boundaries, which is prescribed as

$$\begin{aligned} \bar{\mathbf{v}} &= d(\bar{\mathbf{u}}) / dt \\ \bar{\mathbf{a}} &= d^2(\bar{\mathbf{u}}) / dt^2 \end{aligned} \quad \text{on } \Gamma_u \quad (4-3)$$

- 2) Traction boundary conditions, also called NEUMANN conditions:

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \bar{\mathbf{t}} \quad \text{on } \Gamma_\sigma \quad (4-4)$$

where $\mathbf{n}$ is the outward normal of the surface of current configuration and $\bar{\mathbf{t}}$ denotes the applied traction on Γ_σ .

- 3) Contact boundary conditions:

a) Normal contact condition

The non-penetration condition is to forbid self-intersection and mutual penetration among contact interface and objects. (kinematic contact conditions)

$$\Omega^A \cap \Omega^B = \emptyset \quad (4-5)$$

where $\emptyset$ denotes a null space.

Furthermore, assuming that two contact boundaries are not welded together or have no surface tension, tensile traction is not allowed on the contacting boundaries, thus

$$p_N \leq 0 \quad \text{on } \Gamma_c \quad (4-6)$$

where p_N is the contact pressure which is equivalent with the normal component of the traction vector regarding to the contact surface. Minus sign “-” denotes compression.

b) Tangential contact condition

According to the classic Coulomb friction law, the tangential friction components are bounded as follows:

$$|\mathbf{P}_T| \leq \mu \left| \int_{A_c} p_N dA \right| \quad (4-7)$$

where $|\mathbf{P}_T|$ indicates the magnitude of tangential contact traction on the contact area A_c and μ is the friction coefficient, which depends on the nature of the corresponding contacting boundaries.

Generally speaking, there are two distinguished states along the tangential direction of the contact interface. The first is the so-called **Stick State** in which a pair of contact boundaries is not allowed to move in a tangential direction. The second case is **Sliding State**, which means that boundaries partners have relative movement between them along the tangential direction.

Stick state:

$$d_T = 0 \quad \text{if} \quad |\mathbf{P}_T| < \mu \left| \int_{A_c} p_N dA \right| \quad (4-8)$$

Here d_T denotes the relative displacement in a tangential direction, which has to be zero.

Sliding state:

$$\mathbf{v}_T \neq 0, \mathbf{v}_T \cdot \mathbf{P}_T < 0 \quad \text{if} \quad |\mathbf{P}_T| = \mu \left| \int_{A_c} p_N dA \right| \quad (4-9)$$

Eq. (4-9) means relative sliding velocity $\mathbf{v}_T$ in a tangential direction is not equal to zero. The vector direction of frictional force $\mathbf{P}_T$, which is acting on the contact zone, is always opposite to sliding direction.

In a word, displacement boundary conditions and traction boundary conditions are the typical prescribed boundary conditions. Contact boundary conditions is so-called uncertain boundary condition.

4.2.2 3-D Extension of contact boundary condition

Constraint condition by contact interaction, which is formally presented in the previous section, can not be used directly in the solution procedure. The previous

description is not sufficient for all complicated details. In this section, we will further present the 3-D profile of contact boundary conditions.

1) Symbol and Definition

Without losing any generality, the contact configuration between two arbitrarily shaped 3-D bodies is shown in Fig. 4-2.

Figure 4- 2 3-D contact configuration and definitions

Assuming that body A and body B will touch each other at contact surface $'S_c^A$ and $'S_c^B$ at time instant t , the figure shows their contact critical state configuration, denoted by $'\Omega_c^A$ and $'\Omega_c^B$. Normally, local Cartesian coordinate system is set at the center of contact interface, and a set of unit vectors $(\mathbf{n}_1^A, \mathbf{n}_2^A, \mathbf{n}_3^A)$ is introduced at center-point $'x_c^A$ on surface $'S_c^A$, for example. $\mathbf{n}_1^A, \mathbf{n}_2^A$ locate at the contacting point on the tangent plane of $'S_c^A$, and are orthogonal to each other, while $\mathbf{n}_3^A$ is perpendicular to the outside of $'S_c^A$. They satisfy

$$\mathbf{n}_3^A = \mathbf{n}_1^A \times \mathbf{n}_2^A \quad (4-10)$$

For convenience, a slice plane is set along of $\mathbf{n}_3^A$ direction between body A and B at time instance t (shown in Fig.4-3).

Figure 4- 3 Slice profile of 3-D contact bodies

Two contact points ${}^t x_c^A$ and ${}^t x_c^B$ at the contact interface is referred as “**contact pair of particle**”, and ${}^t \mathbf{P}^A$ and ${}^t \mathbf{P}^B$ are contact force applying on these two points. The instantaneous velocities at the contact points are denoted by ${}^t \mathbf{v}^A$ and ${}^t \mathbf{v}^B$. In fact, contact interaction happens at two sides of the contact pair simultaneously, without any *master-slave* relationship. However, under some specific circumstance for clarification, we define one of particles, eg. ${}^t x_c^A$, as a hitting particle and denoted by ${}^t x_c^{hit}$ too, while other particle, eg. ${}^t x_c^B$, as a target particle, denoted by ${}^t x_c^{tar}$. Furthermore, if there is more than one hitting particle, we can define a set of hitting particles as

$$\Gamma_c^{hit} = \left\{ {}^t \mathbf{x}_c^{hit} \mid x(\mathbf{x}_c^A, t) \cap {}^t S_c^B \neq \emptyset, \mathbf{x}_c^A \in {}^t S_c^A \right\} \quad (4-11)$$

Similarly, we define a set of target particles as

$$\Gamma_c^{tar} = \left\{ {}^t \mathbf{x}_c^{tar} \mid x(\mathbf{x}_c^B, t) = x(\mathbf{x}_c^A, t), \mathbf{x}_c^B \in {}^t S_c^B, \mathbf{x}_c^A \in \Gamma_c^{hit} \right\} \quad (4-12)$$

In the case of self-contact, we are more used to address the two side objects of contact pair by “*hitting and target particle*”. The target particle can be any particle belonging to the global-boundary-remainder of the hitting particle. It can also be a particle belonging to the local-boundary-remainder of the hitting particle. Thus, a boundary may contact with itself, see Fig. 4-4.

Figure 4- 4 Self contact within single body

The hitting particle and the target particle must belong to two distinct particle sets, but these two distinct particle sets may both belong to the same contact surface or body. In this way, the relationship among the contact particle, contact particle set, contact surface, and contact body can be expressed as

$$x_c \subset \Gamma_c \subset S_c \subset \Omega_c \quad (4-13)$$

Suppose that when contact occurs, the outer surfaces of contact boundaries are tightly closed, and then the outer normal vectors of contact partners are antiparallel.

$$\mathbf{n}_3^A = -\mathbf{n}_3^B \quad (4-14)$$

According to the *Newton's third law*, we have

$${}^t\mathbf{P}^A + {}^t\mathbf{P}^B = \mathbf{0} \quad (4-15)$$

The above contact force in the local coordinate system is

$$\begin{aligned} {}^t\mathbf{P}^i &= {}^tP_3^i \cdot {}^t\mathbf{n}_3^i + {}^tP_1^i \cdot {}^t\mathbf{n}_1^i + {}^tP_2^i \cdot {}^t\mathbf{n}_2^i \\ &= {}^t\mathbf{P}_N^i + {}^t\mathbf{P}_T^i \quad (i = A, B) \end{aligned} \quad (4-16)$$

where ${}^t\mathbf{P}_N^i$ and ${}^t\mathbf{P}_T^i$ are normal and tangential components of ${}^t\mathbf{P}^i$, which follows

$$\begin{aligned} {}^t\mathbf{P}_N^i &= {}^tP_3^i \cdot {}^t\mathbf{n}_3^i \\ {}^t\mathbf{P}_T^i &= {}^tP_1^i \cdot {}^t\mathbf{n}_1^i + {}^tP_2^i \cdot {}^t\mathbf{n}_2^i \end{aligned} \quad (i = A, B) \quad (4-17)$$

At the same time, instantaneous velocities of particles in the local coordinate system have similar expression

$$\begin{aligned} {}^t\mathbf{v}^i &= {}^t\mathbf{v}_3^i \bullet {}^t\mathbf{n}_3^i + {}^t\mathbf{v}_1^i \bullet {}^t\mathbf{n}_1^i + {}^t\mathbf{v}_2^i \bullet {}^t\mathbf{n}_2^i \\ &= {}^t\mathbf{v}_N^i + {}^t\mathbf{v}_T^i \quad (i = A, B) \end{aligned} \quad (4-18)$$

Here, ${}^t\mathbf{v}_N^i$ and ${}^t\mathbf{v}_T^i$ are normal and tangential components of ${}^t\mathbf{v}^i$, which follows

$$\begin{aligned} {}^t\mathbf{v}_N^i &= {}^t\mathbf{v}_3^i \bullet {}^t\mathbf{n}_3^i \\ {}^t\mathbf{v}_T^i &= {}^t\mathbf{v}_1^i \bullet {}^t\mathbf{n}_1^i + {}^t\mathbf{v}_2^i \bullet {}^t\mathbf{n}_2^i \end{aligned} \quad (i = A, B) \quad (4-19)$$

2) Normal contact condition

Normal contact condition is an importance and most critical step in the whole contact checking procedure. It is not only the judgment on whether the objects fall into contact status, but also the necessary requirement to the contact pairs when the objects already encounter. At the same time, it performs as the sufficient condition to apply tangential contact force.

a) non-penetration condition

Non-penetration condition refers to the case when the configuration of any objects is not allowed to penetrate into others in the whole process of motion and deformation.

By assuming that the corresponding contact boundaries are relatively smooth, at least locally smooth, we can link every particle ${}^t\mathbf{x}^B \in {}^tS_c^B$ with a particle ${}^t\mathbf{x}_\xi^A \in {}^tS_c^A$ via the minimum distance definition,

$${}^td = d(\mathbf{x}^B \rightarrow \xi) = \min_{{}^t\mathbf{x}_\xi^A \in {}^tS_c^A} |{}^t\mathbf{x}^B - {}^t\mathbf{x}_\xi^A| \quad (4-20)$$

where the independent variable of the middle term “ $\mathbf{x}^B \rightarrow \xi$ ” means that any arbitrary point $\mathbf{x}^B$ of surface ${}^tS_c^B$, which can match the closest location ${}^t\mathbf{x}_\xi^A$ on surface ${}^tS_c^A$. Then, non-penetration condition is measured along the direction of ${}^t\mathbf{n}_3^B$, so normal gap is defined as

$${}^td_N = ({}^t\mathbf{x}^B - {}^t\mathbf{x}_\xi^A) \bullet {}^t\mathbf{n}_3^B, \quad \forall \mathbf{x}^B \quad (4-21)$$

Non-penetration condition can also be described as bellowed:

For any given point of surface ${}^tS_c^B$,

$${}^t d_N = ({}^t \mathbf{x}^B - {}^t \mathbf{x}_\xi^A) \cdot {}^t \mathbf{n}_3^B \geq 0, \quad \forall \mathbf{x}^B \quad (4-22)$$

$d_N > 0$ means that surfaces ${}^t S_c^B$ disconnect with ${}^t S_c^A$; $d_N = 0$ means that these two surfaces just touch each other; $d_N < 0$ means that the overlap takes place, where the penetration happens between ${}^t \Omega_c^A$ and ${}^t \Omega_c^B$.

Figure 4- 5 Distance of contact points pair

b) Normal contact pressure

As mentioned above, contact force's normal component is only compressive force without considering adhesion and welding between interfaces. From Eq. (4-15) and Eq. (4-17),

$${}^t \mathbf{P}_N^B \leq 0, \quad {}^t \mathbf{P}_N^A = -{}^t \mathbf{P}_N^B \geq 0 \quad (4-23)$$

3) Tangential contact condition

Tangential status on contact interface has three cases: sliding with friction, sliding without friction, and stick. From the view of constitutive modeling, there are two kinds of models: non-friction model and Coulomb friction model, which are

sufficient to describe the basic tangential contact cases.

a) Non-friction model

When the contact bodies are absolutely smooth, or the friction between is negligible, we can treat the tangential contact force to be zero. It is simply written as

$${}^t\mathbf{P}_T^A = {}^t\mathbf{P}_T^B = \mathbf{0}, \forall t \quad (4-24)$$

b) Coulomb friction model

When the friction is not negligible, Coulomb friction model is widely used in engineering analysis for its simplicity and easy manipulation. However, there are a lot of more precise friction models, which can be chosen, in traditional contact mechanics.

Coulomb friction model assumes that the tangential contact force, the value of ${}^t\mathbf{P}_T^i$, could not exceed its limits $\mu \bullet |{}^t\mathbf{P}_N^i|$, and

$$|{}^t\mathbf{P}_T^i| = \left[\left({}^t\mathbf{P}_1^i \bullet {}^t\mathbf{n}_1^i \right)^2 + \left({}^t\mathbf{P}_2^i \bullet {}^t\mathbf{n}_2^i \right)^2 \right]^{1/2} \leq \mu \bullet |{}^t\mathbf{P}_N^i| \quad (i = A, B) \quad (4-25)$$

where μ is frictional coefficient. When $|{}^t\mathbf{P}_T^i| < \mu \bullet |{}^t\mathbf{P}_N^i|$, there is no relative sliding between contact interface, therefore

$${}^t\bar{\mathbf{v}}_T = {}^t\mathbf{v}_T^A - {}^t\mathbf{v}_T^B = \mathbf{0} \quad \text{if} \quad |{}^t\mathbf{P}_T^i| < \mu \bullet |{}^t\mathbf{P}_N^i| \quad (4-26)$$

In the above equation, ${}^t\bar{\mathbf{v}}_T$ denotes the relative sliding velocity of particle pair.

When $|{}^t\mathbf{P}_T^i| = \mu \bullet |{}^t\mathbf{P}_N^i|$, there will be relative tangential sliding between contact interface, hence

$${}^t\bar{\mathbf{v}}_T = {}^t\mathbf{v}_T^A - {}^t\mathbf{v}_T^B \neq \mathbf{0} \quad \text{if} \quad |{}^t\mathbf{P}_T^i| = \mu \bullet |{}^t\mathbf{P}_N^i| \quad (4-27)$$

and,

$${}^t\bar{\mathbf{v}}_T \bullet {}^t\mathbf{P}_T^i = ({}^t\mathbf{v}_T^A - {}^t\mathbf{v}_T^B) \bullet {}^t\mathbf{P}_T^i < 0 \quad (4-28)$$

Eq. (4-28) represents that the relative tangential sliding velocity is always opposite to frictional force at interaction point. The frictional force prevents the motion tendency.

For better description on friction phenomena, additional discussion on the μ in Eq. (4-26) and (4-27) is made as below

- Frictional coefficient μ can be replaced by static frictional coefficient μ_s and dynamic friction coefficient μ_d . Generally, $\mu_d < \mu_s$.
- In a 3-D contact problem, a contact interface can be expressed as 2-D plane at least locally under a local coordinate system, shown in Fig. 4-6. The frictional coefficient is associated with texture direction as the interface might have different texture configurations, which are frequently seen in geotechnical engineering. In such case, it demands the vectorization of μ according to texture direction. It makes difficult to impose the tangential force.

Figure 4- 6 Vectorization of frictional coefficient μ

The complexity of the tangential force is not fully covered by the above mentioned cases only. The behavior of the contact interface would be further discussed in detail, which is described in the next section.

4.3 Constitutive Equation for Contact Interfaces

If the contact behavior of different material only described with normal locker and

c, ϕ value in the Coulomb friction model, it might be too rough. More detailed contact behavior among the contact interfaces is given in this section. For the sake of more precision needed to resolve the mechanical behavior in contact interface, different approaches have been established over the centuries. Although current version of 3-D NMM in this study has not yet directly employed the contents of this part, constitutive equations on contact interface are extremely necessary for future development. Hence, concise introduction and literatures are provided here.

4.3.1 Normal contact formulation

There are two main techniques to describe contact conditions in the normal direction: the constraint formulation of the non-penetration condition, and elastic or elasto-plastic constitutive laws of approaching contact area.

1) Stopped constraint formulation

This formulation assumes that the contact interface is smooth in micromechanical level. The non-penetration condition can be considered as a purely geometrical constraint. In this case, it is not necessary to specify constitutive relations in the contact interface. The mathematical description of non-penetration is stated as $d_N \geq 0$ (see Eq. (4-22)). Since adhesive stresses is not allowed in the contact interface throughout whole chapters in this research, the contact pressure always satisfies $p_N \leq 0$ (see Eq. (4-6)). This classical way to formulate contact constraint has been used by numerous researches, see [Johnson (1985)] or [Kikuchi and Oden(1988)].

In [Moreau (1974)], this constraint formulation is express by

$$d_N \geq 0, \quad p_N \leq 0, \quad p_N \bullet d_N = 0 \quad (4-29)$$

which is known as *HERTZ-SIGNORINI-MOREAU* conditions for frictionless contact [Wriggers (2002), p57]. It means, one has the conditions $d_N = 0$ and $p_N < 0$ for contact. If a gap between exists, then $d_N > 0$ and $p_N = 0$ hold.

The Eq. (4-29) leads to a non-smooth contact law for the normal contact compressive

force, as shown in Fig. 4-7.

Figure 4- 7 contact force versus normal gap

2) *Constitutive equation for normal contact*

Take geotechnical engineering projects for instance, ideal smooth contact face does not exist in real practice (shown in Fig. 4-8). The constitutive equations which include deformation of the micro structure on the contact surface are necessary for those problems with “high contact precision” requirement. The investigation to constitutive models for different material surface is based on the experiments, e.g. see [Greenwood and Williamson (1966)] or [Barton and Choubey (1977)].

Figure 4- 8 Rough surface geometry of rock mass [Barton and Choubey (1977)]

Most of the normal interface laws can be written in the form:

$$p_N = f(d_N) \quad \text{or} \quad d_N = h(p_N) \quad (4-30)$$

where f and h are nonlinear functions. For example, depending on a statistical model of the micro-geometry, the constitutive relation [Zavarise (1991)] for contacting surface in normal direction yields an exponential equation,

$$p_N = \frac{c_1 \cdot (1617646.152 \frac{\sigma}{m})^{c_2}}{5.589^{(1+0.0711c_2)}} \exp \left[-\frac{1+0.0711c_2}{(1.363 \cdot \sigma)^2} \cdot d^2 \right] \quad (4-31)$$

c_1 and c_2 are mechanical constants which express the nonlinear distribution of the surface hardness, σ and m are statistical parameters of the surface profile, representing the surface roughness and the mean absolute asperity slope.

In one word, most of constitutive models for normal contact could be viewed as nonlinear springs between the contact interfaces. Compared with Fig. 4-7, normal contact compliance law can be simply expressed as Fig. 4-9.

Figure 4- 9 Contact compliance law

4.3.2 Tangential contact formulation

The interfacial behavior related to frictional response is very important in most engineering applications. *Tribology* is related to these problems. Tribology is involved in situations, such as adhesion, wearing, lubrication, thermal contact or electric contact, which are beyond the scope of our study. More details refer to [Gohar (2008)]. This study will only restrict itself to more simple constitutive equations for frictional component.

1) *Coulomb law*

When the tangential component of contact force is triggering a certain limit (Eq. (4-7)), the contacting pairs no longer stick but slide between. Typically, this is described by the *Coulomb law* (see Eq. (4-9)), as in Fig. 4-10.

Figure 4- 10 *Coulomb's* friction law

Notably, the friction coefficient is influenced by other parameters like the surface roughness, the relative sliding velocity and so on. One such friction law incorporating the relative velocity in engineering practice is given by

$$\mu(\mathbf{v}_T) = \mu_D + (\mu_S - \mu_D)e^{-c|\mathbf{v}_T|} \quad (4-32)$$

where μ_S is the static friction coefficient; μ_D is the dynamic friction coefficient; c describes the speed of decaying from static value to dynamic one, shown in Fig. 4-11.

Figure 4- 11 Velocity dependent *Coulomb's* friction law

2) Regularization of the coulomb law

A regularization of the stick-slide behavior are proposed by [Oden and Pires(1983)]. They are founded on a functional form to yield a smooth transition from the state of stick to sliding. The formulation is

$$\mathbf{P}_T = -\mu\varphi^i(\mathbf{v}_T)|\mathbf{P}_N| \quad (4-33)$$

where the function φ^i describes different smooth transition strategy[Raous 1999], as shown in Fig. 4-12.

Figure 4- 12 Regularization of *Coulomb's* friction law

3) Elasto-plastic model for friction

The elasto-plastic constitutive model for friction is firstly suggested by [Courney-Pratt and Eisner (1957)] through the results of experimental observations, as depicted in Fig. 4-13 [Courney-Pratt and Eisner (1957)].

Figure 4- 13 Friction coefficient versus tangential movement

Thereafter, Michalowski and Mroz (1978), Curnier (1984), Wiggers (1987), Laursen and Simo(1993) developed various constitutive equations for frictional problem in the elasto-plasticity framework. The branch of constitutive model divides tangential motion d_T into a elastic stick part d_T^e and a plastic sliding part d_T^p , depicted in Fig. 4-14.

Figure 4- 14 Kinematical split of slide state and elastic stick state

Finally, they generalize the classical *COULOMB* frictional cone to fit a more applicable and general sliding surface, as shown in Fig. 4-15.

Figure 4- 15 Coulomb friction cone to fit general slide surface

4.4 Contact Checking Algorithm

4.4.1 Significance and Difficulties

In the previous section, the basic formulation of contact problem, the different constitutive models describing the contact interface have been discussed. There is, however, another important topic has not been discussed sufficiently yet. It is about how to warn potential contacting zones and to locate contacting zones reliably and efficiently. It is so-called *contact checking procedure* (searching/detection).

1) *Why it is necessary to discuss this topic?*

Although contact problem has been considered for hundreds of years, contact checking issue has not been paid enough attention by researchers, even after that contact mechanics has already become a mature discipline. No one seems to realize that it would become an important topic in numerical simulation. Intuitively, applying equivalent contact boundary conditions accurately is crucial to a contact problem. Through these treatments on contact constraints, we are able to analyze the contact mechanism among materials at least qualitatively. To the question of “when and where the contact happens”, it was supposed to be relatively simple by mistake. Consequently, the major focus of the contact literature in the early stage is how to implement the contact constraints assuming that the possible contact points are already known [Benson and Hallquist (1990)]. In fact, this misunderstanding is plausible as incipient contact problems limit themselves in simple one-to-one contact cases in 2-D. Their non-complex geo-configuration, non-fine mesh, and less contact body make researchers easy to neglect the importance of “*contact detection*” part in algorithm.

Contact detecting has attracted attention since 1990s. Along with the highly developed computer technique, scholars are ambitious to utilize the numerical simulation to go beyond the framework of structural static mechanics, in more complicate and dynamic engineering application (e.g., a car crash or fragmentation of brittle material; rock fall hazard in geotechnical engineering). These efforts bring new desire on the topic of contact checking strategy, as researches find that contact

adds a significant cost to the overall solution even when the ratio of the number of contact points to the number of elements is small.

2) The difficulties of the topic come from few aspects as below:

Firstly, in engineering applications, contact bodies have arbitrary geometries and undergo large displacement and large rotations. Large sliding among contacting boundaries is not predictable. Contact may occur or disappear at non-predictable places on any contact boundary involved at any time instant. Meanwhile, the area of contact interface can change their size and locations. Additionally, once the fracturing processes are considered, new contact surfaces are generated due to the splitting of material mass into pieces during the time/load step. Altogether, the algorithm has to be well designed to cover complicated situations in geometrics.

Secondly, diverse application fields have different requirement to the contact algorithm. A general contact checking algorithm, in principle, is not obligatory to distinguish application areas, but contact situation and key issues varies. For example, numerical methods are mostly used in two major areas.

- a)* Mechanical engineering, such as the automobile collapse analysis. Its calculation involves performing large plastic deformation (crash and buckling). Large deformation will cause complex self-contact issue.
- b)* Geotechnical engineering, for discontinuous blocky system such as tunnel, excavation, and rock slope. These rocks do not undergo large deformation, but large displacement/rotations and un-regular shape itself. All these contribute the complexity of contact problem. Therefore, suitable algorithm is required to fit different practical applications.

