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Implementation of a two-dimensional discrete element method to describe granular materials composed of elliptical cohesionless particles

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ABSTRACT

IMPLEMENTATION OF A TWO – DIMENSIONAL DISCRETE ELEMENT METHOD TO DESCRIBE GRANULAR MATERIALS COMPOSED OF ELLIPTICAL COHESIONLESS PARTICLES

by
Juan José Martínez Alvez

This work is aimed at developing a discrete element simulation that models the contact between elliptical grains or particles in granular materials. The goal is to implement an algorithm to carry out collision detection between ellipses as well as ellipsoidal objects. The practical issue here is that the real shape of macroscopic grains can be approximated better using elliptical curves than using spherical curves. In addition, the simulation model will also be valid for spheres, since these objects are special cases of ellipsoids.

An accurate contact detection algorithm was investigated by means of two different formulations. The first formulation determines the minimum distance of one ellipse with respect to another ellipse and vice versa and finds the two closest points. Then it analyzes the position of these two points. However, this formulation is not robust enough to determine all the contact detections tested. The first formulation fails in cases when the distance between centers is unrealistically close and the major and minor axes are large. The second formulation determines the overlap distance. This method was successful in each of the realistic cases tested. The second formulation, as well as the first formulation, fails in unphysical cases, i.e., the distance between the centers of the ellipses is much smaller than the size of the major and minor axes of the ellipses. The implementation of a contact force formulation with minimum overlap distance will remove any possibility that these cases occur.

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by
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IMPLEMENTATION OF A TWO – DIMENSIONAL DISCRETE ELEMENT METHOD TO DESCRIBE GRANULAR MATERIALS COMPOSED OF ELLIPTICAL COHESIONLESS PARTICLES

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“HONOR YOUR FATHER AND MOTHER!”

To my parents: Juan Martínez Echevarría and Evelyn Alvez Millayes

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NOMENCLATURE

a_i, a_j	Ellipses i and j half length in the x axis
b_i, b_j	Ellipses i and j half length in the y axis
c	Ellipses half length in the z axis
C_x, C_y	Center of Curvature's position in moving coordinate axes of the x and y axes, respectively
d	Distance between the centers of Ellipses i and j
G_x, G_y	Center of Curvature's position in fixed coordinate axes of the x and y axes, respectively
h	Penetration distance
P_i, P_j	P_i is the elliptic curve i nearest point of the center of the local coordinate axes of the other elliptic curve j; P_j is found in the same way but reverse i and j
X, Y	Position of an ellipse point using fixed coordinate axes
X_C, Y_C	Position of the center of the elliptic curve in fixed coordinate axes

Greeks

ρ	Radii of curvature
ϕ	Angle in z-axis that defines the orientation of moving coordinate axes with respect to fixed coordinate axes
θ	Variable that defines the angle of the points in the parametric curve
θ_i^*, θ_j^*	Angle that minimizes the Ellipse i in the coordinate axes of Ellipse j and vice versa, respectively
$\hat{n}$	Unit outward normal vector

CHAPTER 1

INTRODUCTION

1.1 Objectives

In this thesis, a computer simulation model was developed to implement a contact detection algorithm between elliptical particles for use in a Discrete Element simulation. The computer simulation is a test of the theoretical formulation and experimental tests of elliptical particles. The computer simulations can be implemented in special circumstances where the experimental tests are very dangerous, expensive, and/or difficult.

1.2 Background Information

Highly specialized automatic machinery is widely used in the industry that transports and processes granular materials. The behaviors of these granular materials have to be understood for the proper design of this machinery.

Granular materials or bulk solids exhibit special behaviors. They can be deformed as solids, they can flow as liquids, and they are compressible like gasses [Peters, 2002]. Granular materials are discontinuous structures, so continuum models are not recommended to simulate these materials. Finite Element Method, Boundary Element Method, and Finite Difference Method are examples of continuum models. Commonly, they do not allow for separation, rotation, large scale deformation and displacement [Nordell, 2002]. Simulations for discontinuous structures can be broadly classified as follows: macroscopic modelling and microscopic modelling. Discrete Element Method (DEM) method is classified as microscopic modelling. DEM keeps track of each particle or body inside a granular material.

In the 1970's, Cundall [1979] developed a discrete model to describe the behavior of granular materials. He is recognized as the founder of the Discrete Element Method, although the technique has its formulation in molecular dynamics simulations commonly used by the physics community to investigate fluid behavior. Since the complete phase space is determined in a discrete element simulation, it is possible with the proper averaging, to compute the bulk transport properties of the granular material. This, in turn, is invaluable in understanding experiments.

There have been reports that have dealt with mechanical interactions in soil machinery [H. Tanaka, 2000]. These reports mostly have been concerned with spherical particles. Recently, some approaches have been implemented for elliptical [Peters, 2002] and general shaped bodies. In these approaches, the particles were modeled as ellipsoidal, sphere cluster [Vu – Quoc, 2000] or general shaped via superquadratics [Williams, 1989; Mustoe, 1993 and 2000].

The elliptical formulation has many advantages because with the modification of the ellipse's length in the x and y axes, it is possible to model an infinite number of ellipses (circles included). For circular particles, the analysis is simple because one only needs the diameters and the distance between centers to know if the particles are in contact. For elliptical particles, the diameters and the distance between centers is not enough to determine if there is contact. The parameters are the distance between centers, length of the ellipse's major and minor axes, and one angle (2D) or three angles (3D).

Circular and spherical shape analysis in many realistic cases is not as accurate as using an elliptical shape. Superquadratics shape analysis is even more realistic. However, it can be computationally expensive. Elliptical particles represent a good compromise between the very precise and computationally expensive superquadratics particles and the less precise and relatively inexpensive circular particles.

This thesis aims to explain and implement two formulations for collision detection, needed in a discrete element simulation of elliptical particles. Chapter 2 introduces the general concepts, which are applied in the entire thesis. Chapter 3 describes the contact detection terminology. In Chapter 3, the formulation is explained in great detail. Chapter 4 gives the results that were obtained with the implementation of the contact detection strategy developed in Chapter 3. Chapter 5 summarizes and analyzes the most important points of the thesis.

1.3 Overview of Discrete Element Method

The grains inside a granular material interact and change shape near the collision point. In the Discrete Element Method (DEM), the particle shape is not allowed to change. Rather, the particle deformation is not necessary to obtain the mechanical behavior of a granular material [Cundall, 1979]. The amount of interpenetration between a pair of particles is considered as a measure of deformation. The amount of penetration is related to the contact force.