Lastly, the process of contact checking operation is quite expensive in computational cost. Since the total number of contacting pair is unknown prior to the solution of the problem, most of the computation time has to be devoted to searching and checking.

For explicit time integration methods, contact checking has to be performed in every time or load step of the numerical simulation. In implicit time integration schemes, a trial-and-error iteration is necessary in each time/load step. If such a check has to be carried out at each iteration step, the checking operations will dominate the overall time for the computation.

Contact checking algorithm is carefully designed to fulfill the efficiency standard as a frequently used subroutine. Besides, the design of contact checking algorithm is also a difficult scheme with strong logic. The contact behavior among bodies always happens at unfolded topological spatial entities layers, which could be surface, facet, edge, and vertex. Obviously, checking every object against all other objects will, of course, work, but is too inefficient to be used when the number of objects is large, especially in 3-D cases. It demands that data structure should be organized well.

All these aspects define a vivid research field in which new fast algorithms are constructed based on different mathematical approaches and computational architectures - an optimal contact warning/ detection/ tracking procedure.

4.4.2 Literatures on contact warning-detection-tracking techniques

Contact algorithm has hitherto been explored tremendously in different research fields and has a lot of category. For instance, the contact algorithm aimed to graphical display and 3-D animation in computer science discipline. It normally is approximate solutions with high calculation speed. Another example is in the area of operation planning, which aims to guide robots' motion. This is known to be hyper-accurate, but lack of general principles in mechanics.

In this study, it focuses on the contact algorithm for mechanical analysis in numerical simulation. This line of researches starts from 90s in the last century. Two well-developed branches of contact checking algorithm are:

- 1) Under continuum mechanics, e.g., FEM, FDM. They focused on large deformation cases (Shell component in automobile design).
- 2) Under dis-continuum mechanics, e.g., DEM, DDA. They focused on large

displacement cases (rock mass in slope or tunneling design).

This study focuses on developing 3-D NMM under Lagrangian framework. All listed algorithm has been proven to applicable in various analytical situation. However, the properties of the different methods make them suitable for different types of problems.

Figure 4- 16 Category of contact algorithm by checking method

Two specific approaches developed under the Lagrangian framework are worth to be mentioned at first, *MSC* and *SSC*. Most of checking algorithm historical evolution begins with discussion of these two approaches.

The *MSC* algorithm is preferred in two-surface contact situations when self-contact within one surface is not expected, since it is more efficient than the *SSC* algorithm in these types of problems. The single-surface algorithm is intended for problems with highly distorted contact surfaces and for situations where self-contact within one surface can occur.

These two methods have successive relationship. *MSC* is raised in early stage to simple contact types (vertex-to-facet, facet-to-facet). It needs to appoint potential contact range artificially and it is for one-to-one contact situation. Although *MSC* is quite limited, it has induced the original foundation for introducing contact mechanics into numerical simulation. In practical application, *MSC* represented approaches require much manual intervention. Furthermore, its simple contact type and non-available for self-contact become an obstacle to further development.

To overcome *MSC*'s limitation, *SSC* is proposed later. *SSC* has committed itself on automatic contact checking. It generates a contact surface to cover each contact body. Through the geometric relationship among entities on contact surface (vertex, edge, facet), automatic contacting judgment works, instead of manual intervention. In terms of automatic fulfillment, *SSC* can be considered as innovation. Actually, direct searching method with brute force searching algorithm (*BFSA*) is one of *SSC* method. When applying *BFSA*, another serious problem merges, which is huge computation burden. Benson and Hallquist (1990) proposed *SSC*, together with Bucket sort algorithm (*BSA*) to reduce the *BFSA*'s computation burden. Even though *BSA* has made great effort compared to *BFSA*, its performance is still normal. It does inspire latent researchers to look for better efficient contact checking procedure, to further reduce the computer time consumption for the contact search with order of N^2 (N is the number of vertex in system).

In summary, *MSC* and *SSC* (with *BFSA*) are actually two extreme cases in dis-continuum contact algorithm in its historical evolution path. Their purpose is to deal with contact boundary conditions in multi-body numerical simulation. The former has high calculation speed, but involves too much manual intervention, especially facing abundant contact pairs or complex contact situation in dynamic analysis. The latter one is automatic, however, with slow calculation speed. Similarly, when calculation quantity is quite large, the analysis is hard to proceed for computer. Therefore, it is necessary to find a balance between these two extreme examples. The approaches developed later-on by other researchers are mostly built to balance these two methods.

In this section, I will firstly categorize the previous works under Lagrange framework. Further instructions will not distinguish the specific algorithm category, as the general contact algorithm is not limited by these groups. Especially in 3-D NMM as mentioned in previous chapter, NMM could be seen as a unified method. Its contact checking algorithm is also compatible to both FEM and DDA.

In general, locating and tracking the contact zone has been split into *three phases*:

- a) *Contact warning*: spatial search for objects which **might possibly** come into contact; (also called global searching)
- b) *Contact detection*: determination of pairs of objects which **actually intersect** and hence are in contact;(also called local searching)
- c) *Contact transferring*: record the state of each contact pair (open-close/lock sliding situation) for reference to next iteration/time/load step contact checking.

These three phases are related to purely geometrical consideration, and only depend on the geometric information of contact bodies.

Phase I:

Fig. 4-17(a) has illustrated a relatively simple case of potential contact by four different discretization bodies. It is not advised to check the contact of one node against each other on other bodies' surface. Another example is given to find possible

contact partners for the black sphere with in a set of spheres as in Fig. 4-17(b). Simply, it is only necessary to check the vicinity area for the black sphere in such case. In the computer science, this feature is referred to as the “nearest neighbor problem” [Knuth (1998)]. Obviously, this step could be called “pre-location” to highly reduce unnecessary local detection operation for real contact.

Figure 4- 17 Discrete contact demonstrations

In this phase, it should be sufficient enough to use relatively rough description on the objects, such as through bounding boxes and surrounding sphere as shown in Fig. 4-18. The coarse description gives the benefit of high speed and low cost on computation efficiency when sorting subroutines.

Figure 4- 18 Bounding box and surrounding sphere of a contact body

It has now been developed some sorting methods to numerical studies. One example is the nested sorting, mentioned in Benson and Hallquist (1990). They firstly

implemented the nested sorting method to find potential solutions for large deformation contact problems in their finite element numerical studies. In Fig. 4-19, the space is separated into divisions of square cells or buckets, each of which is surrounded by eight neighbors in 2-D and twenty-six buckets in 3-D.

(a) Position cells in 2-D view

(b) Position buckets in 3-D space

Figure 4- 19 Nest sorting searching algorithm

[Benson and Hallquist (1990) p148] [Oldenburg and Nilsson (1994) p370]

In the process of contact searching (e.g., case in Fig. 4-20), it is only necessary to search the central colored bucket. Therefore, it will result in a scheme with almost $O(N)$ operations through programming carefully.

Figure 4- 20 Bucket search for contact

A relatively more delicate 3-D sorting routine was referred to as “*Hierarchical ordering*”(HO) in Zhong and Nilsson (1989). The method of HO is more intuitively, where it tries to construct a tree-like data structure over the surface of the mesh. Under a given time step or displacement increment of one global search, HO method can set up a hierarchical structure. The generated hierarchical structure then is used to determine the potential contact location, among bodies, part of bodies, surfaces or parts of the surfaces (refer to [Zhong (1993)]). Further development on this branch, continued by Oldenburg and Nilsson (1994), they suggested the *linear position code*. In their method, a lot of small square boxes were gained through dividing search domain, and their positions were kept in position index codes through all the lines. With the help of this single index, it was not difficult to locate their neighbors. The location of contact bodies and their neighbors were easily determined simultaneously.◦

Another algorithm was introduced by Belytschko and Neal (1991) for global searching. In their *pinball algorithm*, they determined contact searching by judging overlapped situation for pinballs through embedding a sphere for each element. Furthermore, Williams and O’Connor (1995) proposed the *heapsort algorithm*. Other advance algorithms were also suggested for efficient global searching, including alternating digital tree method [Bonnet and Peraire (1991)], Double-Ended Spatial Sorting (DESS) algorithm [Perkins and Williams (1995)], NBS algorithm [Munjiza and Andrews (1998)], a space filling curve technique [Diekmann *et al.* (2000)].

Wriggers P (2002) summarized sorting strategies as

- *Grid cell algorithms.* This kind of algorithm is to contain discrete solids into uniform cells through subdividing the simulation space, as in Fig. 4-21 (a). . Such algorithm is quite suitable for equally distributed elements within cells, while it does not work well for the case when elements in some cells cluster together. Adaptive grids are used to extend the algorithm to consider heterogeneous element distribution, as in Fig. 4-21(c), which unluckily increases the cost of computing for the adaptive grids.
- *Octree method.* This algorithm only keeps cells containing finite elements in the tree structure, as in Fig. 4-21 (b). Searching time is highly dependent on first construction of the octree, mentioned in Williams and O'Connor (1999), which results in high speed of creating octree and evaluating ($O(N\log N)$ operation) in its spatial searching with the help of techniques such as balancing tree branches and minimizing octree depth (e.g., [Williams and O'Connor (1999)]; [Knuth (1998)]).
- *Spatial heapsort algorithm.* This method sorts a list of elements by increasing co-ordinates along the axes of the simulation space, which is proposed by Williams and O'Connor (1995). This algorithm could be combined with body-based cells, as in Fig. 4-21(d). This algorithm has the advantage that it does not require special data structure, thus it is not sensitive to object/element's spatial distribution. This advantage helps to reduce computational storage, 10 times less than octree method. The time performance is of order of $O(N\log N)$ to sort an unordered set of N elements.
- *Double-Ended Spatial Sorting (DESS) algorithm.* This method and similar other methods are insensitive to the object size, developed by Perkins and Williams (1995). The feature of insensitivity to object size makes them suitable for discrete finite element analysis when sizes of finite elements chunk broken off are not ex-ante predictable. It has a performance of order $O(N\log N)$, and N is the number of contacting objects.

Figure 4- 21 Different sorting strategies [Wriggers (2002)]

Phase II:

Once two blocks are detected to have potential real contact through Phase I, it has to further determine the real position of the contact. It is better to get the specific contact position at which level for the contact object pairs, and their contact direction. It is also the main task of the Phase II. Actually, the second stage of contact detecting process is the essential part of the contact checking algorithm. The advantage and disadvantage of different checking algorithm are originated from the design of Phase II.

Although the contacting check algorithm for 2-D problem is not completed yet, it has still well-developed, e.g. DDA contacting searching, common plane algorithm of UDEC, etc. 2-D studies being of little interest in this thesis because of abundant literatures existed, their further discussion is to assist the complete understanding to 3-D algorithm. It will be concentrated on 3-D contact detection techniques in this section.

a) Master-Slave contact method (*MSC*)

For historical reasons, studies on contact problem in early stage do not involve with large displacement, large deformation, and self-contact. Such simplified contact algorithms need to artificially predict contact boundaries or its probably happening range in advance. More specifically, users manually identify the potential contacting zone, and make the *Master surface* to be the one side of surface with the relatively coarse mesh, convex face, and hard material property. The other surface is endowed with *Slave surface* as defined. Contact checking and contact object matching are only operating on the manually pre-assigned contact surface. If consequent contact interaction is out of this range, this method will miss it.

The *M-S* contact algorithm is only suitable for one-to-one contact analysis. The artificially pre-assigned potential contact sets (*M-S* surface) reduce the searching range and increase the hitting rate of detection, however, it has to involve human-intervention.

b) Single surface contact algorithm (*SSA*) and brute force searching algorithm (*BFSA*).

The concept of single contact surface was firstly raised by Benson and Hallquist (1990). The term of “single” is corresponding to the traditional two-surface contact algorithm (*MSC*). It suggests cover each contact body with a single exterior surface. Then, it will automatically implement contact checking operations within a single surface or among those single surfaces. The innovation of the single surface concept gives a fresh idea to the contact checking algorithm, and turns a new page on its

development. After the concept of single surfaces, the contact mechanics start to enter computer era. The problem of self-contact after large deformation becomes readily solvable.

Originally, the method of *SSA* does not involve Phase I, which is called “direct checking algorithm”, or exhaustive searching, or brute force searching algorithm. It is proposed before the concept of single surfaces. It is the simplest approach through testing all possibilities for contact interaction by trivial contact search algorithm. It is easily to imagine that it could engage large computer burden. The required calculations amount in *SSA* is proportional to second power of the boundary objects (segments, edges, vertexes) number, as discussed in the previous sections.

Even though Benson and Hallquist utilized the nested sorting logic (phase I checking process) and nearest neighbor local searching logic, which attempted to reduce the computation costs, their extension method was still under the framework of direct searching. In other words, they did not make full use of hierarchical order among the contact objects in the contact system essentially. This induced the possibility to reduce large non-necessary contact checking to decrease the large computing burden. Several latter enhanced contact checking(searching) algorithms follow such original intention.

c) Hierarchy Territory algorithm (*HTA*)

Compared to direct searching algorithm, hierarchy territory algorithm (*HTA*) [Zhong and Nilsson (1996)] classified the information in the contact system to avoid the non-necessary non sense contact checking judgment. It was firstly realized in finite element program of DYN3D, and used to analyze the car crash and thin wall construction collision. DYN3D later on developed into nowadays widely used commercial software LSDYNA. *HTA* classified contact system information into 4 hierarchies: contact bodies, contact surfaces, contact facets and contact vertexes. In order to increase the contact searching efficiency, each contact hierarchy object could assign its corresponding territory. The contact checking is to determine whether contact objects have entered into others' territory to match. In this way, the contact

checking is narrowed down to find out the distance relationship between contact vertex and contact facet. The idea is then extended to my proposed 3-D NMM contact checking algorithm.

d) Splitting pinball method (SPM)

The splitting pinball method [Belytschko and Yeh (1993)] was built upon the concept of “pinball hierarchy”. The thought of the method is to assign each contact body into its corresponding spherical space in the system. The spherical space is split into smaller ones gradually, which creates “pinball hierarchy”. By this way, contact checking and the match between contacting partners are simplified to occur among the layers of pinballs. The specific contact base position is determined through searching among the layers of pinballs step by step. When the detailed position and sizes of pinballs are in determination, it is relatively simple to judge the overlapping status among the pinballs. Its detailed steps are sketched in Fig. 4-22.

In other words, the interpenetration check can be simplified by enforcing it only on a set of spheres embedded within the elements in the pinball contact algorithm. Once it is detected to have interpenetration of parent pinballs, the parent pinball is split into a hierarchy of descendent pinballs.

(b) Level 1

(c) Level 2

(d) Level 3

Figure 4- 22 Interpenetration detection among active pinballs and their descendants

e) Inside-outside search algorithm (*IOA*)

The technique of inside-outside searching algorithm (*IOA*) is applied to match node and segment in FEM. When a contact is found approaching a surface segment, the algorithm will perform a local search process, which helps to determine the candidate contact point on the contact surface and the distance. Whereas implementing *IOA* might come across some exceptional situations, as in Fig. 4-23.

Figure 4- 23 Special situations in matching a contact node with a contact segment

Fig. 4-23 gives the special case of multiple contact candidates, which is known as “*deadzone*” in FEM [Zhong and Nilsson (1990)]. To the problem of “*deadzone*”, it defines the *mesh normal vector* to impose the contact condition to aid the matching process in the inside-outside algorithm, which was suggested by [Wang and Nakamachi (1997)]. It gains the normal of a node by taking average on all surface normal vectors of its adjacent element segments, as in Fig. 4-24.

Figure 4- 24 Definition of mesh normal

With the definition of mesh normal and simply judgment on which segment the node projects along the mesh normal direction, contacting node will exclusively match with one contacting segment.

The so-called “inside-outside” is to determine whether projection point falls at the same side of edges along the natural edge sequence of the segment, as shown in Fig. 4-25.

Figure 4- 25 The inside-outside logic for contact searching

f) Common plane method (*CPM*)

The common plane method is proposed by [Cundall (1988)], which is used in 3-D DEM. The “common plane” is analogous to an auxiliary rigid plane, which is hanging loosely between the contacting blocks (see Fig. 4-26).

Figure 4- 26 Visualization for positioning of common-plane in response to block geometry [Itasca Consulting Group (2003)]

Along with the movement of contacting blocks, the rigid plate could real-time translation or rotation until the contacting blocks contact. At this moment, the plane, where the rigid plate stays, is the Common Plane (abbreviated as C-P). After determining C-P, the contact checking between is turned into contact checking between blocks and C-P, whatever the shape and orientation of the contacting blocks. Hence, it becomes relatively simple to search the candidate of contact pairs and judge the contacting relationship among blocks.

In FEM, similar procedure was referred to as “*Mortar method*” [Simo *et al.* (1985)]; [McDevitt and Laursen (2000)], which is a special technique to enforce contact constraints in the discretized system for non-matching meshes. Mortar side in the interface is defined by the so-called “intermediate contact surface”, as shown in Fig. 4-27.

Figure 4- 27 Definition of intermediate mortar surface

g) Penetrated edges method (*PEM*)

The penetrated edges method [Chen *et al.* (2004)] fits for the contact judgment between convex polyhedrons. When contact happens between two convex polyhedrons in the space, there will be non-empty intersection set among blocks. The non-empty intersection is called “*penetrated body*”. The edges of the penetrated body are also of the convex polyhedrons, and these edges are called “*penetrated edges*”. In order to determine the contact mode between blocks, the penetrated edges are classified into 5 types, as shown in Table 4-1.

Table 4- 1 Penetrated edge type

Type	Edge feature	Length Feature
1	2 original point	With Length
2	1 original point; 1 truncation point	With Length
3	1 original point; 1 truncation point	Non-Length
4	2 truncation point	With Length
5	2 truncation point	Non-Length

Table 4- 2 Contact types and corresponding penetration information

Contact type	Penetrated Edge Property
Vertex-to-vertex	$N_A^{original} = N_B^{original} = 1$ $\begin{cases} N_A^i > 0, N_B^i > 0 & i = 3 \\ N_A^i = 0, N_B^i = 0 & i \neq 3 \end{cases}$
Vertex-to-edge	$N_A^{original} + N_B^{original} = 1$ $\begin{cases} N_A^3 > 0, N_B^5 = 0 & \text{if } N_A^{original} = 1 \\ N_B^3 > 0, N_A^5 = 0 & \text{if } N_B^{original} = 1 \end{cases}$
Edge-to-edge	$\begin{cases} N_A^i = 1, N_B^i = 1 & i = 5 \\ N_A^i = 0, N_B^i = 0 & i \neq 5 \end{cases}$
Edge-to-edge overlap	$N_A^1 + N_A^2 + N_A^4 = 1$ $N_B^1 + N_B^2 + N_B^4 = 1$ $2 \leq N_A^{original} + N_B^{original} \leq 4$
Vertex-to-facet	$N_A^{original} + N_B^{original} = 1$ $\begin{cases} \sum_i N_B^i = 0 & \text{if } N_A^{original} = 1 \\ \sum_i N_A^i = 0 & \text{if } N_B^{original} = 1 \end{cases}$
Edge-to-facet	$N_A^1 + N_A^2 + N_A^4 + N_B^1 + N_B^2 + N_B^4 = 1$
Facet-to-facet	$N_A^1 + N_A^2 + N_A^4 + N_B^1 + N_B^2 + N_B^4 \geq 3$

where $N_A^{original}$ represents the number of points that contacting body is in penetrated body. N_A^i is the number of penetrated edge in the contact type index I in block A.

According information of penetrated edges and the number of function points in the penetrated body of the contacting body, it could determine the contact mode between contact pairs.

h) Inscribed sphere method (ISM)

The method of inscribed sphere method [Ahn *et al.* (2009)] is proposed to avoid the

difficulty in determination of the unit normal in edge-to-edge, edge-to-vertex, and vertex-to-vertex cases. Its basic idea is through installing an inscribed sphere into each vertex, as shown in Fig. 4-28.

Figure 4- 28 Inscribed spheres and penetrated plane

The real contact happens between the inscribed sphere, and contact force direction can be gained through connecting the center of the sphere. The type of vertex-to-facet and vertex-to-edge could also be changed into one or more contact mode of sphere-to-sphere.

Figure 4- 29 Exaggerated free drop test process

This algorithm is actually an approximate method, which avoid the difficulty of

direct determination. However, when more than 3 facets exist to form one vertex in rock engineering, it is hard to get reasonable inscribed sphere. Especially, the detailed geometric shapes of sharp vertex have significant effect on strains between blocks and the motion direction of the blocks.

Phase III:

The purpose to record the information is also to decrease the computation costs. In DDA [Shi (1988)]/NMM [Shi (1996b)], Phase III is also called “*contact transfer*”. The contact transfer is to transfer the contact position and status of same contact pairs from the current time step/load step/iteration step to the next step. In this way, it fulfills the requirement of continuous description to the contact process in time domain.

As the number of contact point is unknown at the beginning of each time step/load step, it has to apply try and error procedure to gain its value. This also involves the problem of initial value setting. Hence, one of the tasks in this Phase is to provide necessary foundational information for choosing initial value setting for the next time step.

4.5 Numerical Treatment of Contact Constraint

After contact checking procedure, locations of contacting zones are confirmed. The contact interface condition in *Section 4.2.1* builds up modified energy functional as an additional constraint to unknown $\mathbf{u}$.

$$\Pi^* = \Pi_u + \Pi_c \quad (4-34)$$

where Π_u is total energy without contact constraint condition in original continuous problem. Π_c indicates the component to total energy caused by contact constraints.

There are several different strategies to find the maximum/minimum of a function subject to constraints, such as

- 1) The Penalty Method
- 2) The Lagrange Multiplier Method
- 3) The Augmented Lagrange Method
- 4) The method of direct elimination of the geometrical contact constraints[Wriggers (2002)]
- 5) The Nitsche method, which enforces geometrical constraints in a weak sense.
- 6) The perturbed Lagrange formulation which combines (1) and (2) in a mixed form [Oden (1981)], [Simo *et al.* (1985)]
- 7) The barrier method [Bazaraa *et al.* 1993]
- 8) The cross-constraint method which combines the penalty and barrier methods. [Zavarise and Wriggers 1997]

Each of them has its advantages and drawbacks. Recently, most standard numerical codes (Ansys, Lsdyna, 3DEC, 2-D DDA/NMM), which are able to handle contact problems, use the first three methods. Hence, this thesis provides detailed discussion on the first three methods. It is worth to notice that the current version of 3-D NMM in this study utilizes the first method.

4.5.1 Penalty method

Penalty scheme is used most widely for its simplicity. It provides adaptable and robust algorithm for many application. However, it is also clear that the penalty method is just an approximation of the correct contact constraints. It approaches the exact result under the penalty parameters $k_N, k_T \rightarrow \infty$. In real computational applications, it is not possible to use very large penalty parameters, since it would lead to an ill condition for the coefficient matrix.

A penetration between contact bodies is accepted in this method, but it needs to be controlled via the so-called *penalty parameters*.

Then, the formulation for the contact contribution is

$$\Pi_c^{PT} = \frac{1}{2} \int_{\Gamma_c} \left[k_N \cdot (d_N)^2 + k_T \cdot \mathbf{d}_T \cdot \mathbf{d}_T \right] d\Gamma \quad (4-35)$$

k_N and k_T represent the penalty parameters. d_N and $\mathbf{d}_T$ are the normal and tangential gap functions. Their definition can be found in *Section 5.2.1* and *5.2.2*. The above equation represents pure stick state. The variation yields

$$C_c^{PT} = \int_{\Gamma_c} (k_N \cdot d_N \cdot \delta d_N + k_T \cdot \mathbf{d}_T \cdot \delta \mathbf{d}_T) d\Gamma \quad (4-36)$$

If it is under frictionless condition in contact interface, the second terms in the bracket are required to be eliminated. The slide condition would lead to

$$C_c^{PT} = \int_{\Gamma_c} (k_N \cdot d_N \cdot \delta d_N + \mathbf{P}_T \cdot \delta \mathbf{d}_T) d\Gamma \quad (4-37)$$

where the second term in bracket follows one of the frictional laws from *Section 4.3.2*.

4.5.2 Lagrange multiplier method

Classic Lagrange multiplier method is pioneer method that is applied as one way to solve block contact problem. It depicts contact strain energy into the produce of unknown contact force λ and penetration distance d . As increased unknown λ , the classic Lagrange multiplier method has to increase system balance equation dimension number[Brunßen *et al.* (2007)]. Meanwhile, it also provides better and more stable results in contact problem solution.

In this formulation, the Lagrange multipliers add constraints to a weak form.

$$\Pi_c^{LM} = \int_{\Gamma_c} (\lambda_N \cdot d_N + \lambda_T \cdot \mathbf{d}_T) d\Gamma \quad (4-38)$$

where λ_N and λ_T are the Lagrange multipliers.

The variation of constraints form is

$$C_c^{LM} = \int_{\Gamma_c} (\lambda_N \cdot \delta d_N + \lambda_T \cdot \delta \mathbf{d}_T) d\Gamma + \int_{\Gamma_c} (\delta \lambda_N \cdot d_N + \delta \lambda_T \cdot \mathbf{d}_T) d\Gamma \quad (4-39)$$

The first term of the right hand side is associated with the virtual work of the Lagrange multipliers along the normal and tangential variation of gap functions. The second term describes the enforcement of the constraints. The physical meaning of the Lagrange multiplier λ_N is the value of contact force $\mathbf{P}_N$. The terms $\lambda_T \cdot \delta \mathbf{d}_T$ and $\delta \lambda_T \cdot \mathbf{d}_T$ are identified as the tangential sticks. In the pure stick case, the relative

tangential motion $\mathbf{d}_T$ should be equal to zero. It leads the physical meaning of λ_T become the reaction force in tangential direction, which is a vector.

When the slide situation happens between the contact interfaces, a tangential friction vector $\mathbf{P}_T$ is calculated from the constitutive laws (see *Section 4.3.2*), which leads

$$C_c^{LM} = \int_{\Gamma_c} (\lambda_N \cdot \delta d_N + \mathbf{P}_T \cdot \delta \mathbf{d}_T) d\Gamma + \int_{\Gamma_c} (\delta \lambda_N \cdot d_N) d\Gamma \quad (4-40)$$

It is similar and easy to get the frictionless functional expression.

4.5.3 Augmented Lagrange multiplier method

The Augmented Lagrange Multiplier Method is extended from Classic multiplier Lagrange Method. It heritages the simplicity of its penalty method, and solve the problem of incremental dimension of system equations in the classic multiplier Lagrange method in the meanwhile. The main idea is to combine either the penalty method or the constitutive interface laws with Lagrange multiplier methods.

The augmented Lagrange functional is described in detail in [Pietrzak and Curnier (1999)].

$$\Pi_c^{AL} = \int_{\Gamma_c} \left(\lambda_N \cdot d_N + \frac{k_N}{2} \cdot (d_N)^2 \right) d\Gamma + \int_{\Gamma_c} \left(\lambda_T \cdot \mathbf{d}_T + \frac{k_T}{2} \cdot \mathbf{d}_T \cdot \mathbf{d}_T \right) d\Gamma \quad (4-41)$$

with the augmented Lagrange multipliers $\hat{\lambda}_N = \lambda_N + k_N \cdot d_N$ and $\hat{\lambda}_T = \lambda_T + k_T \cdot \mathbf{d}_T$

The variation is

$$C_c^{AL} = \int_{\Gamma_c} (\hat{\lambda}_N \cdot \delta d_N + \delta \lambda_N \cdot d_N) d\Gamma + \int_{\Gamma_c} (\hat{\lambda}_T \cdot \delta \mathbf{d}_T + \delta \lambda_T \cdot \mathbf{d}_T) d\Gamma \quad (4-42)$$

Note that λ_N and λ_T is not an additional variable, but an estimate of the correct contact force. To approach the real contact force, another local iterative process is necessary. The advantage of this numerical treatment is that satisfaction of non-penetration constraint can be improved even if penalty parameters k_N and k_T are much smaller than that in the pure penalty method via repeated application of the augmentation procedure.

Chapter 5 Contact Mechanics -- 3-D NMM

5.1 Overview

Many aspects of contact problem have been discussed in the previous chapter, and specific techniques have been reviewed systematically. This section will try to find a tractable solution procedure for contact problem, based on 3-D NMM characteristics, requirements and the aspects covered. The following parts will be discussed in this section. The difficulties and characteristics of NMM contact checking algorithm will be stated firstly. Detailed checking procedure will be introduced. Then, penalty method will be selected as the treatment of contact constraint, and general contact solution procedure in 3-D NMM (implicit time integration) are analyzed finally.

The process of locating and tracking the contact zone is split into three operation phases: *Contact Warning*, *Contact Detection*, and *Contact Transferring*. A new hierarchical contact system is introduced to establish efficient scheme. The background mathematical mesh, one special definition of NMM, with mathematical patterns has been firstly utilized for contact warning phases. The contact detection phase matches lower level primitive hierarchies, and confirms the contact type of each contact pair candidate. Finally, four basic types of contact pair have been transformed into only two essential contact modes: *point to plane mode* and *crossing lines mode*. The detailed contact information are recorded under the re-formed contact mode environment, and also transferred to the next iteration or time/loading step.

5.2 Difficulties and Characteristics of Contact Technique in NMM

The contact checking algorithm in 3-D NMM has three phases: warning, detection, transferring. Not all the contact checking algorithm mentioned in the previous section is suitable for the NMM requirement, because of its particular features. In

fact, the specific techniques that fit for NMM are not constrained from the classification of Phase I or Phase II discussed in previous chapter. In other words, the function under the Phase II framework can be applied to fulfill the global searching requirement, and vice versa.

Notably, the inadequacy for the searching algorithm in *Section 4.4* might not be their weakness. Each algorithm has its own usage and range of application, therefore, it is a “*hasty generalization*” way to prove the advantage of one method through criticizing other algorithms. Instead, one should make use of previous knowledge in order to find proper contact algorithm, based on fully understanding past NMM theory and its application features. This is a better way of heritage and future extension.

Particular Features of NMM and applications:

- 1) Designed application of NMM is for geotechnical engineering calculation. The shape of rock mass is quite random, which makes the complexity of the contact types, compared to cases in mechanical engineering. This demand is similar to DDA and DEM.
- 2) FEM chooses tetrahedron and hexahedron as basic element in 3-D cases, which produces triangular and convex quadrilateral components of the contact surfaces. On the contrary, NMM can choose arbitrary shaped polyhedron as its manifold element, which produces corresponding arbitrary polygon facets of contact surfaces.
- 3) NMM is born with mathematical mesh in the background. The mathematical cells, generated by this mesh, normally are implicitly hidden, and are only employed in calculation. As its natural regularity, mathematical cell enclosures manifold element as “halo”. Actually, the background mesh is not only one part of definition, but also can be utilized into contact checking procedure. Hence, it replaces buckets or position boxes of manifold element, even contact territories of manifold element.

Due to the listed particular features, many contact checking algorithm, suitable for either continuing or discontinuing framework, cannot be applied directly onto 3-D NMM. It requires further improvements or even combination. The contribution of this research is to explore a viable and efficient notion to enable 3-D NMM with handling capacity to contact problem, from these previous works. Those algorithms, which are not applied here, are not consistent with 3-D NMM conception in some sense.

Take inside-outside algorithm (*IOA*) as an example, it is proposed under FEM. The components of contact surface are mainly triangular and convex quadrilateral segment as mentioned. The Inside-outside algorithm works well under these conditions, as these two kinds of shape are all convex, and it is very easy to determine whether one projection point is inside relative to all the edges of the surface segment or not, simply making use of fencing edge equations. Studies show the inside-outside algorithm is a highly efficient contact local detection algorithm [Wang and Nakamachi (1997)]. However, the second particular features above disable the usage of inside-outside algorithm into 3-D NMM. Necessary modification must be done if one wants to continue with logic of inside-outside algorithm.

Another example is the penetrated edges method (*PEM*). The basic prerequisite of *PEM* is that two contact bodies are convex, at least locally convex, to guarantee their intersection to be convex too [Chen *et al.* (2004)]. The first particular feature states that rock mass has random shapes, and some local position might be concave, where the prerequisite of *PEM* does not satisfy. Even though any arbitrary shape can be decomposed into sets of convex element, there is no stable encoding to realize the massive decomposition process up until now. If utilizing the current subdivision algorithm directly [Chazelle and Dobkin (1985)], it will bring disproportional overburden to the NMM structure, and reduce the whole efficiency. Fortunately, the mathematical cells in recent stage are composed by tetrahedron or hexahedron [He and Ma (2010)], hence, some of the thought in this algorithm can be imported into warning process (Phase I global searching). This technique can be employed to

detect the overlapped mathematical cells, which are found extremely proper.

The basic idea of 3-D NMM contact checking algorithm is built upon the concept of *entrance mode*. There are various contact types in the 3-D view. For example, an edge cluster of even one vertex has a large amount of possible combinations, and many derivative contact situations are generated by two 3-D vertex. Other contact types are similar. For convenience, we classify them into 7 *basic contact types*, as shown in Fig. 5-1.

Figure 5- 1 Basic contact types between two 3-D blocks

The first one among them, vertex-to-facet, is relatively easy to handle. To judge whether one vertex penetrates a facet or not, only vertex coordinates and plane equations for the facet are needed, which are easy to get. If we can get a viable

scheme to transform any of the 7 types of contact pair into the “*point-to-plane*” mode, the contact checking procedure become much simpler.

This idea is similar to the entrance theory in 2-D DDA [Shi (1988)]. The “*crossing-lines*” mode is discovered during the coding, for example the contact type (b) is difficult to transform into “*point-to-plane*” mode. Inspired by Dr. Shi Genhua, “*crossing-line*” mode is defined finally.

In the designed 3-D NMM, two entrance modes are defined.

- a) point-to-plane mode
- b) crossing-line mode

5.3 Contact Checking Procedure in 3-D NMM

The procedure of contact checking algorithm in 3-D NMM is to: locate contact pair candidates→determine contact pair candidates’ type→transform into entrance mode→screen real contact pair and calculate penetration depth→record real contact pair information. They are realized specifically by the bellowing 6 processes.

Step 1: Setup Process

Setup process is to setup contact hierarchies and outer normal vector of hierarchies. Based on the outline of contact checking algorithm, new definitions are now introduced to prepare for the establishment of efficient scheme. It is so-called ***hierarchical contact system***. The contact system of 3-D NMM are divided into 5 levels, which are contact body, contact manifold element, contact facet, contact edge, and contact vertex. Obviously, a hierarchical relation exists among those ***contact hierarchical objects/contact hierarchies***. Fig. 5-2 assumes a solid polyhedron as a ***contact body*** is placed in mathematical mesh, and the polyhedron is discretized into many manifold elements according to the NMM definition. There are two kinds of element here. One is internal element, and the other is external element, which is attached by contact boundary surface. The latter one is referred to as “***contact manifold element***”. Contact manifold element, itself, is a collection of facet. We

define the external facets as *contact facet*, which are on the contact boundary. Each contact facet is again defined by *contact edge*. Contact edge normally embodies two *contact vertexes*.

Figure 5- 2 Contact system of 3-D NMM

The tree structure of hierarchical contact system and its referred concepts are depicted in Fig. 5-3.

Figure 5- 3 Hierarchical contact system in 3-D NMM

It is also obvious that contact can occur only on one side of the contact facet. We need distinguish the positive side from negative side. The side of the segment, on which contact can occur, will be referred to as the positive side. The local indexes of the vertexes on the contact facet will always be numbered in a counter-clockwise order, as shown in Fig. 5-4.

Figure 5- 4 Contact facet with external normal

With the NMM discretization, the contact boundary may be no longer smooth all the time. Vertexes may not stay on a common plane. A normal vector on the positive side of the facet can then be averaged as

$$\tilde{N} = nor \left[\frac{\sum_{i=1}^{n-1} \mathbf{e}_i \times \mathbf{e}_{i+1}}{n} \right] \quad (5-1)$$

where n is the total edge sum of the facet, $\mathbf{e}_i$ is unit vector of edge i .

Step 2: Warning Process

Warning process is to do contact warning with single block generation methodology. In this process, we focus on the mathematical cells which enclosure manifold element, not the contact body itself. As mentioned before, NMM has regular mesh. Mathematical cells enclosure the contact manifold element, meanwhile also enclosure the contact body. If we concentrate to observe these mathematical cells in the whole process, it is not hard to find that the responding mathematical cells have already overlapped before the real contact occurs. It is shown in Fig. 5-5. When two contact bodies continue to approach along the arrow direction, the frame of mathematical cells would overlap prior to real contact.

Figure 5- 5 Frames of the mathematical cell coming into contact

Because of this, we can provide warning to the contact interaction in advance. In this way, contact checking scope and calculation quantities are reduced significantly; hitting efficiency increases at the same time. This is the main task of this process. Here, we define the frame of mathematical cell set as territory of contact body. Its 2-D representation is in Fig. 5-6.

Figure 5- 6 Overlapped territory of two contact bodies

The absence of an ***overlapped territory*** means that further testing on lower-level hierarchical elements can be trivially rejected. In other words, there is no contact interaction in current stage. When an overlapped territory is detected, the testing continues operating on lower elements' level, which are also enclosed and intersected by ***overlapped territory of elements***.

Concerning with geographic features of mathematical cell in current 3-D NMM, tetrahedron and hexahedron is classic convex polyhedron. We utilize ***single block cutting methodology*** [He and Ma (2009)] to detect overlapping cells.

Each mathematical cell, say a cube, is formed by a set of six planes. The intersection part of two cells can be considered as a union of two sets of planes, as the vertexes of intersection body must satisfy Half-space requirements for those 12 planes.

Single block cutting methodology can determine the topological expression of union parts, and then use simplex integration formulation to gain the volume of the intersection body. Fig. 5-7 gives the intersection examples of some hexahedron cell pairs.

Figure 5- 7 Examples for the intersection body of two mathematical cells

When the value of volume is positive, it indicates that overlapping happens, and contact warning is activated. Under this strategy, we find both contact body pairs and potential contact manifold element pairs. Further contact locating is at the external facet of manifold element and at descendent level of *primitive hierarchies* (primitive hierarchies includes facet, edge, vertex), which is the task for next step. From the following steps, contact checking procedure enters Phase II.

Step 3: Matching Process

Matching process is to setup contact territory and match hierarchical contact pair. The definition of the contact territory follows the criterion that all candidate objects

approaching the target object will be caught and tested for contact matching before the interpenetration occurring. As shown in Fig. 5-8, Fig.5-9, Fig. 5-10, Fig. 5-11, D_c is the territory expansion, which is controlled by the prescribed maximum relative vertex displacement (equivalent to maximum displacement ratio in 2-D NMM) in a special time step.

Figure 5- 8 Contact territory of contact facet

Figure 5- 9 Front view of contact territory associated with a contact facet

Figure 5- 10 Contact territory of contact edge

Figure 5- 11 Contact territory of contact vertex

Assisting by territory, we can easily match the primitive hierarchies of contact element pairs. Normally, the matched types do not have 7 types as in Fig. 5-1, instead, there are only four **essential types**: vertex-to-vertex, vertex-to-edge, vertex-to-facet, and edge-to-edge. The reason is that edge-to-facet, facet-to-facet, and even edge-to-edge (parallel) are finally decomposed to the combination of 4 essential types. Up until now, the operations above are called **first matching check**.

After the matching check guaranteed by territory overlapping detection, **second matching check** is designed to avoid possible missing contact pairs, because 3-D contact situation are more complex than 2-D situation. Second matching check is built on the concept of a **target neighbor**. A target neighbor is a collection of one of primitive contact hierarchies and its neighboring contact facet (including its belongings). Since three primitive contact hierarchies are vertex, edge, and facet. Thus, the target neighbor can be categorized into three groups: the vertex-centered target neighbor, the edge-centered target neighbor, and the facet-centered target neighbor, as shown in Fig. 5-12.

Figure 5- 12 Target neighbors

Even though the second matching check might increase the scope of contact detection locally, it ensures its hitting ratio. Meanwhile, it also balances the overall cost of computer time as economical operation.

General remarks:

- 1) To build connective network of contact hierarchies, a natural way is to follow the sequential order of Step 1's tree structure. Thus, each contact hierarchy is defined by specifying all its contact hierarchies at one level lower in a prescribed order. However, it is not the efficient connectivity definition. For example, it requires ergodic operation on whole data structure to determine one target neighbors of one vertex. Actually, alternative way is to rewrite the data structure at initialization stage before calculation. Extension from the lowest-level hierarchy, the information of the vertex starts to expand to include its parent hierarchies'

indexes and neighbored primitive hierarchies' indexes, not only original coordinate. Similar extensions are operated for edge and facet level. Obviously, it requires more storage space but saves computer time for repeatedly extracting the contact vertex information for the contact boundary. It can also be considered as an example of the trade-off between the efficiency and storage cost in the contact checking process.

- 2) Since the expansion of contact territory, it is possible that some particular contact pair belongs to multiply types. A vertex might match to a facet partner, and at the same time, it also matches to an edge partner. For these phenomena, it follows the rule of “complex to simple”, which is vertex-to-vertex > vertex-to-edge > vertex-to-facet > edge-to-edge (crossing). The purpose is to avoid misjudge to complex situation.
- 3) During the twice matching checks, contact pair with edge-to-edge type is searched independently. After finishing the matching operation between vertex and primitive hierarchies, additional checking is run between every edge pairs on the contact boundary. This operation can keep away from the edge penetration problem, as illustrated in Fig. 5-13. The edge penetration problem normally happens when we select relative coarse mathematical mesh.

Figure 5- 13 Edge penetration problem

- 4) The purpose of the contact matching process is: firstly, to extract the primitive hierarchies that are candidates for contact in this time/loading step from all defined contact primitive hierarchy in the structure; Then, to generate *contact pair candidates*; Finally, to confirm the type of them.

Step 4: Transform Process

Transform process is to transform contact pair candidates with essential types to entrance mode. In the four essential contact types, vertex-to-facet and edge-to-edge (crossing) are very easy to handle, and transform to two given entrance modes correspondingly. These two contact pairs have only one entrance mode accordingly.

The situation that requires transforming is under the contact type of edge-to-edge (parallel), vertex-to-edge, and vertex-to-vertex., If choosing relative fine background mathematical mesh, these three contact types have low probability to occur. For the robust and stable coding purpose, it is still necessary to deal with them carefully.

1) Edge-to-edge parallel

Set up an auxiliary section plane along directional vector of edge, so that the 3-D contact type can be treated as a 2-D contact case, shown in Fig. 5-14. The contact between two 2-D angle has sufficient reference in [Shi (1988)]. It is worth to notice that entrance lines of 2-D contact algorithm should correspond to the entrance planes of 3-D contact cases. By this logic, this type of contact pair will be transformed to one or more pairs of first kind of entrance mode. Furthermore, each 3-D parallel edges contact case should generate a pair of 2-D vertex-vertex contact models along the edge direction.

Figure 5- 14 Auxiliary section planes for 3-D parallel contact edges' type case

2) Vertex-to-edge

Each edge is generated by two crossing facets. Through the above-mentioned match sorting, the vertex-to-edge here specifies the case when vertex is located right above the angle bisector of the edge, and it cannot directly transform to any entrance modes in geometric sense. In this case, we have to track the motion velocity of the vertex in last time step. Corresponding entrance mode is targeted by extending vector of vertex velocity. It means that the transforming here is path-dependent, which is different with pure contact judgment based on geometric conditions in previous description. If unavailable still, one possible way to define a normal vector on the edge is to take the average of all normal vectors which can be gained from the geometries of all facets sharing the same point of interests, as shown in Fig. 5-15. Setup an auxiliary plane to perpendicular to the average normal direction, so that vertex-to-edge is transformed to point-to-plane mode.

Figure 5- 15 Auxiliary plane for non-distinguished contact edge

3) *Vertex to vertex*

Similar problems arise at the sharp corner as shown in Fig. 5-15. In the demonstrated case, the vertex presented 3-D corner is very complicated, such as Fig. 5-17 and Fig. 5-18.

Figure 5- 16 Auxiliary plane for non-distinguished contact vertex

Actually, these two cases are referred to as “a vertex in the valley” [Zhong and Nilsson (1990)]. We have to setup local section plane and sample 3-D vertex-to-vertex cases with 2-D slices, to help judgment. It is worth to notice that a vertex in such valley may have more than one contact pair involving. In other words,

it has more than one entrance mode.

Figure 5- 17 Vertex-to-concave vertex

Figure 5- 18 Vertex-to-complex vertex

Step5: Judging Process

Judging process is to judge real contact pair under definition of entrance mode and penetration criteria. Entrance mode is to finally determine whether two contact pair candidates have met or not, and at the same time to guide the selection of the right location to add contact constraints to prevent the contact bodies from penetrating each other.

2-D NMM contact interaction judgment is via screening the sign of triangular area generated by contact point and entrance edge. Intuitively, if points P_1 , P_2 and P_3 rotate in the same direction as the rotation of coordinate axis from OX to OY (see Fig. 5-19). When vertex P_1 passes through entrance edge, the rotate direction will change if we still hold the order of three points. It means that the area of mentioned triangle will change to negative, formulated as [Shi (1988)]

$$\Delta = \begin{vmatrix} 1 & x_1 + u_1 & y_1 + v_1 \\ 1 & x_2 + u_2 & y_2 + v_2 \\ 1 & x_3 + u_3 & y_3 + v_3 \end{vmatrix} < 0. \quad (5-2)$$

(x_i, y_i) and (u_i, v_i) are the coordinates and displacement increments of P_i , $i = 1, 2, 3$ respectively at a time instance. This simple formula is still correct when these three points move simultaneously.

Figure 5- 19 Judgment for penetration in 2-D NMM

Later on, we would see that it is similar for 3-D entrance modes. Different from 2-D, contact judgment monitors the volume of the auxiliary tetrahedron. Indeed, we try to construct such auxiliary tetrahedron for both *mode 1* and *mode 2* that a unified formula can be used to describe the relative position between the contact pairs. More specifically, as below:

a) Point-to-plane mode:

There are two arbitrary shaped polyhedral elements coming into contact, as shown in Fig. 5-20.

Figure 5- 20 Point to plane mode

Suppose P_0 is the vertex of element, $P_1P_2P_3P_4P_5$ is the contact facet of element. In fact, one face can be defined by three vertexes. In practice, several vertexes might not keep in the same common plan, and we have to find the most representative two neighboring edges for the facet beforehand. It means we take three vertexes out of the several vertexes to form a bottom triangular face of auxiliary tetrahedron. For example, we can take P_1, P_2, P_3 , since the cross product of these two edges have the largest value of projection vector on the average normal for this facet. It is expressed as,

$$P_iP_{i+1}P_{i+2} \exists \max \left\{ (\mathbf{e}_i \times \mathbf{e}_{i+1}) \cdot \tilde{\mathbf{N}}, \forall i \in 1 \sim n \right\} \quad (5-3)$$

where $\tilde{\mathbf{N}}$ is the average normal of the facet (defined by Equation 5-10), $\mathbf{e}_i$ is unit vector of edge i . “ $\exists$ ” denotes “choose from”, n is the total edge sum of the facet. Furthermore, the auxiliary tetrahedron has been established from $P_0P_1P_2P_3$ vertexes. We are able to simultaneously observe the volume of tetrahedron easily, and judge the contact situation for the contact pair candidate.

Let (x_i, y_i, z_i) and (u_i, v_i, w_i) are the coordinates and displacement increments of vertex P_i ($i = 0 \sim n$). After the displacement increments are applied, the new positions of vertexes are depicted as P'_i ($i = 0 \sim n$) and the normal distance between the point and facet is

$$d'_N = \frac{1}{A_0} \begin{vmatrix} 1 & x_0 + u_0 & y_0 + v_0 & z_0 + w_0 \\ 1 & x_1 + u_1 & y_1 + v_1 & z_1 + w_1 \\ 1 & x_2 + u_2 & y_2 + v_2 & z_2 + w_2 \\ 1 & x_3 + u_3 & y_3 + v_3 & z_3 + w_3 \end{vmatrix} \quad (5-4)$$

where $A_0 \approx \sqrt{\begin{vmatrix} y_2 - y_1 & z_2 - z_1 \\ y_3 - y_1 & z_3 - z_1 \end{vmatrix}^2 + \begin{vmatrix} x_2 - x_1 & z_2 - z_1 \\ x_3 - x_1 & z_3 - z_1 \end{vmatrix}^2 + \begin{vmatrix} x_2 - x_1 & y_2 - y_1 \\ x_3 - x_1 & y_3 - y_1 \end{vmatrix}^2}$, neglecting the second and third order infinitesimal terms on denominator.

If $d'_N < 0$, the point P'_0 will pass through the facet of $P'_1 P'_2 P'_3 P'_4 P'_5$, which means a penetration takes place.

b) Crossing-lines mode:

When two edges belonging to different manifold elements approach close to each other until the happening of real contact, crossing-lines mode fits well. Similarly, we can construct an auxiliary tetrahedron as following steps, shown in Fig. 5-21.

Figure 5- 21 Crossing-lines mode

Suppose $\overline{P_1P_2}$ is an edge of element, $\overline{P_3P_4}$ is other contact edge of element. Extract these two edges from the model, and build up spatial auxiliary tetrahedron with four vertexes, as in Fig. 5-22a. Fig.5-22(a)~(c) illustrates the changing situation of auxiliary tetrahedron during the approaching and penetrating process.

(a)

(b)

(c)

Figure 5- 22 Auxiliary tetrahedron changes during two edges approaching

Clearly, the volume of auxiliary tetrahedron also experiences the process from positive to negative. There is no harm in treating $\triangle P_1P_4P_2$ as the bottom of tetrahedron. Assume the contact point P_H and P_T are known and located at the line $\overline{P_1P_2}$ and $\overline{P_3P_4}$, the length from P_H to P_T demonstrates the shortest distance between two edges. P_3^{proj} is the projection point of P_3 on the plane of $\triangle P_1P_4P_2$. Let (x_i, y_i, z_i) and (u_i, v_i, w_i) be the coordinates and displacement increments of vertex P_i ($i = 1 \sim 4, H, T$). Thus

$$\gamma_T = \frac{|\overrightarrow{P_1P_T}|}{|\overrightarrow{P_1P_2}|} \quad (5-5)$$

$$\gamma_H = \frac{|\overrightarrow{P_3P_H}|}{|\overrightarrow{P_3P_4}|} \quad (5-6)$$

Because $\overrightarrow{P_3^{proj}P_3}$ and $\overrightarrow{P_HP_T}$ are relatively small. It can represent each other in

geometric sense, where their included angle is ignorable. Therefore,

$$\frac{\overline{P_H P_T}}{P_3^{proj} P_3} \approx 1 - \gamma_H \quad (5-7)$$

Finally, the normal distance between the two crossing edges is

$$d_N' = \frac{1 - \gamma_H}{A_0} \begin{vmatrix} 1 & x_3 + u_3 & y_3 + v_3 & z_3 + w_3 \\ 1 & x_1 + u_1 & y_1 + v_1 & z_1 + w_1 \\ 1 & x_4 + u_4 & y_4 + v_4 & z_4 + w_4 \\ 1 & x_2 + u_2 & y_2 + v_2 & z_2 + w_2 \end{vmatrix} \quad (5-8)$$

where $A_0 \approx \sqrt{\begin{vmatrix} y_4 - y_1 & z_4 - z_1 \\ y_2 - y_1 & z_2 - z_1 \end{vmatrix}^2 + \begin{vmatrix} x_4 - x_1 & z_4 - z_1 \\ x_2 - x_1 & z_2 - z_1 \end{vmatrix}^2 + \begin{vmatrix} x_4 - x_1 & y_4 - y_1 \\ x_2 - x_1 & y_2 - y_1 \end{vmatrix}^2}$, neglecting the

second and third order infinitesimal terms on denominator.

In the same way, $d_N' < 0$ means the occurrence of a penetration. For convenience, we adjust the index of vertexes to get a uniform expression d_N' for both two modes.

$$d_N' = \frac{1 - \gamma}{A_0} \begin{vmatrix} 1 & x_1 + u_1 & y_1 + v_1 & z_1 + w_1 \\ 1 & x_2 + u_2 & y_2 + v_2 & z_2 + w_2 \\ 1 & x_3 + u_3 & y_3 + v_3 & z_3 + w_3 \\ 1 & x_4 + u_4 & y_4 + v_4 & z_4 + w_4 \end{vmatrix}, \quad \begin{matrix} \gamma = 0, \text{mode} & 1 \\ \gamma = \gamma_H, \text{mode} & 2 \end{matrix} \quad (5-9)$$

For mode 1, re-indexed as 0-1, 1-2, 2-3, 3-4

For mode 2, re-indexed as 1-2, 2-4, 3-1, 4-3

Step 6: Recording process

Recording process is to record contact pair information for next iteration step or time step. The recording information includes contact pair index, contact pair types, the number of entrance modes for current contact pair, open-closed state, penetration normal depth, relative tangential displacement, new contact identity.

5.4 Penalty Treatment of Contact Constraints in 3-D NMM

Among several numerical treatments of contact constraints mentioned in Section 5.1, the penalty method is not the most accurate method. However, it does not introduce

any new unknowns, it is relative simple to realize in coding. The current 3-D NMM uses this method to introduce contact constraints into system functional.

Penalty terms due to the constraint condition are added to Π_c as follows:

$$\Pi_c^{\text{Penalty}} = \frac{1}{2} \int_{\Gamma_c} (k_N \cdot (\bar{d}_N)^2 + k_T \cdot (\bar{d}_T)^2) dA, \quad k_N, k_T > 0 \quad (5-10)$$

1) *Normal contact matrix*

From Eq. (5-9),

$$\begin{aligned} d_N' &= \frac{1-\gamma}{A_0} \begin{vmatrix} 1 & x_1+u_1 & y_1+v_1 & z_1+w_1 \\ 1 & x_2+u_2 & y_2+v_2 & z_2+w_2 \\ 1 & x_3+u_3 & y_3+v_3 & z_3+w_3 \\ 1 & x_4+u_4 & y_4+v_4 & z_4+w_4 \end{vmatrix} \\ &= \frac{1-\gamma}{A_0} \left\{ V_0 + \begin{vmatrix} 1 & u_1 & y_1 & z_1 \\ 1 & u_2 & y_2 & z_2 \\ 1 & u_3 & y_3 & z_3 \\ 1 & u_4 & y_4 & z_4 \end{vmatrix} + \begin{vmatrix} 1 & x_1 & v_1 & z_1 \\ 1 & x_2 & v_2 & z_2 \\ 1 & x_3 & v_3 & z_3 \\ 1 & x_4 & v_4 & z_4 \end{vmatrix} \right. \\ &\quad \left. + \begin{vmatrix} 1 & x_1 & y_1 & w_1 \\ 1 & x_2 & y_2 & w_2 \\ 1 & x_3 & y_3 & w_3 \\ 1 & x_4 & y_4 & w_4 \end{vmatrix} + \begin{vmatrix} 1 & u_1 & v_1 & w_1 \\ 1 & u_2 & v_2 & w_2 \\ 1 & u_3 & v_3 & w_3 \\ 1 & u_4 & v_4 & w_4 \end{vmatrix} \right\} \quad (5-11) \end{aligned}$$

$$\text{where } V_0 = \begin{vmatrix} 1 & x_1 & y_1 & z_1 \\ 1 & x_2 & y_2 & z_2 \\ 1 & x_3 & y_3 & z_3 \\ 1 & x_4 & y_4 & z_4 \end{vmatrix}.$$

Set C_{ij} is the algebraic complement of determinant V_0 about element v_{ij} , denoted as,

$$C_{ij} = (-1)^{i+j} \cdot V_{ij} \quad (5-12)$$

where V_{ij} is cofactor of V_0 about element v_{ij} . For example, $C_{12} = (-1)^{1+2} \cdot \begin{vmatrix} 1 & y_2 & z_2 \\ 1 & y_3 & z_3 \\ 1 & y_4 & z_4 \end{vmatrix}$.

Thus, neglecting the infinitesimal terms (last term in Eq. (5-20)), the increment of normal penetration distance is

$$\Delta d_N = \frac{1-\gamma}{A_0} \left\{ \begin{aligned} & (C_{12} \ C_{13} \ C_{14}) \begin{bmatrix} u_1 \\ v_1 \\ w_1 \end{bmatrix} + (C_{22} \ C_{23} \ C_{24}) \begin{bmatrix} u_2 \\ v_2 \\ w_2 \end{bmatrix} \\ & + (C_{32} \ C_{33} \ C_{34}) \begin{bmatrix} u_3 \\ v_3 \\ w_3 \end{bmatrix} + (C_{42} \ C_{43} \ C_{44}) \begin{bmatrix} u_4 \\ v_4 \\ w_4 \end{bmatrix} \end{aligned} \right\} \quad (5-13)$$

Let

$$\begin{aligned} \mathbf{H} &= \frac{1-\gamma}{A_0} [T_\alpha(x_1, y_1, z_1)]^T \begin{bmatrix} C_{12} \\ C_{13} \\ C_{14} \end{bmatrix} \\ \mathbf{G} &= \frac{1-\gamma}{A_0} \left\{ [T_\beta(x_2, y_2, z_2)]^T \begin{bmatrix} C_{22} \\ C_{23} \\ C_{24} \end{bmatrix} + [T_\beta(x_3, y_3, z_3)]^T \begin{bmatrix} C_{32} \\ C_{33} \\ C_{34} \end{bmatrix} + [T_\beta(x_4, y_4, z_4)]^T \begin{bmatrix} C_{42} \\ C_{43} \\ C_{44} \end{bmatrix} \right\} \end{aligned}$$

for mode 1 (5-14)

$$\begin{aligned} \mathbf{H} &= \frac{1-\gamma}{A_0} \left\{ [T_\alpha(x_1, y_1, z_1)]^T \begin{bmatrix} C_{12} \\ C_{13} \\ C_{14} \end{bmatrix} + [T_\alpha(x_2, y_2, z_2)]^T \begin{bmatrix} C_{22} \\ C_{23} \\ C_{24} \end{bmatrix} \right\} \\ \mathbf{G} &= \frac{1-\gamma}{A_0} \left\{ [T_\beta(x_3, y_3, z_3)]^T \begin{bmatrix} C_{32} \\ C_{33} \\ C_{34} \end{bmatrix} + [T_\beta(x_4, y_4, z_4)]^T \begin{bmatrix} C_{42} \\ C_{43} \\ C_{44} \end{bmatrix} \right\} \end{aligned}$$

for mode 2 (5-15)

Then,

$$d_N' = (1-\gamma) \cdot (d_N + \mathbf{H}^T \mathbf{D}_\alpha + \mathbf{G}^T \mathbf{D}_\beta) \quad (5-16)$$

where $\mathbf{D}_\alpha$ and $\mathbf{D}_\beta$ are the cover displacement on manifold MP α and β respectively.

The potential energy due to the normal spring is

$$\begin{aligned} \Pi_N &= (1-\gamma)^2 \frac{k_N}{2} (d_N')^2 = (1-\gamma)^2 \frac{k_N}{2} \left(\mathbf{H}^T \mathbf{D}_\alpha + \mathbf{G}^T \mathbf{D}_\beta + \frac{V_0}{A_0} \right)^2 \\ &= (1-\gamma)^2 \frac{k_N}{2} \left(\mathbf{D}_\alpha^T \mathbf{H} \mathbf{H}^T \mathbf{D}_\alpha + \mathbf{D}_\beta^T \mathbf{G} \mathbf{G}^T \mathbf{D}_\beta + 2 \mathbf{D}_\alpha^T \mathbf{H} \mathbf{G}^T \mathbf{D}_\beta \right. \\ &\quad \left. + 2 \left(\frac{V_0}{A_0} \right) \mathbf{D}_\alpha^T \mathbf{H} + 2 \left(\frac{V_0}{A_0} \right) \mathbf{D}_\beta^T \mathbf{G} + \left(\frac{V_0}{A_0} \right)^2 \right) \end{aligned} \quad (5-17)$$

Thus, in the case of tetrahedron cover cell, the sub-matrices due to the normal spring can be obtained and assembled into global stiffness matrix and global loading vector as

$$\begin{aligned}
(1-\gamma)^2 k_N \mathbf{H}_{\alpha(r)} \mathbf{H}_{\alpha(s)}^T &\rightarrow \mathbf{K}_{\alpha(r)\alpha(s)}, (r, s = 1, 2, 3, 4) \\
(1-\gamma)^2 k_N \mathbf{H}_{\alpha(r)} \mathbf{G}_{\beta(s)}^T &\rightarrow \mathbf{K}_{\alpha(r)\beta(s)}, (r, s = 1, 2, 3, 4) \\
(1-\gamma)^2 k_N \mathbf{G}_{\beta(r)} \mathbf{H}_{\alpha(s)}^T &\rightarrow \mathbf{K}_{\beta(r)\alpha(s)}, (r, s = 1, 2, 3, 4) \\
(1-\gamma)^2 k_N \mathbf{G}_{\beta(r)} \mathbf{G}_{\beta(s)}^T &\rightarrow \mathbf{K}_{\beta(r)\beta(s)}, (r, s = 1, 2, 3, 4) \\
-(1-\gamma)^2 k_N (V_0 / A_0) \mathbf{H}_{\alpha(r)} &\rightarrow \mathbf{F}_{\alpha(r)}, (r = 1, 2, 3, 4) \\
-(1-\gamma)^2 k_N (V_0 / A_0) \mathbf{G}_{\beta(r)} &\rightarrow \mathbf{F}_{\beta(r)}, (r = 1, 2, 3, 4)
\end{aligned} \tag{5-18}$$

2) Tangential contact matrix

When the Eq. (4-25) is fulfilled, the tangential displacement along the contact surface is not allowed. Assume $P_1^{proj}(x_p, y_p, z_p)$ is the projection point of vertex P_1 on reference entrance plane $P_2P_3P_4$. After a time step, P_1 and P_1^{proj} move to P_1' and $P_1^{proj'}$, as shown in Fig. 5-23.

Figure 5- 23 Representation of shear displacement

There is a tangential penalty spring between P_1' and $P_1^{proj'}$ to prevent the tangential displacement on the surface. The vector theory has been used to determine the tangential displacement which should not happen.

$$\left(d_T'\right)^2 = \left|\overrightarrow{P_1'P_1^{proj'}}\right|^2 - \left(d_N'\right)^2 \quad (5-19)$$

Considering two cases of *mode 1* and *mode 2*, similarly, we have

$$\left(d_T'\right)^2 = (1-\gamma)^2 \cdot \left[\left|\overrightarrow{P_1'P_1^{proj'}}\right|^2 - \left(\overrightarrow{P_1'P_1^{proj'}} \cdot \tilde{\mathbf{N}}\right)^2 \right] \quad (5-20)$$

where $\tilde{\mathbf{N}}$ denotes the average normal of reference entrance facet. Then,

$$\begin{aligned} \Pi_T &= (1-\gamma)^2 \frac{k_T}{2} (d_T')^2 \\ &= (1-\gamma)^2 \frac{k_T}{2} \left\{ \begin{aligned} &\begin{bmatrix} x_1 + u_1 - x_p - u_p \\ y_1 + v_1 - y_p - v_p \\ z_1 + w_1 - z_p - w_p \end{bmatrix}^T \begin{bmatrix} x_1 + u_1 - x_p - u_p \\ y_1 + v_1 - y_p - v_p \\ z_1 + w_1 - z_p - w_p \end{bmatrix} \\ &- \begin{bmatrix} x_1 + u_1 - x_p - u_p \\ y_1 + v_1 - y_p - v_p \\ z_1 + w_1 - z_p - w_p \end{bmatrix}^T \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T \begin{bmatrix} x_1 + u_1 - x_p - u_p \\ y_1 + v_1 - y_p - v_p \\ z_1 + w_1 - z_p - w_p \end{bmatrix} \end{aligned} \right\} \\ &= (1-\gamma)^2 \frac{k_T}{2} \left\{ \begin{aligned} &\begin{bmatrix} x_1 + u_1 - x_p - u_p \\ y_1 + v_1 - y_p - v_p \\ z_1 + w_1 - z_p - w_p \end{bmatrix}^T \left[\mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T \right] \begin{bmatrix} x_1 + u_1 - x_p - u_p \\ y_1 + v_1 - y_p - v_p \\ z_1 + w_1 - z_p - w_p \end{bmatrix} \end{aligned} \right\} \\ &= (1-\gamma)^2 \frac{k_T}{2} \left\{ \begin{aligned} &\begin{bmatrix} x_1 - x_p \\ y_1 - y_p \\ z_1 - z_p \end{bmatrix}^T \left[\mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T \right] \begin{bmatrix} x_1 - x_p \\ y_1 - y_p \\ z_1 - z_p \end{bmatrix} + 2 \cdot \begin{bmatrix} u_1 - u_p \\ v_1 - v_p \\ w_1 - w_p \end{bmatrix}^T \left[\mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T \right] \begin{bmatrix} x_1 - x_p \\ y_1 - y_p \\ z_1 - z_p \end{bmatrix} \\ &+ \begin{bmatrix} u_1 - u_p \\ v_1 - v_p \\ w_1 - w_p \end{bmatrix}^T \left[\mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T \right] \begin{bmatrix} u_1 - u_p \\ v_1 - v_p \\ w_1 - w_p \end{bmatrix} \end{aligned} \right\} \quad (5-21) \end{aligned}$$

Therefore,

$$\begin{aligned}
\Pi_T &= (1-\gamma)^2 \frac{k_T}{2} (d_T')^2 \\
&= (1-\gamma)^2 \frac{k_T}{2} \left\{ \begin{aligned} &\begin{bmatrix} x_1 - x_p \\ y_1 - y_p \\ z_1 - z_p \end{bmatrix}^T \begin{bmatrix} \mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T \end{bmatrix} \begin{bmatrix} x_1 - x_p \\ y_1 - y_p \\ z_1 - z_p \end{bmatrix} \\ &+ 2 \cdot \mathbf{D}_\alpha^T \left[T_\alpha(x_1, y_1, z_1) \right]^T \begin{bmatrix} \mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T \end{bmatrix} \begin{bmatrix} x_1 - x_p \\ y_1 - y_p \\ z_1 - z_p \end{bmatrix} \\ &- 2 \cdot \mathbf{D}_\beta^T \left[T_\beta(x_p, y_p, z_p) \right]^T \begin{bmatrix} \mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T \end{bmatrix} \begin{bmatrix} x_1 - x_p \\ y_1 - y_p \\ z_1 - z_p \end{bmatrix} \\ &+ \mathbf{D}_\alpha^T \left[T_\alpha(x_1, y_1, z_1) \right]^T \begin{bmatrix} \mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T \end{bmatrix} \left[T_\alpha(x_1, y_1, z_1) \right] \mathbf{D}_\alpha \\ &- \mathbf{D}_\alpha^T \left[T_\alpha(x_1, y_1, z_1) \right]^T \begin{bmatrix} \mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T \end{bmatrix} \left[T_\beta(x_p, y_p, z_p) \right] \mathbf{D}_\beta \\ &- \mathbf{D}_\beta^T \left[T_\beta(x_p, y_p, z_p) \right]^T \begin{bmatrix} \mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T \end{bmatrix} \left[T_\alpha(x_1, y_1, z_1) \right] \mathbf{D}_\alpha \\ &+ \mathbf{D}_\beta^T \left[T_\beta(x_p, y_p, z_p) \right]^T \begin{bmatrix} \mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T \end{bmatrix} \left[T_\beta(x_p, y_p, z_p) \right] \mathbf{D}_\beta \end{aligned} \right\} \quad (5-22)
\end{aligned}$$

Set

$$\begin{aligned}
\tilde{\mathbf{H}} &= \left[T_\alpha(x_1, y_1, z_1) \right]^T \\
\tilde{\mathbf{G}} &= \left[T_\beta(x_p, y_p, z_p) \right]^T
\end{aligned}
\quad \text{for both mode} \quad (5-23)$$

Lastly, the sub-matrices due to the shear spring are obtained and assembled to the global stiffness matrix and global loading vector as

$$\begin{aligned}
& (1-\gamma)^2 k_T \tilde{\mathbf{H}}_{\alpha(r)} [\mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T] \tilde{\mathbf{H}}_{\alpha(s)}^T \rightarrow \mathbf{K}_{\alpha(r)\alpha(s)}, \quad (r, s = 1, 2, 3, 4) \\
& -(1-\gamma)^2 k_T \tilde{\mathbf{H}}_{\alpha(r)} [\mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T] \tilde{\mathbf{H}}_{\beta(s)}^T \rightarrow \mathbf{K}_{\alpha(r)\beta(s)}, \quad (r, s = 1, 2, 3, 4) \\
& -(1-\gamma)^2 k_T \tilde{\mathbf{H}}_{\beta(r)} [\mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T] \tilde{\mathbf{H}}_{\alpha(s)}^T \rightarrow \mathbf{K}_{\beta(r)\alpha(s)}, \quad (r, s = 1, 2, 3, 4) \\
& (1-\gamma)^2 k_T \tilde{\mathbf{H}}_{\beta(r)} [\mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T] \tilde{\mathbf{H}}_{\beta(s)}^T \rightarrow \mathbf{K}_{\beta(r)\beta(s)}, \quad (r, s = 1, 2, 3, 4) \\
& -(1-\gamma)^2 k_T \tilde{\mathbf{H}}_{\alpha(r)} [\mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T] \begin{bmatrix} x_1 - x_p \\ y_1 - y_p \\ z_1 - z_p \end{bmatrix} \rightarrow \mathbf{F}_{\alpha(r)}, \quad (r, s = 1, 2, 3, 4) \\
& -(1-\gamma)^2 k_T \tilde{\mathbf{G}}_{\beta(r)} [\mathbf{E} - \tilde{\mathbf{N}} \cdot \tilde{\mathbf{N}}^T] \begin{bmatrix} x_1 - x_p \\ y_1 - y_p \\ z_1 - z_p \end{bmatrix} \rightarrow \mathbf{F}_{\beta(r)}, \quad (r, s = 1, 2, 3, 4)
\end{aligned} \tag{5-24}$$

3) Friction force matrix

For the sliding mode, except the normal spring, a pair of frictional forces will be added instead of a tangential spring. Based on the *Coulomb's friction law*, the frictional force is calculated as

$$|\mathbf{f}| = \text{sign} \cdot \mu \cdot k_N d_N \tag{5-25}$$

where “sign” is assigned as “+” or “-” according to the direction of relative sliding, μ is the friction coefficient, $k_N d_N$ is the normal force.

As shown in Fig. 5-23, the tangential vector of relative sliding on the contact facets is

$$\mathbf{d}_f' = \overrightarrow{P_1' P_1'^{proj'}} - \left(\overrightarrow{P_1' P_1'^{proj'}} \cdot \tilde{\mathbf{N}} \right) \tilde{\mathbf{N}} \tag{5-26}$$

Then, the potential energy due to frictional force $\mathbf{f}$ is

$$\begin{aligned}
\Pi_f &= \mathbf{f} \cdot \mathbf{d}_f' = |\mathbf{f}| \cdot |\mathbf{d}_f'| \\
&= |\mathbf{f}| \cdot \begin{bmatrix} u_1 - u_p \\ v_1 - v_p \\ w_1 - w_p \end{bmatrix}^T \begin{bmatrix} \frac{d_{fx}'}{|\mathbf{d}_f'|} \\ \frac{d_{fy}'}{|\mathbf{d}_f'|} \\ \frac{d_{fz}'}{|\mathbf{d}_f'|} \end{bmatrix} \\
&= |\mathbf{f}| \cdot \mathbf{D}_\alpha^T \bar{\mathbf{H}} - |\mathbf{f}| \cdot \mathbf{D}_\beta^T \bar{\mathbf{G}}
\end{aligned} \tag{5-27}$$

where

$$\bar{\mathbf{H}} = \begin{bmatrix} T_\alpha(x_1, y_1, z_1) \end{bmatrix}^T \begin{bmatrix} \frac{d_{fx}'}{|\mathbf{d}_f'|} \\ \frac{d_{fy}'}{|\mathbf{d}_f'|} \\ \frac{d_{fz}'}{|\mathbf{d}_f'|} \end{bmatrix}, \quad \bar{\mathbf{G}} = \begin{bmatrix} T_\beta(x_p, y_p, z_p) \end{bmatrix}^T \begin{bmatrix} \frac{d_{fx}'}{|\mathbf{d}_f'|} \\ \frac{d_{fy}'}{|\mathbf{d}_f'|} \\ \frac{d_{fz}'}{|\mathbf{d}_f'|} \end{bmatrix} \tag{5-28}$$

Without losing the generality, the sub-matrix due to the frictional force are obtained and assembled to the global loading vector as

$$\begin{aligned}
(1-\gamma)|\mathbf{f}| \bar{\mathbf{H}}_{\alpha(r)} &\rightarrow \mathbf{F}_{\alpha(r)}, \quad (r=1,2,3,4) \\
-(1-\gamma)|\mathbf{f}| \bar{\mathbf{G}}_{\beta(r)} &\rightarrow \mathbf{F}_{\beta(r)}, \quad (r=1,2,3,4)
\end{aligned} \tag{5-29}$$

4) General remarks

However, we need to pay attention to some of limitation on this method: 1) **Efficiency**: Extra contributions from contact are added to the original system matrix (stiffness and inertia matrix), and these additional terms change the skyline and the profile of the system matrix. It increases the burden of matrix equation solver, also brings limitation on matrix solution method, hence reduce efficiency. 2) **Accuracy**: As we know, the penalty parameters control the range of penetration tolerance. The accuracy of solution is depended on the choice of penalty parameters. In the implicit

analysis, too small penalty parameters may result in too big penetrations, which may produce unacceptable results. 3) **Numerical unstable:** One way to reduce the error is to increase the value of penalty parameters. However, it also cannot exceed a certain value, because too large value will make the coefficient matrix in balance equation under ill-condition.

5.5 General Procedure in 3-D NMM Contact Program

This part would propose a general incremental solution format with contact treatment capacity for 3-D NMM. It combines above-mentioned techniques to generalize solution procedure, including mechanics condition of contact interface, contact checking algorithm, the penalty way of introducing contact constraint into system functional based on generalized variational principle.

1) Try and error iteration-----Open-closed iteration

After understanding several aspects of the contact problem, it is clear that contact handling process is not only a pure mechanics process or pure geometric judgment; it is also time-dependent and involves three kinds of classic non-linearity. Especially, it involves the contact non-linearity after the numerical manifold discretization, which arises from the fact that the total number ${}^{cp}N$ of real contact pair is unknown prior to the solution of the problem. However, the solution is affected by the exact value of ${}^{cp}N$ in turn. This phenomenon is particularly serious in the case of more than two contact bodies. It seems self-contradictory, as it requires information of B to gain A , which is influenced by B around. For such problem, normally trial-and-error iteration procedure is proper, which is actually named the open-close iteration in 2-D DDA/NMM.

The proposed 3-D NMM applies incremental formulation with implicit solution. In each time step, assembling and solving system of equations are repeated to determine correct contact pair position, and to apply contact springs to the right location. This trial-and-error iteration procedure is generally depicted as:

- a) Through contact checking algorithm (Step 1 2 3), target potential contact pair candidates, say, there are number of ^{cp}N . According the result of the last time step (e.g., location of vertex, position of known contact pairs), the initial value of contact pair position and intensity are assumed for the first iteration step $^{try1}N \leq ^{cp}N$.
- b) Based on the loading condition, recorded element information (e.g., element strain, velocity of vertex) in the prior time step, and initial guess value ^{try1}N , the inequality constraints are overwritten to the equality constraints in kinematics and dynamics, which would be used as definite condition to reorganize the global systematic formula.
- c) Re-call the subroutine of contact checking algorithm, determine the real contact pair position under presumed guess value, denoting the number of real contact pair ^{res1}N . Additionally, apply inequality constraints condition in Section 5.2.2 as verification condition. If the resulted ^{res1}N is consistent with the presumed ^{try1}N completely, also all ^{res1}N pairs satisfy the verification condition, the solution is done in this time step. Otherwise, return back to *step a)* to redefine the initial guess value and iteration solution until the verification condition bounds.

The followed example is to simply demonstrate the iteration process. Detailed verification condition will be explained in the next part.

Assume at time instance t_n , one contact system has only four potential contact pair candidates, denoted by CP1, CP2, CP3 and CP4, as shown Fig. 5-24.

Figure 5- 24 Simplified general contact system

Depending on the result at time instance t_n , the real contact happens at CP1 & CP3 position. The penalty springs are applied immediately at these two positions. Contact situation at this moment is recorded as pseudo code format of “1010”, where “1” denotes contact close; “0” denotes open.

When calculating the contact solution at time instance t_{n+1} , it is no harm to presume that the contact situation does not change initially. Let it be the value “1010”. Then, apply all other definite boundary conditions at the current time step. Later on, assemble global balance equation to gain the new position of all vertexes, indicated as I_1 .

Re-call the subroutine of contact checking algorithm to verify penetration status for the known array I_1 . The result shows that the contact state changes to “0110” (different with initial value “1010”). There is inappropriate presumption in previous iteration.

Return global balance equations to their original formulation at time instance t_n , and presume the contact state as “0110”, which refers to the result of last iteration; Calculate again to gain new solution I_2 ; recall contact checking and get another new state “1110”.

Such iteration continues until the contact state of I_n is consistent with presumed value. Record contact information and finally complete the time step t_{n+1} .

2) Verification conditions and corresponding operations on the contact interface

Besides the normal verification condition above, there are more strict contact interface verification conditions in 3-D NMM. The contact states on the interface have totally three kinds: stick, slide, and separate. Verification conditions are described to the three kinds consequently, shown in Table 5-1.

Table 5- 1 Verification of contact situation in 3-D NMM

Contact State		Verification
Separate		$\left({}^{t+\Delta t}\mathbf{x}^B - {}^{t+\Delta t}\mathbf{x}^A \right) \cdot {}^{t+\Delta t}\mathbf{n}_3^B \geq \varepsilon_s,$ <p>If not, turn to “stick state”; record the position of contact</p>
Contact	Stick	<p>a) ${}^{t+\Delta t}\mathbf{P}_N^A = -{}^{t+\Delta t}\mathbf{P}_N^B \geq 0$, if not, turn to “separate state”</p> <p>b) $\left {}^{t+\Delta t}\mathbf{P}_T^i \right - \mu \left {}^{t+\Delta t}\mathbf{P}_N^i \right < 0 \quad (i = A, B)$, if not, turn to “slide state”</p>
	Slide	<p>a) ${}^{t+\Delta t}\mathbf{P}_N^A = -{}^{t+\Delta t}\mathbf{P}_N^B \geq 0$, if not, turn to “separate state”</p> <p>b) $\left({}^{t+\Delta t}\mathbf{u}_T^A - {}^{t+\Delta t}\mathbf{u}_T^B \right) \cdot {}^{t+\Delta t}\mathbf{P}_T^A < 0$, $\left {}^{t+\Delta t}\mathbf{u}_T^A - {}^{t+\Delta t}\mathbf{u}_T^B \right < \varepsilon_s$, if not, turn to “stick state”</p>

where ε_s is the numeral mite in contact checking procedure

According to the verification condition, the following operations are listed below in Table 5-2:

Table 5- 2 Detailed operation corresponding to the change of contact state

State Changes	Corresponding Operation
Separate to separate	No change
Separate to slide	Apply the normal spring and a pair of friction force
Separate to stick	Apply the normal and tangential springs
Slide to separate	Release the normal spring and a pair of friction force
Slide to slide	No change
Slide to stick	Release the friction forces and apply the tangential spring
Stick to separate	Release the normal and tangential springs
Stick to slide	Release the tangential spring and apply a pair of friction force
Stick to stick	No change

3) *3-D NMM codes flowchart*

Figure 5- 25 Flowchart of 3-D NMM program with contact treatment function

Chapter 6 Calibration Examples

In this chapter, the author is going to examine the precision and robustness of the 3-D NMM algorithm developed. At first, the algorithm is examined and tested (*Section 6.1* and *6.2*) with three conventional continuous-based examples focusing on the analysis of the accuracy on deformation description with the 3-D NMM. The implementation of the contact algorithm in 3-D NMM is also tested and verified with some discontinuous-based examples and case studies (*Section 6.3 – 6.6*). Summary of each section is described as follow:

The classic example of “a free falling block” is used to verify the predictability of the 3-D NMM to simulate the problem under continuous environment in *Section 6.1*. Serial tests are followed by analyzing the effect of MC size and cutting plane orientations direction through a plane structure, which also verifies the convergence and stability of the continuum algorithm in *Section 6.2*. *Section 6.3* utilizes a case of “a cube sliding on an inclined plane” to examine the numerical contact algorithms (especially face-to-face, vertex-to-face), when imposing frictional boundary conditions. In *Section 6.4*, the precision of the 3-D NMM is examined by comparing with the analytical solutions from the parametric study on “a roof wedge falling” case. In order to further demonstrate the function of 3-D analysis, a “3-D tetrahedral wedge sliding” case is designed and demonstrated the analytical ability of current algorithm in *Section 6.5*. Finally, application problems such as dominos run and dougong/bracket structure crushing are analyzed and discussed in *Section 6.6*.

6.1 Movement of a Free Falling Block

Since the primary aim of the 3-D NMM is to predict the stability and motion of a discontinuous system, the developed program is validated by simulating the free-falling process of a single block.

Figure 6- 1 Falling cube under gravity

In the 3-D space (shown in Fig. 6-1), the geometry of a single cube (the size is $1.25 \text{ m} \times 1.25 \text{ m} \times 1.25 \text{ m}$) can be defined by using the physical covers and mathematical covers mentioned in the previous chapters. Mesh spacing have been set to 0.5, a total of 328 manifold elements are generated finally. The cube falls under the only influence of the gravity. The acceleration of gravity is 10 m/s^2 . This example uses the adaptive time step which initiated at 0.05s.

(a) Velocity history

(b) Displacement history

Figure 6- 2 Comparison between NMM results and analytical results on displacement & velocity history

The displacement and the velocity time history are shown in Fig. 6-2. The dots are the results of numerical simulation from 3-D NMM, while the curved lines as exact value from the analytical solution. The error of the numerical solution has less than

0.1% in the maximum absolute difference, which illustrates the credibility of the NMM calculation accuracy.

6.2 Effect of MC Size and Orientation

The NMM consists of independent MCs and PCs, thus the generation of the cover based manifold elements is not restricted to the MC configurations, instead, the concerned physical domain can be obtained by intersection with MCs. The following examples are to investigate the effect of the MC size and the cutting plane orientations. A plate structure is generated by cutting a cube and the density of the MC is variable. The orientation of the cutting planes to produce the same geometry plate can be different.

6.2.1 MC size effect (quasi-static condition)

In a quasi-static condition the MC size effect towards the solution is examined below (Example I). A $2\text{ m} \times 2\text{ m} \times 0.1\text{ m}$ plate is subjected to the gravity load with $g=10\text{m/s}^2$ and fixed at four corners. The material properties are assumed to be $E=10\text{kPa}$, $\nu=0.3$, $\rho=12\text{ kg/m}^3$. Its geometry of the typical mesh design is shown in Fig. 6-3 in which the faces of the plate are conformed parallel to the axis planes.

Six mathematical cover size of $s= 0.52, 0.32, 0.22, 0.12, 0.08$ and 0.05 are used to examine the MC size effect. After intersecting with the physical plate, 190, 684, 1104, 3706, 8100 and 19200 manifold elements are respectively generated. In order to clarify the quasi-static responses of the 6 models, five measurement points in total are set at the middle of the panel for every edge for each case (Fig. 6-3). The calculated results are converging and stable with the increase of the mesh density as shown in Fig. 6-4 and the analysis are listed in Table 6-1.

Total MElem no. = 1104
 Total Facet no. = 5266
 Total Point no. = 6116
 Current blk no. = 1

(a) Mesh design #1

Time step 30000->15000

(b) Location of measurement points

Figure 6- 3 Geometry of typical mesh design for *mesh density effect study*

The maximum displacement of case 6 (*refinement 5*) is illustrated in Fig. 6-5. It is found that the results converge well and all the four edges are adequately symmetric,

e.g. M1~4 curves in Fig. 6-5 represent the deformation history of four middle points from the up, down, left and right side.

The results converge to the closed-form solution when the mesh density increases. The validity of the 3-D NMM calculation is supported by the consistent results given by the FEM analysis solution.

Figure 6- 4 Total deformation convergence test

Table 6- 1 Solution history at the center of panel

Name	Base Solution	Refinement 1	Refinement 2	Refinement 3	Refinement 4	Refinement 5
Total Deformation	0.16404 m	0.25027 m [+34.45%]	0.34334 m [+27.11%]	0.37919 m [+9.45%]	0.39694 m [+4.47%]	0.39973 m [+0.76%]
Mesh properties	Spacing: 0.52 Elements: 190 Vertexes: 1156	Spacing: 0.32 Elements: 684 Vertexes: 3812	Spacing: 0.22 Elements: 1104 Vertexes: 6116	Spacing: 0.12 Elements: 3706 Vertexes: 20184	Spacing: 0.08 Elements: 8100 Vertexes: 44282	Spacing: 0.05 Elements: 19200 Vertexes: 76800

Figure 6- 5 Deformation of case 6 at the maximum displacement loading step

6.2.2 MC orientation effect (dynamic condition)

In dynamic condition, the MC orientation effect is tested by *Example II*, where a $2\text{ m} \times 2\text{ m} \times 0.1\text{ m}$ plate is subjected to a constant point load $L=5\text{ kN}$ at the center with four fixed corners. The material properties of the plate are the same as the previous example (*Example I*), but the program are set under fully dynamical mode for these examples. Two different orientations of the mathematical mesh (Orientation 2 and 3) are shown in Fig. 6-6 while the orientation 1 is same as *Example I*.

(a) Mesh design #2

(b) Mesh design #3

Figure 6- 6 Geometry of mesh designs for *mesh orientation effect study*

The Z displacement histories of the center point are shown in Fig. 6-7, from which it can be seen that the orientation of the MCs has negligible effect on the plate maximum displacement at the plate center. The maximum displacement is accurate

and stable after converging, and the convergence time is similar when the total element number is almost same. The details of results are shown in Table 6-2.

Figure 6- 7 Z displacement histories of center point

The results show that the orientation of the MCs has little effect to the simulation result. This ensures the accuracy and modeling efficiency of the 3-D NMM decreases the mesh division complexity in FEM, and increases the modeling efficiency. It also supports the validity of the 3-D NMM dynamic algorithm.

Table 6- 2 Mesh design comparison

Name	Mesh Design 1	Mesh Design 2	Mesh Design 3
" Results"	Peak disp.: 0.39598 m Stable disp.: 0.255538 m Stable time: 48.86s.	Peak disp.: 0.40054 m Stable disp.: 0.252278 m Stable time: 49.16s	Peak disp.: 0.40878 m Stable disp.: 0.253667 m Stable time: 46.34s
Mesh properties	Spacing: 0.32 Elements: 684 Direction: 0 0, 90 0, 90 90	Spacing: 0.31 Elements: 608 Direction: 0 0, 90 30, 90 120	Spacing: 0.28 Elements: 618 Direction: 30 0, 90 30, 90 120

Note: When the absolute curvature is smaller than 0.01%, it is regarded as "stable status".

6.3 Cube Sliding on an Inclined Plane

6.3.1 Problem Statement

This example is designed to test the numerical algorithms to study the face-to-face contact mode (or vertex-to-face mode), and also the stability of the system in applying friction boundary condition. This example is quite common and widely seen in engineering application. A matrix sliding cube is put on an inclined plane, and the movement of the sliding cube is observed.

6.3.2 Analytical Solution

The general equation of motion for a rigid block on an inclined plane subject to *Coulomb* frictional resistance force can be expressed as a single degree-of-freedom system by taking its coordinate system parallel to the plane direction, as shown in Fig. 6-8. The analytical solution for the displacement d after time t from the resting state is:

$$d = \frac{1}{2} g (\sin \alpha - \tan \phi \cos \alpha) t^2 \quad (6-1)$$

where g is the acceleration of gravity, α is the slope angle of inclined plane, and ϕ is the friction angle of plane surface.

Figure 6- 8 General model for sliding cube on an inclined plane

6.3.3 3-D NMM Model

The physical model shown in Fig. 6-9 consists of two contact bodies. The bottom wedge with inclined plane is fixed and only the sliding cube is allowed to move under the pure gravity. The mechanical properties and calculation parameters are in Table 6-3.

Table 6- 3 Mechanical properties and calculation conditions in “Cube sliding”

Parameters	Value
Density ρ (kg/m ³)	2650
Young’s modulus E (GPa)	50
Poisson’s ratio ν	0.25
Penalty spring stiffness P	$20E$
The slope of inclined plane α	24
Gravity acceleration g (m / s ²)	10

Figure 6- 9 Physical model for sliding cube

After the intersection between the physical model and mathematical covers, 280 tetrahedron manifold elements are finally generated, as shown in Fig. 6-11 (after generating hexahedral division in Fig. 6-10).

Figure 6- 10 Hexahedron manifold elements with mathematical domain in “Cube sliding”

The black-colored frame in the figure is the emphasized territory of mathematical covers, which are generated from the interaction with physical domain.

```

Input Block no. = 2
Tetra Elemt no. = 280
Total Facet no. = 1373
Total Point no. = 1620
Current blk no. = 1

```

Figure 6- 11 Tetrahedron manifold elements for calculation in “Cube sliding”

Seven different friction angle values, with 0, 5, 10, 15, 20, 24, 25, have been assigned on the sliding surface.

6.3.4 Results and Discussion

A comparison between the analytical solutions from Eq. (6-1) and 3-D NMM solutions is shown in Fig. 6-12. The 3-D NMM results show a satisfactory agreement with the time-dependent displacement functions predicted by the analytical solutions. It demonstrates that the 3-D NMM is able to capture essential aspects of the displacement over the sliding distance.

Figure 6- 12 Comparison between the analytical results and 3-D NMM results in “Cube sliding”

The dots in Fig. 6-12 denote the numerical result of 3-D NMM program from time 0 to 1.0 second with time interval of 0.01 second, where else the curve lines represented the analytical results. The maximum error shown is less than 0.001% for all different friction angles tested, and these matched results proved that the 3-D NMM code is accurate enough for geotechnical problems. Since the 24 degree is the critical friction angle in this example, some interesting phenomena can be observed during calculation. A little sliding occurs when the friction angle is set as same as the slope of inclined plane α . The small extent sliding is due to the initial unstable dynamical interaction between the cube and the inclined plane, because the gravity load is acting to the system suddenly at begin. However, the difference between the curve of 24° and 25° is difficult to find in the Fig. 6-12's precision level. If the calculation are divided into two phases, and friction angle is set to a higher value than the critical value at the first phase. After few time steps calculation, the system becomes stable. Then, the friction angle reduces to 24° . This phenomenon will not occur.

6.4 Roof Wedge Falling

6.4.1 Problem Statement

The stability of a rock mass located at the roof of a tunnel is always under the priority concern. The stabilizing effect of the in-situ stresses and the influence of joint friction are significant factors that affect the structure stability of tunnels. Under the effect of these two factors, tunnel surface could stay stable without any artificial supports. Meanwhile, sudden change of the intensely strong in-situ state of stress and joint friction state could be one of the reasons to induce rock burst. A simple model in this example is firstly used to examine the accuracy of the 3D-NMM analysis prior utilizing it to analyze the stability of the complex tunnel structure later on.

As shown in Fig. 6-13, a roof wedge is generated by three joints which are dipping at 65° with dip directions of 30° , 150° , and 270° . The height of the wedge is 1 meter. An in-situ state of stress which consists of two principal stresses parallel to the tunnel roof, equal to -0.05MPa . The vertical principal stress is set to zero.

Figure 6- 13 Physical model for a roof wedge

6.4.2 Analytical Solution

It is fortunate that the simplified model of falling wedge has a theoretical solution. A closed-form solution of the support force for stabilization of the wedge in the roof was derived by [Goodman *et al.* (1982)], and is given by the equation

$$\frac{A_0}{W} = 1 - \sum_{i=1}^{n-1} \frac{\sigma_{n,i} A_i \sin(\phi_i - \alpha_i) (k_{s,i} / k_{n,i}) [\cos \alpha_i \cos i_i + \tan \alpha_i \sin(\alpha_i - i_i)]}{W \cos \phi_i (k_{s,i} / k_{n,i}) [\cos \alpha_i \cos i_i + \tan \phi_i \sin(\alpha_i - i_i)]} \quad (6-2)$$

where

n = number of faces on the block;

i = index denoting the face of the block;

A_0 = required force to stabilize the wedge;

W = weight of the wedge;

$\sigma_{n,i}$ = normal stress acting on the i^{th} face of the wedge;

A_i = area of the face of wedge;

ϕ_i = friction angle on the face of the wedge;

α_i = complement of the dip angle of the joint which creates the face;

$k_{s,i}$ = shear stiffness of the i^{th} joint;

$k_{n,i}$ = normal stiffness of the i^{th} joint;

i_i = roughness angle of the i^{th} joint.

For this particular case, where:

1. All joints have the same dip angle;
2. The initial stress state in the plane parallel to free face of the block is hydrostatic;
3. All joints have the same ratio between normal and shear stiffness.

The critical friction coefficient required for stability of the wedge without any support can be expressed by Eq. (6-3), as follows:

$$\tan \phi = \frac{W + \sigma_n \sum A_i \sin \alpha}{\sigma_n \sum A_i \sin \alpha - W \tan \alpha} \quad (6-3)$$

6.4.3 3-D NMM Model

The physical model in this example contains seven bodies. Six lateral bodies are fixed and only the central tetrahedron wedge is allowed to move under gravity. The mechanical properties and conditions are listed as in Table 6-4.

For clearer visualization of the targeted subject, the six surrounding bodies are hidden. The position of the movable central wedge (transparent) and fixed points are shown in Fig. 6-14. Each three-color crossing represents a fixed point.

Table 6- 4 Mechanical properties and conditions for “Roof wedge falling” example

Parameters	Value
Density ρ (kg/m ³)	2000
Young's modulus E (GPa)	50
Poisson's ratio ν	0.25
Penalty spring stiffness P	$20 \cdot E$
Critical frictional angle ϕ in analytical solution	34.402^0
In-situ horizontal principal stress σ (MPa)	-0.05
Gravity acceleration g (m/s ²)	10

Figure 6- 14 Position of the movable wedge and fixed points

Similarly, the hexahedron manifold elements with corresponding mathematical covers are presented in Fig. 6-15.

Figure 6- 15 Hexahedron manifold elements with mathematical domain in “Roof wedge falling”

After the intersection between the physical model and mathematical covers, 454 manifold elements are finally generated.

6.4.4 Results and Discussion

The calculation consists of two stages. Firstly, the friction angle is set to 89 degree. After a period of 2 second, the designed system becomes stable with proper systematic damping. Through reducing the friction gradually, it could reach the case when central wedge starts to fall down. The 3-D NMM simulation yields a friction angle 36.354° , and the closed value from the analytic solution for the critical friction angle is 34.402° . The failure of the wedge is shown in Fig. 6-16. The systematic damping is a governing parameter (from 0 to 1) in Author’s 3-D NMM version. It presents that how much velocity of each cover has been transfer to next time step, also indicts how many percent of energy loss in total during a time step. If the value

set to “0”, it means the simulating system is under quasi-static condition. While “1” means the fully dynamic version.

Figure 6- 16 Failure of roof wedge

Although, the final result of this example has an error of 5.67% compared to the analytical solution, it illustrates the reliability of the contact algorithm and the imposed initial stress. It proves that the calculation precision of 3-D NMM which has satisfied the practical requirements in the rock engineering.

6.5 Tetrahedral Wedge Sliding

6.5.1 Problem Statement

Rock-slope failure is a major hazard in cutting highways and railways in mountainous area. A tetrahedral wedges sliding is one of most common phenomena (shown in Fig. 6-17). It is caused by the intersection of two separate planes, for example, two joints sets. The slope surface and two planes create a wedge that will tend to slide outwards even under the pure gravity due to the lack of frictional resistance. In this case, stability analysis is important in terms of both cost estimation

before and during construction and safety during and after construction.

Figure 6- 17 Wedge failure at the side of road¹

6.5.2 Analytical Solution

The stability analyses of tetrahedral wedges in rock slopes are commonly conducted using stereographic projection technique [Goodman (1976)], engineering graphics [John KW (1968)], versatile sequential vectorial operations [Hoek and Bary (1981)], and closed-form equations based on limit equilibrium [Low BK (1997)].

Among the theories stated, the vectorial procedure of Hoek and Bray (1981) is chosen to check the analytical ability of 3-D NMM to understand this kind of problem.

Definitions and notations of the geometry are illustrated in Fig. 6-18. The discontinuities are denoted by Plane 1 and 2. The crest surface of the slope is denoted by Plane 3 and Plane 4 presenting the slope face. To solve this problem, the parameters required are: the unit weight of rock mass γ , the height H of the crest of the slope above the intersection, the dip ψ and dip direction α of each plane,

¹ Refer to Ahmad Rosli Blog(2008-11-02):http://geologimalaysia.blogspot.com/2008_11_01_archive.html

the cohesion modulus c and the friction angle ϕ for planes 1 and 2 and the average water pressure u on each of the planes 1 and 2². If the slope face overhangs the toe of the slope, an index η is assigned the value of -1; if the slope does not overhang, $\eta = +1$.

Figure 6- 18 Definition of the slope geometry

Other terms used in the solution are:

F = factor of safety against wedge sliding calculated as the ratio of the resisting to the actuating shear forces.

A = area of a face of the wedge

W = weight of the wedge

N = effective normal reaction on a plane

S = actuating shear force on a plane

x, y, z = co-ordinate axes with origin at 0. The z axis is directed vertically upwards.

The y axis is in the dip direction of plane 2.

$\vec{a}$ = unit vector in the direction of the normal to plane 1 with components (a_x, a_y, a_z)

² If it is assumed that the discontinuities are completely filled with water and that the water pressure varies from zero at the free faces at a maximum at some point on the line of intersection, then $u_1 = u_2 = \frac{\gamma_w H_w}{6}$ where H_w is the overall height of the wedge.

$\vec{b}$ =unit vector in the direction of the normal to plane 2 with components (b_x, b_y, b_z)

$\vec{f}$ =unit vector in the direction of the normal to plane 4 with components (f_x, f_y, f_z)

$\vec{g}$ =vector in the direction of the line of intersection of plane 1 and 4 with components (g_x, g_y, g_z)

$\vec{i}$ = vector in the direction of the line of intersection of plane 1 and 2 with components (i_x, i_y, i_z)

$$i = -i_z$$

q = component of $\vec{g}$ in the direction of $\vec{b}$.

r = component of $\vec{a}$ in the direction of $\vec{b}$.

$$k = |\vec{i}|^2 = i_x^2 + i_y^2 + i_z^2$$

$$l = W / A_2$$

$$\left. \begin{array}{l} p = A_1 / A_2 \\ n_1 = N_1 / A_2 \\ n_2 = N_2 / A_2 \\ |li| / \sqrt{k} = SA_2 \end{array} \right\} \text{Assuming contact on both planes}$$

$$\left. \begin{array}{l} m_1 = N_1 / A_2 \\ \text{denominator of } F = S_1 / A_2 \end{array} \right\} \text{contact on plane 1 only}$$

$$\left. \begin{array}{l} m_2 = N_2 / A_2 \\ \text{denominator of } F = S_2 / A_2 \end{array} \right\} \text{contact on plane 2 only}$$

Analysis Procedure:

The factor of safety of a tetrahedral wedge against sliding along a line of intersection could be calculated by:

1. $(a_x, a_y, a_z) = \{\sin \psi_1 \cdot \sin(a_1 - a_2), \sin \psi_1 \cdot \cos(a_1 - a_2), \cos \psi_1\}$
2. $(f_x, f_y, f_z) = \{\sin \psi_4 \cdot \sin(a_4 - a_2), \sin \psi_4 \cdot \cos(a_4 - a_2), \cos \psi_4\}$
3. $b_y = \sin \psi_2$
4. $b_z = \cos \psi_2$
5. $i = a_x b_y$

$$6. \quad g_z = f_x a_y - f_y a_x$$

$$7. \quad q = b_y(f_z a_x - f_x a_z) + b_z g_z$$

8. If $nq/i > 0$, or if $n \cdot (f_z - q/i) \cdot \tan \psi_3 > \sqrt{1 - f_z^2}$ and no wedge is formed and the calculations should be terminated.

$$9. \quad r = a_y b_y + a_z b_z$$

$$10. \quad k = 1 - r^2$$

$$11. \quad l = (\gamma H q) / (3 g_z)$$

$$12. \quad p = -b_y f_x / g_z$$

$$13. \quad n_1 = \{(l/k)(a_z - r b_z) - p u_1\} \cdot p / |p|$$

$$14. \quad n_2 = \{(l/k)(b_z - r a_z) - u_2\}$$

$$15. \quad m_1 = (l a_z - r u_2 - p u_1) \cdot p / |p|$$

$$16. \quad m_2 = (l b_z - r p u_1 - u_2)$$

17. a) if $n_1 > 0$ and $n_2 > 0$, there is contact on both planes and

$$F = (n_1 \cdot \tan \phi_1 + n_2 \cdot \tan \phi_2 + |p| c_1 + c_2) \sqrt{k} / |l|$$

b) if $n_2 < 0$ and $m_1 > 0$, there is contact on plane 1 only and

$$F = \frac{m_1 \cdot \tan \phi_1 + |p| c_1}{\{l^2(1 - a_z^2) + k u_2^2 + 2(r a_z - b_z) l u_2\}^{\frac{1}{2}}}$$

c) if $n_1 < 0$ and $m_2 > 0$, there is contact on plane 2 only and

$$F = \frac{m_2 \cdot \tan \phi_2 + c_2}{\{l^2 b_y^2 + k p^2 u_1^2 + 2(r b_z - a_z) p l u_1\}^{\frac{1}{2}}}$$

d) if $m_1 < 0$ and $m_2 < 0$, contact is lost on both planes and the wedge floats as a result of water pressure acting on planes 1 and 2. In this case, the factor of safety falls to zero.

6.5.3 3-D NMM Model

Based on the definition given, two cases are designed to test the 3-D NMM accuracy,

and examine whether the failure mode could be performed as expected by sliding through the specific planes (shown in Fig. 6-19 and Fig. 6-21). 4 planes' Dip and Dip Direction (DD), with stereographic projection are shown in Fig. 6-20.

Figure 6- 19 Physical models for two sliding tetrahedral wedge

Figure 6- 20 4 planes' Dip and DD, with stereographic projection for two sliding tetrahedral wedge

The mechanical properties and conditions are listed in Table 6-5.

Table 6- 5 Mechanical properties and conditions in “Tetrahedral wedge sliding”

Parameters	Value
Density ρ (kg/m ³)	2500
Young’s modulus E (GPa)	50
Poisson’s ratio ν	0.25
Penalty spring stiffness P	$20 \cdot E$
Gravity acceleration g (m / s ²)	10

For case (a), the calculation involves 292 manifold elements with mesh size 0.5 and Case (b) has totally 752 manifold elements with mesh size 0.5.

Figure 6- 21 Hexahedron manifold elements with mathematical domain in “Tetrahedral wedge sliding”

6.5.4 Results and Discussion

According to analytical solution procedure, the geometric parameters and critical frictional angles for two cases are given as below:

Table 6-6 gives two planes in case (a)'s dip and dip direction based on theoretical calculation, which assumes that only friction angle exists in sliding planes and cohesion is set to 0. The analytical calculation procedure and its corresponding result are shown in step 1-16 in the table. In the analytical solution table, the critical friction angle under the example setting could be gained through adjusting the friction angle until the factor of safety turning into 1. At the same time, failure mode *F1* is also gained, which indicates that contact happens simultaneously on the two planes in the process of sliding.

Similarly, Table 6-7 gives the critical friction angle and its failure mode *F2*, which implies that the sliding is only along the plane 1.

The process in 3-D NMM calculation is divided into two stages. Firstly, friction angle is set to 89 degree to ensure a definite stable system built and the dynamical ratio sets to 0.5 by increasing its systematical damping.

Table 6- 6 Geometric parameter and analytical solution for case (a) sliding tetrahedral wedge

Definition		Step 1,2,3,4		step 5,6,7,8		step 9-16		
the unit weight of rock	γ	25	ax	0.699521	1	0.573014201	r	0.490195
height H of the crest of the s		1	ay	0.103296	g_z	-0.42159465	k	0.759709
			az	0.707107	q	-0.65139278	l	12.87557
Dip - Plane 1	ψ_1	45			$\eta q/i$	-1.13678296	p	1.373898
D D - Plane 1	α_1	36.6	fx	0.707107	$\eta(f_z - q/i) \tan \psi_3$			
Dip - Plane 2	ψ_2	55	fy	0.707107	$\text{SQRT}(1-F_z^2)$	-1	n1	7.218889
D D - Plane 2	α_2	-45	fz	6.13E-17			n2	3.846461
Dip - Plane 3	ψ_3	0						
D D - Plane 3	α_3	0	bx	0			m1	9.104406
Dip - Plane 4	ψ_4	90	by	0.819152			m2	7.385122
D D - Plane 4	α_4	0	bz	0.573576				
cohesion - Plane 1	c_1	0						
friction angle - Plane 1	ϕ_1	37.41485						
cohesion - Plane 2	c_2	0						
friction angle - Plane 2	ϕ_2	37.41485						
Conclusion								
aver. water press. - P1	u_1	0	a) if $n1 > 0$ & $n2 > 0$, contact on both planes					
aver. water press. - P2	u_2	0	b) if $n2 < 0$ & $m1 > 0$, contact on plane 1					
			c) if $m1 < 0$ & $m2 > 0$, contact on plane 2					
overhang index	η	1	d) if $m1 < 0$ & $m2 < 0$, contact is lost on both pla					
* the wedge floats as a result of water pressure acting on plane 1 and 2								
						F1	1.000001	Factor of safety
							0.764968	1.000000657
							0.535637	Failure mode
						F4	0	F1

Table 6- 7 Geometric parameter and analytical solution for case (b) sliding tetrahedral wedge

Definition		Step 1,2,3,4		step 5,6,7,8		step 9-16		
the unit weight of rock	γ	25	ax	0.4089678	i	0.384304	r	0.803011
height H of the crest of the s		2	ay	0.6063197	g_z	-0.08078	k	0.355173
			az	0.6819984	q	-0.1289	l	26.59584
Dip - Plane 1	ψ_1	47			$\eta q/i$	-0.33542	p	4.786418
D D - Plane 1	α_1	52	fx	0.4114551	$\eta(f_z - q/i) \tan \psi_3$		m1	30.50311
Dip - Plane 2	ψ_2	70	fy	0.8075262	SQRT (1-Fz2)	-0.77265	m2	-15.398
D D - Plane 2	α_2	18	fz	0.4226183				
Dip - Plane 3	ψ_3	10						
D D - Plane 3	α_3	45	bx	0			m1	18.13832
Dip - Plane 4	ψ_4	65	bxy	0.9396926			m2	9.096312
D D - Plane 4	α_4	45	bz	0.3420201				
cohesion - Plane 1	c_1	0						
friction angle - Plane 1	ϕ_1	47						
cohesion - Plane 2	c_2	0						
friction angle - Plane 2	ϕ_2	50						
Conclusion								
aver. water press. - P1	u_1	0	a) if $n1 > 0$ & $n2 > 0$, contact on both planes		F1	0.837304	Factor of safety	
aver. water press. - P2	u_2	0	b) if $n2 < 0$ & $m1 > 0$, contact on plane 1		F2	1	1	
			c) if $m1 < 0$ & $m2 > 0$, contact on plane 2		F3	0.433763	Failure mode	
overhang index	η	1	d) if $m1 < 0$ & $m2 < 0$, contact is lost on both plane*		F4	0	F2	
* the wedge floats as a result of water pressure acting on plane 1 and 2								

After a period of 0.5 second, dissipate the system vibration due to suddenly imposed gravity. The friction angle will decrease gradually until the wedge starts to fall, meanwhile, the critical friction angel is gained numerically in the starting time of falling down. The 3-D NMM simulation results are presented in Table 6-8.

Table 6-8 shows the consistency between the analytical solution and 3-D NMM numerical solution. In case (a), the error is 1.850%, and the error is only 1.372% for case (b), both having less than 2% error. One possible reason for the error term is that analytical solution is gained from assuming contacting block as rigid block; while on the other hand, blocks in 3-D NMM allow deformation.

Table 6- 8 Comparison between the analytical and 3-D NMM solution in
“Tetrahedral wedge sliding”

	Case (a)	Case (b)
Analytical solution	37.415 ⁰ /37.415 ⁰	47.000 ⁰ /50.000 ⁰
3-D NMM solution	38.107 ⁰ /38.107 ⁰	47.645 ⁰ /50.000 ⁰
Absolute difference	1.850%	1.372%

Although there is approximately 2% error, the accuracy level is high enough to satisfy practical requirement. Besides, the error term tends to be conservative in this case, as the numerical calculation results give higher factor of safety.

In the second stage of testing, the friction angle is further decreased to the critical value for stability. The wedges will start to slide, and its failure mode could be observed. This is to check whether the 3-D NMM results are consistent with the prediction of the analytical solution. The failure procedure based on the numerical simulations result is shown in Fig. 6-22. As expected, contact faces are always on the two planes in case (a) throughout the process of wedge sliding, until flipping and overturn in the numerical results. While the sliding face in case (b) is exactly plane 1, sliding wedge is separated with plane 2 after a short sliding period, and then succeeding sliding is along plane 1. The sliding situations in the numerical process are in line with the analytical prediction, as shown in Fig. 6-23.

Case (a)

Case (b)

Figure 6- 22 Failure procedures for case (a) and (b) in “Tetrahedral wedge sliding”

Time step 30000-> 0
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

Time step 30000-> 174
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

Time step 30000-> 325
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

Time step 30000-> 727
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

Case (a)

Time step 30000-> 0
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

Time step 30000-> 171
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

Time step 30000-> 300
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

Time step 30000-> 572
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

Case (b)

Figure 6- 23 Failure procedures according the predicted mode in “Tetrahedral wedge sliding”

6.6 Application Examples

In this section, two relatively complicate examples are demonstrated to test the robustness and applicability of the proposed 3-D NMM algorithm, especially the contact algorithm. Two applicable examples are given. One is the 3-D dominos run with sequential contact happening, which is normally studied in 2-D simulation studies. The other is a 3-D dougong/brackets structure, which is commonly found in practical construction engineering.

6.6.1 Dominos run

A typical 3-D domino run problem shown in Fig. 6-24 is numerically investigated using the 3-D NMM. The numerical model consists totally 19 Domino blocks with the size of $291.4\text{ mm} \times 184.8\text{ mm} \times 37.1\text{ mm}$ and the approximate spacing of 239.1 mm setting on a horizontal surface.

The mechanical properties and conditions are listed as below:

Density $\rho = 2000\text{ kg/m}^3$

Young's modulus $E = 200\text{ GPa}$

Poisson's ratio $\nu = 0.3$

Penalty spring stiffness $P = 10 \cdot E$

Gravity acceleration $g = 10\text{ m/s}^2$

Frictional angle $\phi = 35^\circ$

Figure 6- 24 Configuration of a dominos run problem

This calculation involves 259 manifold elements with mesh size 0.75, as shown in Fig. 6-25.

Input Block no. = 20
Tetra Elemt no. = 259
Total Facet no. = 1440
Total Point no. = 1844
Current blk no. = 1

Figure 6- 25 Hexahedron manifold elements with mathematical domain for “dominos run”

In the initial state, the first block has been leaned when the scenery is setup, acting as the initial momentum in the system. To begin the test, the first block will topple onto the second block through gravity, which induces a toppling process, shown in Fig. 6-26. The numerically obtained results are consistent with the experimentally observed phenomenon [Bates (2004)].

(a)0s

(b)0.924s

(c)1.848s

(d)2.772s

(e)3.696s

(f)4.530s

(g) Top view of dominos run at 4.530s

Figure 6- 26 Dominos run process modeled by the 3-D NMM

A failure of dominos run under zero friction angle (Fig. 6.26), dominos run could not be realized in absolute smooth horizontal surface. It is demonstrated by setting the frictional angle between the blocks and the horizontal surface is set to 0, the first block will skid smoothly without friction, which could induce non-interaction to the section block.

Figure 6- 27 Failure of Dominos run without friction

In order to check the consistency of the algorithm, additional numerical experiment is done. Except the toppling of the first block under gravity with friction, an initial rotation velocity is imposed to the last block in the 3-D dominos system, and it smashes itself to the second-to-last block. This initial setting will produce a simultaneous toppling process in both side of the 3-D dominos system, as shown in Fig. 6-28.

The numerical result shows that the two-side simultaneous domino motion will stop at the time of 2.05 second, where the ninth block and the tenth block will lean against each other as “ Λ ” shaped.

Time step: 501 -> 1
Accumulated Time = 0 s
Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(a)0s

Time step: 501 -> 101
Accumulated Time = 0.475115 s
Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(b)0.475s

Time step: 501 -> 201
Accumulated Time = 0.933100 s
Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(c)0.933s

Time step: 501 -> 301
Accumulated Time = 1.391084 s
Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(d)1.391s

Time step 501-> 401
Accumulated Time = 1.849069 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(e) 1.849s

Time step 501-> 845
Accumulated Time = 2.050582 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(f) 2.051s

Time step 501-> 500
Accumulated Time = 2.302874 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(g) Top view of dominos run at 2.302s

Figure 6- 28 Two-end dominos run process modeled by the 3-D NMM

The aim of the example here is to test the accuracy of one contracting mode: point-to-plane mode, mentioned in *Chapter 5*. The following verification example in next section aims to examine the performance of another contact mode: crossing lines mode.

6.6.2 Dougong/Brackets structure

The *dougong* style (also known as corbel arch, and Tou-Kung) a wooden brackets structure, build up from fixed layers of crossbeam fixed on top of columns. This unique structural component of interlocking wooden brackets is one of the most important elements in traditional Chinese architecture. Dougong was widely used in the Spring and Autumn Period in Chinese history (770 BC-467 BC). This architecture style is also commonly found in the modern development, for example, the design of *China Pavilion* in *World Expo 2010*, Shanghai. The main structure of the China Pavilion, "The Crown of the East", has a distinctive roof, made of traditional dougong or brackets, as shown in Fig. 6-29.

Figure 6- 29 “The Crown of the East” in Expo. 2010

The stability analysis to such dougong structure and its damage features are both important to production safety and also to prevent from potential threat of terrorist attack.

In this example, a simplified dougong structure sample, which is lack of stability, is studied in 3-D NMM for its collapsing process if it was subjected to pre-damage. The aim is to test the consistency of crossing lines mode in the 3-D contact algorithm. As

shown in Fig. 6-30, the numerical example is designed, the whole structure is put on a flat plane, and built up by 3 poles and 12 beams, where the 12 beams are allocated into 4 different layers superposed to each other, as in a hexahedral location.

Figure 6- 30 Design of “dougong” structure model

The simulation model has a total height of 1004.3 mm. the height of each pole is 450 mm with hexagon cross section of 150 mm edge. The lengths of beams in different layers are different, and the longest beam is 1500 mm with hexagon cross section with 80 mm edge. One of the poles has been imposed by thorough-crack with a dip of 27.2 degree, which is the only one fault in the designed dougong structure for numerical simulation. Under this case, the structure could be crashed down by the force of gravity and insufficient frictional resistance.

It is worth to note that, such positioning makes the contact type to be mainly *crossing lines mode*, caused by face-to-face contact (In *Chapter 5*). It was mentioned that such contact mode is dependent for detection and treatment. The key problem that we

concerned is “Whether the whole process of crashing-down damage satisfy the non-penetration contact condition?”. If it always satisfies the non-penetration contact condition in the whole process, it will provide a strong support on the ability of 3-D NMM to solve similar contacting problems.

The mechanical properties and conditions are listed as below:

Density $\rho = 2500 \text{ kg/m}^3$

Young's modulus $E = 20 \text{ GPa}$

Poisson's ratio $\nu = 0.25$

Penalty spring stiffness $P = 10 \cdot E$

Gravity acceleration $g = 10 \text{ m/s}^2$

Again, the physical model interacts with the mathematical background (Fig. 6-31). The numerical calculation follows such mesh.

Figure 6- 31 Hexahedron manifold elements with mathematical domain in “dougong” structure

For this case, the structure is modeled with 326 manifold elements. There are totally 798 contact pairs at the end of the first time step, where 628 contact pairs of them are

determined to be crossing lines mode. Total calculation runs through 500 time steps in 3.68 seconds. The total CPU time is about 25 minutes for the whole problem on a general computer with Intel E8500 and 3G RAM.

Some configurations of the structure are shown in Fig. 6-32.

Time step: 501 -> 1
Accumulated Time = 0 s
Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(a) 0s

Time step: 501 -> 10
Accumulated Time = 0.309224 s
Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(b) 0.309s

Time step: 501 -> 30
Accumulated Time = 0.527249 s
Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(c) 0.527s

Time step: 501 -> 50
Accumulated Time = 0.742059 s
Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(d) 0.743s

Time step: 501 -> 100
Accumulated Time = 1.146350 s
Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(e) 1.146s

Time step: 501 -> 200
Accumulated Time = 1.793070 s
Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(f) 1.794s

Time step 501-> 500
Accumulated Time = 2.419680 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(g) 2.419s

Time step 501-> 499
Accumulated Time = 3.043482 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(h) 3.043s

Time step 501-> 500
Accumulated Time = 3.668285 s

Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(i) 3.668s

Figure 6- 32 Failure process of “dougong” sample modeled by the 3-D NMM

Even though quantitative analysis has not been given to these verification examples, qualitative studies are employed on the applying and releasing of contact conditions to demonstrate the phenomenon process. The whole modeling process from pre-processing to calculation results are relatively easy to operate, and the 3-D NMM shows its stability in running different cases. It has already proven and demonstrated the efficiency of the algorithm and its strong power of the implemented contact

algorithm.

As the limitation of current preliminary version for the algorithm, it has used the tetrahedron-based background mesh of 0th-order cover function and 1st-order weight function (in *Chapter 3*). Correspondingly, the strain description is relatively rough right now. In the future, it is worth and meaningful to continue further development on accurate material models and high order manifold element.

Chapter 7 Engineering Application---Rock Slope Stability Analysis

7.1 Introduction

The primary purpose to design the NMM is to utilize them to engineer practice, especially to rock engineering. 3-D NMM has unfolded its versatile ability both in the aspect of methodology and of its potential ability to solve different engineering problem during the process of its development. For example, It could be utilized in stability analysis like slope stability, dam stability, tunnel stability.

This chapter pays its attention to its engineering application through systematically analyze one example of rock slope stability to present its potential application abilities. Although the design of the application might have minor disparity with real practice in engineering as limitation of time and real engineering experience, it could act as a tentative investigation to the application ability of proposed algorithm.

In the following sections, *Section 7.2* will shortly discuss about background in rock slope stability analysis, including the importance, current technique limitation on slope stability analysis, the classification for slope engineering based on literatures and engineering practice, the typical failure mode, causes of landslides, and current techniques. *Section 7.3* briefly describes the design of rock slope scenario as application example. *Section 7.4* then gives the modeling with the proposed 3-D NMM program, and *Section 7.5* applies stabilisation measures to discuss the results. Summary and discussion are in *Section 7.6*.

7.2 Background for Rock Slope Engineering

7.2.1 Slope stability

This part mainly discusses about the importance and practical background on slope stability, and limitation of current techniques.

A landslide or landslip is a geological phenomenon which includes a wide range of ground movement, such as rock falls, deep failure of slopes and shallow debris flows, occurring in coastal and mountainous environments.

Recent years, geological activity is relatively frequent globally. In China, Yushu county in northwestern China's Qinghai Province was jolted by a 7.1-magnitude earthquake on April 14, 2010, and a 8.0-magnitude earthquake hit Wenchuan in Sichuan China in May 12, 2008, which killed at least 68,000 people only for Wenchuan earthquake³. Part of its damage are caused by landslides that triggered by earthquake. In May 23, 2010 of Jiangxi province of China, a train from Shanghai to Guilin province derailed in the mountainous area in its Dongxiang county⁴. One of potential causality to its derailment could be subsequent landslide induced by previous rainstorm.

It could be seen that the damage for landslide are serious, and it is quite important to have proper tools to understand the mechanism of landslide. Up to now, the majority of slope stability analyses performed in practice use traditional limit equilibrium approaches or stereographic and kinematic analysis, involving methods of slices that have remained unchanged for decades essentially.

Such analytical methods provides prompt and accurate solution to some specific and relatively simple failure mode (e.g. wedge failure), but it becomes inadequate if the slope fails as a result of complex mechanisms (e.g. internal deformation and brittle

³ This information is based on Wikipedia website. Refer to: Jacobs, Andrew; Edward Wong, Huang Yuanxi (2009-05-07). "China Reports Student Toll for Quake". New York Times. <http://www.nytimes.com/2009/05/08/world/asia/08china.html>. Retrieved 2009-05-14.

⁴ Refer to Wikipedia website: http://en.wikipedia.org/wiki/2010_Jiangxi_train_derailment.

fracture, progressive creep, liquefaction of weaker soil layers, etc.).

The finite element method represents an alternative approach for slope stability problem, which is versatile and requires fewer a priori assumptions. It is thought to contribute to the particular field of slope engineering. Based on continuous analysis, finite element method applies elastic-plastic material model to describe in-situ soil properties, which are more suitable for finding potential circular sliding surface in soil slide [Griffiths and Lane (1999)]. It is still difficult in term of simulating the consequence of slope failure. It is also hard to use FEM to analyze stability for slope which is mainly composed by discrete rock. In fact, such discrete rock massed slopes are widely found in nature, and some of them exist near highway and open pit mining.

Naturally, it is intuitive that rock slope sliding could involve complex situations and mechanism. In the aspect of discontinuum modeling, DDA and DEM are more advantageous for rock slopes controlled by discontinuity behavior. Rock mass is considered as an aggregation of distinct, interacting blocks subjected to external loads and assumed to undergo motion with time.

As the combination of DDA and FEM, NMM shares the common features mentioned above, and it also has an advantage in the slope stability analysis. It is worth to notice that current studies in literatures seldom include 3-D version solution on rock slope stability analyses. Hence, it is significant to utilize 3-D NMM to explore such engineering problem.

7.2.2 Functional classifications for rocks in slope engineering

“Rock is any naturally formed aggregate or mass of mineral matter, whether or not coherent, constituting an essential and appreciable part of the earth’s crust”[A.G.I, (1957)].

There are different ways to classify rock according to analysis purpose. The particular use to which rock is put may require additional specification, such as,

using R.Q.D (Rock Quality Designation) [Deere *et al.* (1967)], mechanical, chemical or biological classification [Bell (1992)] and so on.

In slope engineering, the main consideration is to differentiate the “rock” from the “soil”. Soils being of little interest in this thesis, their classification will not be discussed here. According to [Duncan and Goodman (1968)], the properties of a given site for a rock excavation depend on the combined effect of rock and discontinuities. In order to assign the rock mass(es) of a particular site to a functional classification, some basic geologic information are required,

- a) Identification and distribution of each rock type;
- b) Average geometry, distribution and character of recurrent discontinuities (e.g., joints, bedding planes, foliation);
- c) Location, geometry and character of major faults and altered zones;
- d) Weathering profile;
- e) Ground water regime.

After Duncan and Goodman (1968) firstly suggested the classification of rock masses, Sancio (1979) reproduced ten types of rock masses with minor expansion to the description, as shown in Table 7-1.

Table 7- 1 Classification of rock masses for surface excavations [Sancio (1979)]

Type	Description	Attribute	Figure
1 Strong Homogeneous Rock	Comparable in strength to concrete and free from discontinuities or chemical defects	Stable vertical slopes of great height
2 Weak Homogeneous Rock	Much weaker than concrete, free from discontinuities or chemical defects	Safe angle depends on height. It can be determined by soil mechanics techniques
3 Terraced Rock	Horizontal beds varying from strong to weak forming a heterogeneous mass. Free from discontinuities or chemical defect	Safe angle varies from point to point. Ground-water regime can be significant. Soft seams can control overall strength
4 Ravelling Rock	Free from defects but susceptible to break up by weathering. Columnar jointed rock, friable sandstones and conglomerates, closely fractured shales.	Base of slope covered with running material. Benches and Walls necessary for protection
5 Slumping Rock	Altered or clay rich rock with very low strength: major fault zones; Montmorillonitic compaction shales; Hydrothermally altered zones; highly weathered zones.	Retaining walls, gabions or rock blankets and horizontal drains required. Frequent maintenance necessary.
6 Sheeted Rock	Hard, Strong rock with planar weaknesses. Roughly parallel to natural slopes; Commonly granitic rocks.	Drainage of sheet joints essential if natural slope is steeper than about 30°. Rock bolts can be used to tie sheets together.
7 Slabby Rock	Hard rock with one strongly developed set of discontinuities which control the strength of the mass. Typically, silty shales and shaly lime-stone.	Support may be required if slab daylight and are inclined more steeply than friction angle ϕ . ϕ determined from direct shear tests and field observations.
8 Buttressed Rock	Hard rock with two sets of weakness planes which dominate the rock mass strength. Line of intersection of weakness planes	Benches or possibly retaining walls necessary to hold blocks if line of intersection is steeper than about 30° and undercut by slope.

		delimits buttresses.	
9	Blocky Rock	Hard Rock with 3 or more sets of weakness planes which dominate the rock mass behavior; typically, quartzite limestone. Jointed granites.	<p>Benches necessary to accumulate fallen rock. Wire mesh and gunite necessary to prevent rock falls, especially if joints are very weak. Rock bolts on pattern can be used.</p>
10	Foliated Rock	Foliated Planes, usually steeply dipping, control rock mass behavior; mica schists, phyllites and slates.	<p>Creep leading to slump-like slides may occur as leaves of rock gradually deform. Particularly severe where rock is highly weathered or foliation is controlled by mica.</p>

These types are differentiated through following criteria:

- a) Rock material strength and deformability;
- b) Frequency of discontinuities;
- c) Orientation of discontinuities;
- d) Number of commonly oriented systems of discontinuities.

The designed example in this section is particularly concerned with one of hard, and strong rocks with planar weaknesses, i.e., with “sheeted rocks” as described in number 6 of Table 7-1.

7.2.3 Typical failure mode of rock slope

According to the rock mass classification in the rock engineering, there are 4 kinds of typical failure modes in rock slope, and they are summarized as follows (Fig. 7-1).

- Planar failure: it is governed by a main set of discontinuities dipping in the direction of the slope (Fig. 7-1 a).
- Wedge failure: it is governed by two main set of discontinuities in which intersection lines towards the slope (Fig. 7-1 b).
- Toppling failure: it involves vertical slabs or rock columns created by vertical discontinuities close to the slope face (Fig. 7-1 c).

- Circular failure: the slip surface is shaped like a shell, and it occurs in severely jointed rock masses and in soils (Fig. 7-1 d).

Figure 7- 1 Typical failure modes in rock slope

Another common damage phenomenon, rock fall, normally happens in a rock slope. It has been a tendency to define rock fall as one of the slope failure mode in engineering practice. In the author's opinion, it is misleading to define it as a mode, as "rock fall" is better to be only seen as a consequence of above listed four basic modes.

The rock slope failures observed in reality are much more complex than the discussed ones. Sometimes, these failure modes could occur simultaneously. Sometimes, real rock slope failure does not belong to any of the modes mentioned. Nevertheless, it is straightforward to define such basic failure mode for

understanding failure mechanism of rock slope. Such definition also provides necessary platform to design verification example to test the 3-D NMM algorithm, as the wedge failure verification example did in *Section 6.5*.

Based on these definitions, one planar failure mode is chosen as a reference case study.

7.2.4 Causes of landslides

During a landslide, it is believed that the action of gravity is the primary driving force. Despite the action of gravity, there are other contributing factors that affect the original slope stability⁵. Typically, pre-conditional factors constitute specific sub-surface conditions that make the area/slope prone to failure. It is also required to have a trigger before being released in the actual landslide.

When the stability of a slope changes from a stable to an unstable condition, landslides occur. Stability changing of a slope could be caused by a number of factors, acting together or alone. Natural causes of landslides include:

- Groundwater (pore-water) pressure acting to destabilize the slope;
- Loss or absence of vertical vegetative structure, soil nutrients, and soil structure (e.g. after a wildfire);
- Erosion of the toe of a slope by rivers or ocean waves;
- Weakening of a slope through saturation by snowmelt, glaciers melting, or heavy rains;
- Earthquakes adding loads to barely-stable slopes;
- Earthquake-caused liquefaction destabilizing slopes;
- Volcanic eruptions.

Landslides could be aggravated by human activities, including: deforestation, cultivation and construction, which destabilize the already fragile slopes

- Vibrations from machinery or traffic;

⁵ Refer to: <http://en.wikipedia.org/wiki/Landslide>

- Blasting;
- Earthwork altering the slope shape or imposing new loads on an existing slope;
- In shallow soils, the removal of deep-rooted vegetation binding colluvium to bedrock;
- Construction, agricultural or forestry activities (logging) changing the amount of water which infiltrates the soil.

7.2.5 Stabilisation techniques for rock slope

Although necessary monitor and avoidance could be done to human activities that trigger slope failure, it is still difficult to manage the unpredictable natural causes of landslides. There are some ways to reduce damage for natural causes of landslides through efficient fostering to potential dangerous slopes. Useful reinforcements are able to reduce the probability of dramatic disaster happening, and significantly lower the loss caused by sliding occurrence.

Generally speaking, stabilisation techniques can be separated into two groups:

- a. Techniques attempting to fix loose blocks in place, such as rock anchoring or bolting, dental concrete buttresses (shown in Fig. 7-2).

Figure 7- 2 Loose rock slab stabilized through bolted concrete buttresses, Rio de Janeiro [Ortigao and Sayao (2004) p393]

b. Techniques attempting to reduce the damage of rock fall, instead of preventing. The term “*risk reduction measure*” is widely used to describe this kind of techniques. As the name suggests, measures do not intend to prevent a rock block from moving out of the slope, but attempt to decrease the possible damage caused by a rock fall. Various measures are listed below.

- Berms to reduce kinetic energy of falling blocks or prevent a block from reaching the nearby property or people
- Ditch trap [Peckover and Kerr (1997)]
- Impact wall
- Barriers or fences [Agostini *et al.* (1988)]
- Protection steel mesh [Ortigao and Sayao (2004)]

7.3 Rock Slope Scenario Study

7.3.1 Scenario setting

Following the definition given above, a rock slope scenario near an express-way is designed, as shown in Fig. 7-3.

(a) ISO review of rock slope example

(b) Front view

(c) Side view

Figure 7- 3 Configuration of designed rock slope example

This designed scenario belongs to a classical No. 6 type in Table 7-1, from *functional classifications for rocks in slope engineering*. Its failure tendency is the type of planar failure mode, according to the *failure mode of rock slope* section.

It is not hard to see that the main set of joints is almost parallel to the slope surface. Their dips get close to the initial natural friction angle of joints. It may cause the sliding of isolated blocks. For example, a natural planar sliding happened at Cerro Verde Mine, Arequipa, Peru (Fig. 7-4).

Natural trigger of rock sliding could be assumed to be heavy rain storm as happened in Shikoku Island and the Tyugoku area of Japan year 2004. According report of [Wang *et al.* (2010)], saturation may cause reduction of rock joint friction angle and shear strength after heavy rain. Its efficient friction angle is less than 16° , which is compared with the initial granite's friction angle that is around $26^\circ \sim 29^\circ$ [Barton and Choubey (1977)].

Figure 7- 4 Typical planar sliding in nature [Ortigao and Sayao (2004) p16&18]

7.3.2 Geometric modeling

The configuration of this case is illustrated in Fig. 7-3. Isolated rock blocks have 3

layers placing in a slope with 32° dip. The whole slope has height of 5.50 m. The thickness of the three layers from above to below are 0.60m, 0.65m, 0.70m. The width of the express-way near the slope is 7.96 m. A transition zone with 9.10° between express-way and slope is designed.

As no crack propagation mechanism implemented in current program, the model is discretized into 45 rock blocks that are likely to move out. The average volume of the rock blocks is 1.22995 m^3 . The smallest block is 0.4155 m^3 , and the largest block is 2.7687 m^3 .

Based on 130 DST tests[Barton (2008)], the residual friction angle for rock joints is around $26^\circ \sim 29^\circ$ with the roughness profile (JRC) and joint wall strength(JCS) description, as shown in Fig. 7-5.

According to their results, a typical rock and joints properties, listed in Table 7-2, are assigned to this scenario example. Other parameters that used in 3-D NMM are also listed in Table 7-2.

Figure 7- 5 Range of joint roughness profile tested and their JRC values and strength envelopes [Barton and Choubey (1977)], based on 130 rock joints tests

Table 7- 2 Parameters for 3-D numerical manifold method computations in “Rock slope” example

Feature	Item tested	Value
Rock mass	Unit weight (kN/m ³)	25.7
	Poisson’s ratio	0.23
	Young’s modulus (GPa)	24.5
Discontinuity	Initial frictional angle (°)	26.4
	Cohesion (MPa)	0.0
	Tensile strength (MPa)	0.0
Analysis parameters	Displacement-allowed ratio	0.01
	Maximum time increment (s)	0.001
	Normal contact spring stiffness (MN/m)	260.0
	Total time steps	10000.0

7.4 Modeling with 3-D NMM

After the 3-D NMM preprocess treatment, the intersection between the physical model and mathematical covers, 1067 tetrahedron manifold elements are finally generated for the case, as shown in Fig. 7-6.


```

Input Block no. = 48
Tetra Elemt no. = 1067
Total Facet no. = 5867
Total Point no. = 7466
Current blk no. = 1

```

Figure 7- 6 Manifold treatments for calculation in “Rock slope” example

The black colored frame is the emphasized territory of mathematical covers, which is interacted with the physical domain.

7.4.1 Case A: Free sliding without lateral constraints

Assuming that only slope bottom, transition zone, and highway are fixed in this example, the 45 isolated blocks in the slope will slide down freely without lateral confinement pressure, where the friction angle has been set to 10° . As the friction angle is smaller than slope grading angle, the blocks in the slope will not stay stable under the force of gravity.

Time step 1001-> 1
Accumulated Time = 0 s

Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(a)0.000s

Time step 1001-> 100
Accumulated Time = 0.378018 s

Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(b)0.378s

Time step 1001-> 200
Accumulated Time = 0.759855 s

Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(c)0.760s

Time step 1001-> 300
Accumulated Time = 1.141692 s

Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(d)1.142s

Time step 1001-> 411
Accumulated Time = 1.565530 s

Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(e)1.566s

Time step 1001-> 500
Accumulated Time = 1.905365 s

Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(f)1.905s

Time step 1001-> 601
Accumulated Time = 2.291020 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(g)2.291s

Time step 1001-> 700
Accumulated Time = 2.669339 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(h)2.669s

Time step 1001-> 800
Accumulated Time = 3.050875 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(i)3.051s

Time step 1001-> 900
Accumulated Time = 3.432712 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(j)3.433s

Time step 1001->1000
Accumulated Time = 3.814549 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(k)3.815s

Figure 7- 7 Rock slope failure process modeled by 3-D NMM

As shown in Fig. 7-7, the slope demonstrates a whole collapse in a large scale. The velocity of the highest blocks would gradually become larger than that of lower level sliding blocks, as larger quantity of potential energy has been transformed to momentum for the highest blocks. The upper layer blocks are then covering up the lower layer of blocks, which forms the block rolling phenomenon by up-front blocks. Normally, block rolling could result in serious damage to local road surface.

Under the remaining 10° friction angle, all the sliding blocks will glide across the 7.960 m road width, leaving no blocks on the road, but causing local damage to the road to some extent.

In order to clearly analyze detailed slope sliding during the process, 9 representative blocks are chosen to depict the displacements from the 45 potential slide blocks, as in shown Fig. 7-8.

Figure 7- 8 Selected measuring blocks in “Rock slope” example

In Fig. 7-8, “B8” means the #8th block in this horizontal Group. “L1” means the #1st layer. “G1” indicates the #1st group in horizontal direction. The displacement curves of the selected 9 block’s centroid are depicted, in Fig. 7-9.

(a) Displacement history in X direction

(b) Displacement history in Y direction

(c) Displacement history in Z direction

Figure 7- 9 Displacement history for selected blocks

From Fig. 7-9, the detailed three direction displacements of the selected 9 blocks can be seen clearly. Based on horizontal axis, 4 blocks of 9 are in the left side, and other 5 are in the right side. From Fig. 7-9(a), it has shown the two-side expansion tendency along the x direction during the sliding process. Based on vertical axis $y=0$, the x-axis displacement curves also are separated into two parts, where 4 blocks are in the upper side, and 5 blocks are in the lower side. This is consistent with observations.

Block sliding along negative y axis direction is very smooth, as shown in Fig.7-9(b). Each curve basically has changed three times in their degree of curvature, which are corresponding to the slides along slope to the transition zone, and then to the road surface. In the figure, the upper most curves are B8_L1_G1, B9_L1_G2, B7_L1_G3, which are almost coincided. It shows that the movement tracks of these blocks along y-axis are quite similar. From Fig. 7-9, these three blocks in fact keep in the same layer “L1”, which is the up-front location of the 9 blocks. Therefore, their accumulated displacement along y-axis is quite small, forming the upmost group of curves, which is consistent with the observation in Fig. 7-7.

More detailed information on block displacement could be gained in Fig. 7-9(c). The blue curve (B9_L1_G2) will be stable in the location of 0.75m, which indicates that block B9_L1_G2 is gliding along the road surface. The violet colored curve (B18_L3_G2) shows that block B18_L3_G2 will start to toppling at 2.8s, and after its toppling, its movement is as free falling body. Its z-axis direction displacement curve presents a clear parabolic curve. The dark blue curve (B17_L3_G3) demonstrates that block B17_L3_G3 loses its original bolstering support and starts to fall at about 2.75s. The non-smoothness of the curve during time period 2.75~3.2s indicates that the falling process of the block during this period has been disturbed by other blocks. Furthermore, the block has occurred one collision with other block or the road surface at about 3.2s, as the displacement curve at time 3.2s has a non-linear jump. After 3.2s, it has the form of a parabolic curve.

Under the analysis on the movement displacement curves for the designed slope sliding, it is obvious that the numerical results based on the algorithm has a great potential to provide more detailed information than traditional experiments. This information is a key and essential to design proper buttress and protection solution. At the same time, it also acts as important prerequisite to the inverse problem analysis.

7.4.2 Case B: Slope failure with lateral constraints

In this part, a further more practical case is studied. The two sides of slope along the road direction (x-axis) are fixed, and in-situ horizontal principal stress $\sigma_h = -0.05MPa$ is imposed. Obviously distinct with 2-D case, these discrete blocks also have crossed configuration along horizontal direction, besides major joints, which are parallel to slope surface. The slope would keep stable under the friction angle of 19.673° .

Fig. 7-10 presents the failure process under friction angle 12° . For clearance, the contour lines for the isolated blocks are shown only.

Time step 1001-> 1
Accumulated Time = 0 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(a) 0.000s

Time step 1001-> 101
Accumulated Time = 0.600000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(b) 0.600s

Time step 1001-> 201
Accumulated Time = 1.200000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(c) 1.200s

Time step 1001-> 301
Accumulated Time = 1.800000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(d) 1.800s

Time step 1001-> 401
Accumulated Time = 2.400000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(e) 2.400s

Time step 1001-> 501
Accumulated Time = 3.000000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(f) 3.000s

Time step 1001-> 602
Accumulated Time = 3.606000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(g) 3.606s

Time step 1001-> 703
Accumulated Time = 4.212000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(h) 4.212s

Time step 1001-> 801
Accumulated Time = 4.800000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(i) 4.800s

Time step 1001-> 900
Accumulated Time = 5.394000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(j) 5.394s

Time step 1001->1000
Accumulated Time = 5.994000 s

Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(k) 5.994s

Figure 7- 10 Rock slope failure process with confining pressure

The failure process for the slope model under this condition is shown in Fig. 7-10. It has a wedge void, which does not follow the defined wedge failure mode in *Section 7.2.3*. In the process of collapsing, its failure mode is similar to the case of planar failure mode, mixed with toppling failure in some locations. The total calculation time takes 6s. Most of the isolated blocks are finally stacked on the express-way, except block #3 (1.822 m^3) in the measure group which is falling outside of the model scope.

Compared with the result of *Case A*, falling rocks have obstructed the highway, and also have damaged the local road surface. In this example, there are totally 19 blocks (sum to 20.841 m^3) left and stacked on the road. From temporary stability of Fig. 7-10 (k), there are two blocks *m* and *n* (4.245 m^3) remaining at the slope, which are still keeping their extreme equilibrium status. If dredging the highway without removing these two blocks, it could cause subsequently potential secondary land-sliding disaster, which is triggered by removing the key block *k* (2.187 m^3) and the blocks left in the transition zone (7.052 m^3).

Therefore, 3-D NMM can also provide suggestive procedure for dredging roads after collapsed sliding slopes. It will not be covered in detail for the reason of concision.

Fig. 7-11 has depicted the historical displacement curves for centroid of the 9 blocks within 6.5 s.

(a) Displacement history in Z direction

(b) Displacement history in Y direction

(c) Displacement history in Z direction

Figure 7- 11 Displacement history for selected measuring blocks in rock slope
example - Case B

7.5 Stabilisation Measures

Under the conditions in *Case B*, the designed example chooses two stabilisation techniques: 1) *concrete buttresses model*, and 2) *barriers of fences model*.

7.5.1 Case C: Stabilisation technique-Concrete buttress

In order to foster the slope, a group of concrete buttresses is located under the falling edges of three block layers, as shown in Fig. 7-12. Concrete buttresses with proper shapes are fastening together with adjacent blocks, which are connected with the bottom of dental buttresses, by rock bolts.

Each buttress is 200mm thick, and lined with 1500mm interval between. The third buttress of the second layer has been shifted to proper location according to the nearby joints distribution. This treatment is consistent with practical engineering

standard.

Figure 7- 12 Configuration of designed concrete buttresses

After 9.85s, all the blocks stay in their original position, as shown in Fig. 7-13.

Time step 1000-> 986
Accumulated Time = 9.850000 s

Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

Figure 7- 13 Rock slope stabilisation by dental concrete buttresses

7.5.2 Case D: Stabilisation technique- Fences barriers

Despite the above method of buttress, practical engineering also use barriers of fences to protect the highway to be damaged or to reduce its damage (as in Fig. 7-14) frequently. As discussed, the method of fence does not prevent falling down of blocks; instead it reduces the damage degree. Normally, such stabilisation technique is much cheaper than the previous one, and it is more suitable for large scope of lower dangerous slopes sliding level. In practice, there might be wire netting between the bollards to prevent spillage of small relics during the slopes sliding. The current 3-D NMM has not yet included mathematical line model, hence the part of wire netting is neglected up until now.

Figure 7- 14 Configuration of road barriers

A group of concrete columns (bollards) with a width of 450 mm and a height of 1700 mm are set at the transition zone between the highway and the potential failure slope. Its direction is the same as exterior normal of the transition zone upper surface. The interval between the columns is 2000 mm, therefore the gap between the columns is

1550 mm. Assuming the bollards are sturdy enough, the simulation result is shown in Fig. 7-15.

Time step 1001-> 1
Accumulated Time = 0 s

Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(a) 0.000s

Time step 1001-> 100
Accumulated Time = 0.891000 s

Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(b) 0.891s

Time step 1001-> 202
Accumulated Time = 1.809000 s

Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(c) 1.809s

Time step 1001-> 302
Accumulated Time = 2.709000 s

Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(d) 2.709s

Time step 1001-> 401
Accumulated Time = 3.600000 s

Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(e) 3.600s

Time step 1001-> 500
Accumulated Time = 4.491000 s

Current Bk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(f) 4.491s

Time step 1001-> 602
Accumulated Time = 5.409000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(g) 5.409s

Time step 1001-> 702
Accumulated Time = 6.309000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(h) 6.309s

Time step 1001-> 801
Accumulated Time = 7.200000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(i) 7.200s

Time step 1001-> 901
Accumulated Time = 8.100000 s
Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(j) 8.100s

Time step 1001->1000
Accumulated Time = 8.991000 s

Current Blk no. = 0
Current Fac no. = 0
Current Edg no. = 0

(k) 8.991s

Figure 7- 15 Road protection from rock slope failure by barriers

The total lasting time of calculation takes 9.0 s, the effect of the bollards is acceptable. Except some of small volume blocks falls outside to the road, most of falling blocks are fended within the transition zone. The spilled small blocks are also stopping at the side of the road. If wire netting is hanged between the columns, it could protect the roads better.

7.6 Summary and Discussion

This study presents a detailed application ability of the developed 3-D NMM formulation. The implementation developed has been successfully applied to analyze the failure process of a rock slope. Good understanding has been obtained.

From the analysis of *Section 7.4*, it could be seen that one important reason to induce the slope failure is the sudden decreasing of the strength for joint faces (e.g., friction angle). The comparison between *Case A* and *Case B* shows the significant role of correctly determining in-situ condition for the rock slopes. Meanwhile, the ability of the developed 3-D NMM procedure to model a fairly complex failure process of a rock slope also highlights the inadequacy of a 2D analysis often used in practice.

In *Section 7.5*, two methods of stabilisation are discussed. The first method of dental concrete buttress provides safer solution, but is relatively more expensive. The latter method is a more economic strategy to the rock sliding for less dangerous cases. In reality, diverse stabilisation methods could be utilized, and they are sometimes not used separately. Some crucial road sections require using various methods simultaneously, which helps to provide efficient and economical way.

As the limitation of current preprocess and the 3-D NMM algorithm itself, the examples now only concentrate on the preliminary studies to the slope stability mechanism. Even though there is still a gap between our designed examples and the real engineering practice, it has moved fitfully toward the engineering application. The simulation works have covered many aspects in rock failure analysis, including collapsing volume estimation, road dredge solution, stabilisation methods, and slope

failure mechanics. It helps to provide meaningful information for these practical engineering designs. It has demonstrated the potential ability of 3-D NMM in the aspect of rock engineering application.

Chapter 8 Engineering Application---Rock Tunnel Stability Analysis

8.1 Introduction

From the very first beginning, human kind starts to utilize underground space for many purposes. However, people normally have the subjective feeling of treating underground space related to unsafe. This partial sense, generally speaking, comes from few aspects as following:

1. Psychological effects: Underground structures sometime are completely enclosed on all sides, which impose psychologically stifling emotion.
2. Culture of “Underworld”: People always associate underground with “darkness”, “misery”, even “death” and “buried”. They buried the dead into ground as a heritage both in East and Western countries.
3. Coalmine accidents: Many reports on mine disasters make people feel unsafe to the underground structure through years.

This study leaves these cultural disputes on the safety issue of underground space aside, and turn back to its scientific consideration to gradually recognize the safety level of underground structures.

In fact, underground structure could be more safe and durable than structure above the ground. For example, there is a widely acceptable knowledge in rock engineering. Engineers place highway and railway tunnels under a sidehill to straighten and shorten a route, and under ridges to avoid extensive surface cuts. Such tunnels tend to be safer than their cut-slope alternatives. There are three reasons. Firstly, the weak rock of the weathered zone is avoided; Second reason is that the span of the tunnels is far smaller than the dip length of the slope, meaning that much smaller key blocks

are involved. Thirdly, tunnels have higher resistant level to earthquake. In other words, they are much safer than above ground structures for earthquake induced shaking. The “5.12” Wenchuan Earthquake has hard-hit the area with 57 tunnels. According to the report [Zhang *et al.* (2009)], among the 18 tunnels investigated in Du-Wen highway, the major damage of the mountain tunnels was mainly happened in the tunnel portals due to spread landslides and rock fall, however, there are no major damage happened in the tunnel.

Because of the improved underground construction technology, safety, and economic concerns, more and more countries and regions strengthen the efforts to exploit the underground space in recent years.

Although underground structure demonstrates its advantages in many aspects, its stability cannot be neglected, such as, tunnels in quite poor rock condition [Rozen (1976)]. Hence, scientists and researchers are continuously purposing efficient analytical tools to discover the failure mechanism in underground engineering and to design better reinforcement scheme. After all, its damage is a potential disaster once it fails.

The prediction of the rock mass response to the excavation of a tunnel is a complex engineering problem. A number of methods are available to analyze tunnels, from the earliest closed-form solutions to the most recent numerical modeling methods. Concentrating the attention to modern numerical modeling methods and rigorous analysis of tunneling problem, normally, we have two groups of approaches [Barla and Barla (2000)]:

Equivalent continuum approach: the rock mass is treated as a continuum with equal in all directions. Input data for the strength and deformability properties, which define a given constitutive material model: elastic, elastic-plastic, etc. to represent the combination of rock mass and discontinuities inside.

Discontinuum approach: the rock mass is represented as a discontinuum and most of

the attention is separated to two parts: the characterization of rock elements and the properties of rock joints. Each discrete block may interact with the neighboring blocks through the joints. The interest of study takes place with reasonable treatment of the contact interaction among the rock mass with special geometry shape.

As many difficulties, current 3-D studies on tunnel analysis are mainly based on the first kind of approaches. They are used to monitor surrounding rock deformation to assess and control the tunnel stability.

In the author's opinion, it is improper to analyze hard rock tunnel with FEM based on the continuum assumption. Strong tectonic discontinuities cut the surrounding rock blocks of tunnel surface into discrete state. It could not reflect the failure process of such blocky system, if only modeling such discrete blocks into one homogeneous body with equivalent strength and only observing its deformation/strain. From the angle of mechanics, block deformation could not substitute the displacement in the block system completely. The enforcement scheme design, based on continuous assumption, might be not safe enough, especially in 3-D situation. Such averaging design of bolt and lining might be not sufficient for locally dangerous blocks. Its corresponding enforcement scheme is either insufficient or extravagant.

To this area, block theory [Goodman and Shi (1985)] could be recognized as a pioneer in 3-D excavation analysis. The principal ideas of block theory are that: 1) many different combinations of discontinuities generate a group of diverse shaped blocks. 2) The group of blocks is divided into five types (Fig. 8-1). 3) It directly identifies the certain critical blocks as "key block" by stereographic projection method or vector analysis. The features of "key block" are finite, removable, and potentially unstable.

Figure 8- 1 Five types of blocks in block theory [Goodman and Shi, 1985]

In this example, we continue to use this concept—“Key Block”. It is a really “key” to handle key block in surrounding blocks when analyzing the stability for hard rock tunnel.

Starting from the concept of block theory, this chapter represents the dynamic analysis on complete failure process for key blocks in tunnel with 3-D NMM. By this way, some regular failure patterns are also recognized, which provides better references to practical rock engineering. Nevertheless, this thesis aims to develop 3-D NMM and its feasibility study on rock engineering application, even more importantly, the example verifies the robustness of the proposed algorithm.

8.2 Rock Tunnel Scenario Study

8.2.1 Scenario setting

Rock falling from the side and roof of tunnel surface is one kind of frequently seen accident during the excavation operation (as shown in Fig. 8-2). Such falling blocks are above mentioned key blocks. Due to the loss of key block, more free-surfaces are exposed, which would produce more massive collapse. Therefore, it is the most important task to find and describe the most critical key block around an excavation in such engineering problem.

The scenario setting in this example is designed under this background.

Figure 8- 2 Rock mass failure in the side of tunnel surface at Shakespeare Cliff⁶

Since the surface of a tunnel excavation have different types: horseshoe-shaped tunnel, circular tunnel, square tunnel, etc., its intersection with a system of joints

⁶ Refer to http://www.subbrit.org.uk/sb-sites/sites/c/channel_tunnel_1880_attempt/index1.shtml

produces blocks with a curved face, or say concave block. The calculation involves the concave blocks, which can be considered to the further test the 3-D contact algorithm (proposed in chapter 4 and 5).

In this example, a horseshoe-shaped tunnel is centered along the global x direction.

The tunnel is located in rock containing three major discontinuities:

- 1) Dipping at 50° with a dip direction of 130°
- 2) Dipping at 45° with a dip direction of 45°
- 3) Dipping at 76° with a dip direction of 90°

Several local tectonic joints are also distributed in the model.

(a) Perspective view

(b) Side view and front view

Figure 8- 3 Scenario setting for a rock tunnel

Under such geometrical settings, totally 12 blocks with diverse shapes are formed, including one key-block (Blk #11) in the roof of tunnel, other key-block (Blk #12) located at the side wall, as shown in the Fig. 8-4 and Fig. 8-6.

#01(63.4423 m³)

#02(86.9571 m³)

Figure 8- 4 Blocks with diverse shapes in tunnel

For clear demonstration, each block is shown in the perspective view with proper transparency, so that the details of each facet could be seen clearly. It is worth to note that the denotation “ $\hat{n}$ ” from the loop center is along the average exterior normal direction, which helps to guarantee the complete description on each block. The random block generation algorithm could be referred to as [He and Ma (2010)]. The

volume of each block is provided by the 3-D simplex integration method (*Section 3.5*). The total volume of rock mass is 277.4533m^3 . The excavation volume of tunnel is 25.6507m^3 .

Overall view of tunnel and input discontinuities is shown in Fig. 8-5.

Figure 8- 5 Overall view of tunnel model

8.2.2 3-D NMM modeling

Similar with the example in Chapter 7, the current NMM program does not have the function to simulate crack propagation. The model in this example is divided into 12 discrete blocks by existent discontinuities directly. In order to present the compatibility between NMM and DDA, the whole model has been placed into a giant tetrahedral manifold pattern (MP). From some point of view [Ma *et al.* (2010)], it is also a 3-D DDA example.

Except the top face, other 5 faces are fixed in the model. The model has unified rock mass parameters and uniform property of discontinuities inside, listed in Table 8-1. Under only gravitational loading, some of such discrete blocks are unstable.

Table 8- 1 Parameters for 3-D tunnel example

Feature	Item tested	Value
Rock mass	Unit weight (kN/m ³)	38.57
	Poisson's ratio	0.25
	Young's modulus (GPa)	24.50
	In-situ principle stress (MPa)	-0.01
Discontinuity	Initial frictional angle (°)	59.00
	Cohesion (MPa)	0.0
	Tensile strength (MPa)	0.0
Analysis parameters	Displacement-allowed ratio	0.003
	Maximum time increment (s)	0.001
	Normal contact spring stiffness (MN/m)	320.00
	Total time steps	10000

8.3 Results Analysis

The calculation consists of two stages. At first, the friction angle is set to 59 degree. The designed system reaches a steady state with proper systematic damping. Secondly, through reducing the friction gradually, it could reach the case until one of key blocks starts to detach out from surrounding.

Unfortunately, current version of 3-D NMM has not yet included bolt model, therefore it could not further discuss on the enforcement scheme. If the tunnel is excavated without any support, it could keep stable against gravity ($g = 9.8 \text{ m/s}^2$) under the friction resistant (59°) and in-situ principle stress only. Gradually reduce the value of friction angle, there are two potential falling blocks in the example, indexed with Blk #11 and Blk #12. Obviously, the locations of these two key blocks are different, and their surrounding geometrical conditions are also different. Hence, they require different friction angles to keep their original locations. Table 8-2 gives their critical friction angles for both two key blocks.

Table 8- 2 Critical friction angle for two key-blocks in tunnel

	Roof Blk#11	Side Wall Blk#12
3-D NMM solution	11.107 ⁰	17.645 ⁰

With surrounding blocks hidden(Block#1 is hidden) for better viewing, Fig. 8-6 ~ Fig. 8-8 give the close-up view of the possible detached key-blocks.

(a)

(b)

Figure 8- 6 Close-up view of the key-blocks

Unexpectedly, the key block #12, located at the side of tunnel, is in a situation relating less-stable compared with the roof block #11. As in the Table 8-2, roof block stands still when side block starts to be detached under the friction angle 15.50° (as shown in Fig. 8-7). Even though the free surface of the roof block is at the bottom and more effective gravity components acting on, it is found that surrounding rock blocks contributes much more normal component of pressure to the roof block as the narrow shape of the block. Furthermore, these three contact faces are in relative embracing position. Conversely, only two faces on the side block are pairing with a relatively large angle, and embedded depth of the side block is much shallow. Therefore, less normal force perpendicular to contact face can be obtained, which lead to insufficient frictional resistance.

Figure 8- 7 Failure of key block located at the side wall

Figure 8-8 gives rock tunnel failure process with a frictional angle of 8° , which means that both two key blocks in this tunnel model will be detached from the surrounding blocks and fall down to the bottom of tunnel.

(a) 0.000s

(b) 0.304s

(c) 0.556s

(d) 0.630s

(e) 0.778s

(f) 0.703s

(g) 0.848s

(h) 0.996s

(i) 1.869s

Figure 8- 8 Failure process of key-blocks in tunnel

The displacements of key blocks are monitored while the calculation is running. Fig. 8-9 plots the displacement history and indicated that the position of them is mainly moving downward. From the curvature change along the curve, we can also identify that block #11 will be completely detached from surrounding at time 0.776s. It later falls to the bottom of the tunnel at 1.172s. Similarly, side block #12 is detached at 0.709s, and falls to the bottom at 1.605s.

(a)Roof block #11

(b)Side block#12

Figure 8- 9 Displacement history of key blocks

8.4 Summary and Discussion

This example focuses on the dynamic analysis to key block failure process with 3-D NMM and gain the critical friction angle for each key block. It fulfills to better test

the feasibility of developed 3-D NMM. Some facts in the example are discussed.

1. In this example, there are totally two key blocks which will be detached from its original location and fall to the bottom of the tunnel. The maximum collapsing volume is 0.148 m^3 under the setting condition, which will not crash as a whole. Enforcement scheme design should focus on how to prevent small block from falling. Generally speaking, lining and rock bolt should be enough for stabilization.

2. This study is also an extension to the “roof wedge falling” examples in *Section 6.4*. It further provides more evidence and reference after correction of 3-D NMM.

3. The program can simulate the whole process of collapse, and it can also get more detailed valuable information (including collapse time, collapse mode, volume velocity, etc.). These provide the fundament for forward and inverse analysis to engineering accidents.

4. The example shows the complexity of the collapse process, which might not one-off happen. Some local collapse might predict that some of surrounding blocks are also at the edge of danger. It can also provide valuable suggestions on preventing secondary failure and tunnel obstacle release operation after accidents.

5. This example further verifies the stability of the contact algorithm and the potential ability to analyze the interactive contact among complex blocks. At the same time, 3-D NMM contact algorithm has been proved as a general contact logic, which should also work well in the platform of 3-D DDA.

There are also some limitations to the example.

1. As limited number of manifold elements, the program gives relatively rough description of the stress/strain field. Even increasing the degree of freedom, current version of 3-D NMM still need be further developed in better stress field description, since it uses 1st-order weight function and 0th-order cover function.

2. Normally, a tunnel analysis should involve the steps as: a) to simulate the initial condition of surrounding rock, b) to excavate the first step, c) to excavate the second step, and then construct primary support for the first step cavern, d) to excavate the third step, and then construct the secondary lining of the first step and primary support of the second step, and so on. This example simplifies the model and excavation steps. It still has rooms to be improved to real practical excavation operations.

Chapter 9 Conclusions

9.1 Summaries and Results

This thesis focuses on the development of 3-D Numerical Manifold Method. It proposes a proper numerical analytical tool suitable for rock engineering application. Based on systematical literature review, the development is divided into 6 steps:

1. Generalize and reinterpret the concept for NMM; Sort the procedure for NMM; create the unified discussion platform for this method;
2. Discover 3-D manifold pattern and concept extension for 3-D requirement; Derive basic equations;
3. Propose a general contact algorithm;
4. Develop new contact treatment solution for 3-D NMM;
5. Verify the proposed algorithm for each individual features;
6. Apply the proposed algorithm into rock engineering problem demonstrate with case scenarios.

The proposed algorithm is proven to be accurate through verification examples, which is also suitable for practical rock engineering calculation.

9.2 Contribution

The main contribution of this novel study is focus on three aspects: conceptual design, technical development, and practical application.

Conceptual Design:

- 3-D NMM is one of the most suitable numerical methods for practical rock engineering application. It has strong ability to solve both continuous and discontinuous problems in more realistic geological conditions. The verification examples have demonstrated that it is suitable to describe the deformation, which is comparable to the classical FEM in this area. Meanwhile, it is capable to

describe displacement and contact interaction among the blocky system, which is comparable to DEM. In other words, the 3-D NMM actually contains the major advantages of these two groups. The compatibility of NMM probably suggests a bright future to the next generation of numerical method.

- The novel 3-D numerical manifold method is considered to be one of the most suitable methods in simulating the complex process from continuum to dis-continuum (Crack propagation phenomena).
- NMM is constructed on “Dual cover system”, inducing simplification on modeling procedure, and separated preparation for physical model and mathematical description. It could also further divide the analytical procedure to speed up, which also reduces one operation of manual intervention (discretize physical model, equivalent to FEM mesh). In fact, this operation is just the bottleneck of modern numerical method.
- Multi-physics simulation: Since physical domain has been separated independently, the physical domain could be divided into many sub-domains. The sub-domains are then decomposed into geometric field sub-domain, temperature field sub-domain, magnetic field sub-domain, and so on. These sub-domains can be combined together either conceptually or technically. NMM brings a new idea to understand multi-physics.
- Discover 3-D manifold pattern, and extending basic concepts in 3-D NMM.

Technical Development:

- Design the system framework and interpreting terminology used in 3-D NMM development.
- Prepare the technical requirements for 3-D NMM, including the equation derivations and simplex integration. All the sub-matrices and force vectors (including the contact constraints matrices) associated with tetrahedron MP are derived

- Develop a general contact algorithm, embedded into 3-D NMM.
- A pre-process modeling tool, 3-D visualization and SOR solver for large sparse matrix are also designed especially for 3-D NMM.
- Calibration and verification of developed 3-D algorithm with examples studying in three aspects:
 - a) Continuum displacement and deformation, and effect of setting Manifold Cover (MC) size and orientation;
 - b) Verification of Discrete blocky system: the total error between numerical results and theoretical results has been investigated;
 - c) Verification to two basic contact modes: *Point to Plane mode* and *Crossing Lines mode*.

Engineering Practical Application:

- Verification of the algorithm through calibrations and tests with practical engineering problems.
- Rock slope stability analysis with 3-D NMM.
 Through systematically analyze one example of rock slope stability to present its potential application abilities; the simulation works have covered many aspects in rock failure analysis, including collapsing volume estimation, road dredge solution, stabilization methods, and slope failure mechanics. It helps to provide meaningful information for these practical engineering designs.
- Tunnel stability analysis with 3-D NMM
 Tunnel example targets the dynamic analysis to key block failure process with 3-D NMM and gain the critical friction angle for each key block. It fulfills to better test the feasibility of developed 3-D NMM. The simulation also shows the whole failure process of the tunnel, which is hard to realize by other methods. Furthermore, it also is able to provide valuable suggestion to design the excavation operation, stabilizing techniques, and so on.

9.3 Conclusion, Recommendation and Future Works

This study is the first attempt to the 3-D NMM algorithm development and to rock engineering applications. To simplify the description on complex discontinuities, the 3-D NMM is constructed based on two domains: mathematical domain and physical domain. It actually separates the integration field and interpolation field, which highly appropriate to address the problem faced in rock engineering analysis. Such treatment is initially proposed by Shi in 1991, unfortunately, due to the insufficient understanding for this novel initiation, the advancement of NMM becomes tardiness and intricate. Recent years, this idea has been employed by other methods, for example, a cell-based Smoothed Point Interpolation Method [Liu and Zhang (2009)], whom realizes the treatment to large nonlinear deformation problem. These examples point another future direction on NMM: adding complex material constitutive model to satisfy the nonlinear large deformation analysis.

Even though quantitative analysis is not provided in this thesis from those verification examples, qualitative studies are employed on the applying and releasing of contact conditions to demonstrate the phenomenon process. The whole modeling process from pre- processing to calculation results are relatively easy to operate, and the 3-D NMM shows its stability in running different cases. It has already proven and demonstrated the efficiency and accuracy of the algorithm and the robustness of the implemented contact algorithm.

The current developed algorithm restraint the use of a tetrahedron-based mathematical mesh of 0-order cover function and 1-order weight function (in Chapter 3). Correspondingly, the strain description should yet to improve its precision. In the future, it is worth to continue further development on accurate material models and high order manifold element.

- Combinations of higher order cover function and weight function;
- Development of different Manifold Pattern;
- Enrich the rock materials database and discontinuities models (joint constitutive model).

In the view of mathematical approach towards the 3-D application problem, this thesis highlighted and attempted to provide the solution in two major aspects – the separation of integration domain against the interpolation domain and the introduction of solution scheme for a defined conditional nonlinear simultaneous inequation-set. The work details can be summarized as follow:

1. The separation of integration domain against the interpolation domain – In the traditional methods (e.g. FEM), the integration and the interpolation process are sharing the same objective domain. With the essence of using the dual-cover system in NMM, the integration domain can be defined independently against the interpolation domain, this operational features ease the effort of mashing/remashing burden required in other various numerical methods and also aids to model the complicated joint network in rock masses.

2. The introduction of solution scheme for a defined conditional nonlinear simultaneous inequations-set –The mathematical expression of the contact condition is just simultaneous inequations. Therefore, with consideration of the contact phenomena into the problem, the mathematical process of solving the set of simultaneous equations which derived from the partial differential equations under the continuum hypothesis is replaced by seeking the solution for the evolved defined conditional nonlinear simultaneous inequation-set. However, especially in the three dimensional domain, the process to achieve the solution is rather sophisticated. With a specific purpose of simulating the dynamic response among a blocky system, a possible solution scheme based on the geometrical and topological relations in physical models are provided in Chapter 4 and 5.

The application examples in Chapter 7 and Chapter 8, show the room for improvement and advancement in this program. For instance, bolt and lining models are normally used for stabilizing slope and tunnel, which is not available in the current version of 3-D NMM. Therefore, three future improvements are suggested:

- Development for 3-D shell, beam and string elements;
- Model of Bolt and lining;

- 3-D crack criterion and its crack propagation analysis.

3-D NMM can be further applied in other form of analysis to cater for geologic hazard and anti-terrorism protection. Numerical functions can develop toward these two practical directions:

- Seismic loading analysis and underground earthquake-proof design;
- Explosive loading analysis and anti-detonation design.

In rock engineering, another significant factor to affect structure stability is underground water. Current model is built on statistically uniform materials; however, it is believed that percolation model based on known crack spatial distribution will be further developed through the evolution of numerical methods. Specifically:

- Fluid-solid coupling, multi-field problem, percolation problem, etc.

Lastly, although this thesis has proposed a general contact algorithm and contact solution suitable for 3-D NMM, the algorithm itself does also require further optimization. For example, its contact checking algorithm and numerical treatment of contact constraint (e.g., penalty method has its limitations as mentioned in Chapter 4).

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