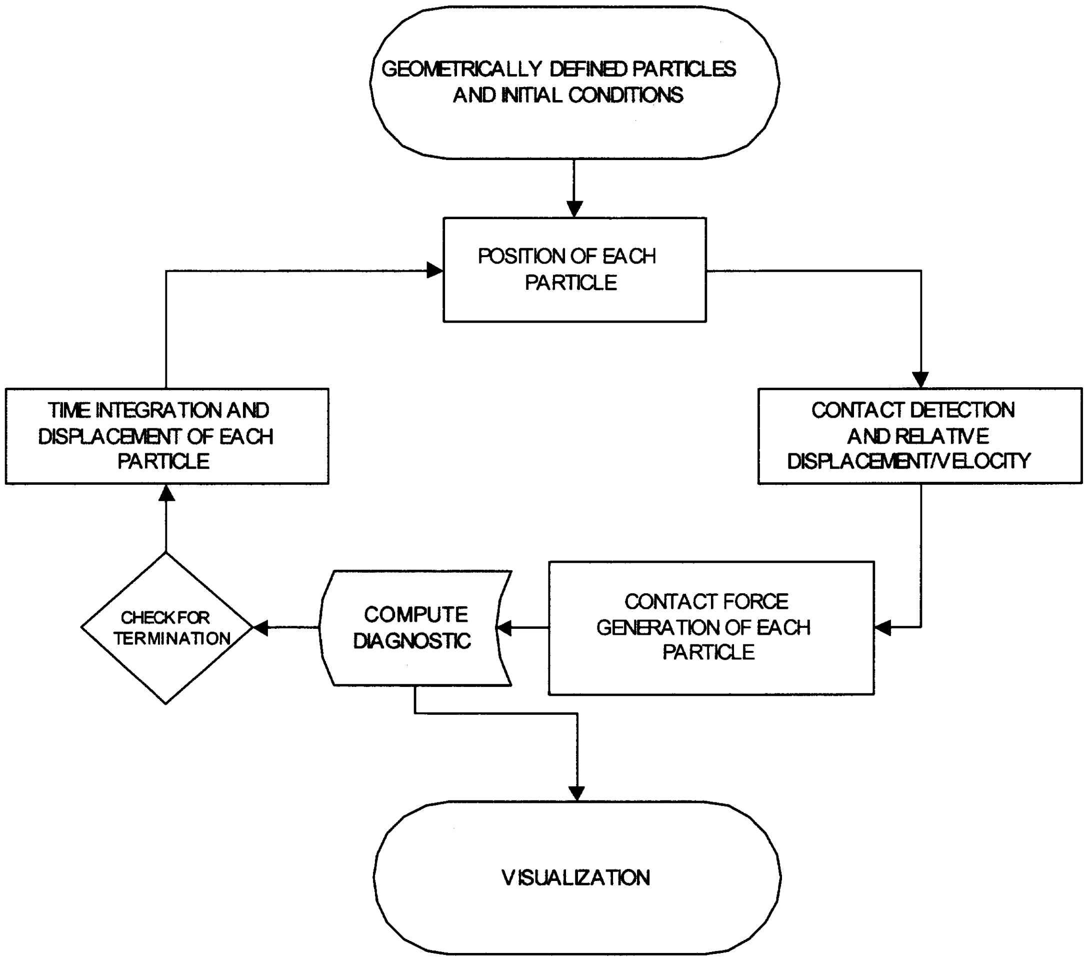


Figure 1.1 General procedure for DEM algorithms.

CHAPTER 2

CHARACTERIZATION OF ELLIPTICAL PARTICLES

This chapter introduces the basic concepts used through the entire thesis. Here, the ellipse is analytically described and parameterized. This involves a description of various coordinate axes and transformations.

2.1 Geometry of the Ellipse

The family of surfaces described by Equation 2.1 is called "quadratics," which includes the ellipse, parabola, and hyperbola. An elliptic curve has to meet the following conditions: $B \neq 0$ *and* $B^2 - 4 \cdot A \cdot C < 0$ or $B = 0, A \neq C,$ *and* $A \cdot C > 0$. For circles, the conditions are $B = 0$ *and* $A = C \neq 0$.

$$A \cdot X^2 + B \cdot X \cdot Y + C \cdot Y^2 + D \cdot X + E \cdot Y + F = 0 \qquad (2.1)$$

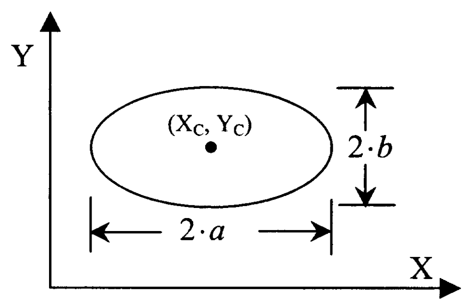


Figure 2.1 Quadratic definition of elliptic curve.

The basic equation that defines the elliptic curve is presented in Equation 2.2, in which the major and minor axes of the elliptic curve are parallel to the coordinate axes [Spiegel, 1995].

$$\left(\frac{X-X_C}{a}\right)^2+\left(\frac{Y-Y_C}{b}\right)^2=1 \tag{2.2}$$

Here X_C and Y_C are the X and Y positions of the centroid of the ellipse. The half length in the x and y axes are called a and b respectively.

2.2 Parametrization of an Ellipse

In order to make the description of the elliptic curve more tractable, it is possible to introduce a parametrization [Lee, 1999], as defined by Equation 2.3.

$$X=a\cdot\cos\theta,\quad Y=b\cdot\sin\theta,\quad Z=0 \qquad for\ \theta\in[0,2\pi] \tag{2.3}$$

This parametrization can also be formulated as a column matrix, i.e.,

$$\begin{bmatrix} X \\ Y \\ Z \\ 1 \end{bmatrix} = \begin{bmatrix} a\cdot\cos\theta \\ b\cdot\sin\theta \\ 0 \\ 1 \end{bmatrix} \qquad \text{for } \theta \in [0, 2\pi] \tag{2.4}$$

Here the center of the ellipse lies at the origin of the coordinate axes, while the major and minor axes are parallel to the coordinate axis.

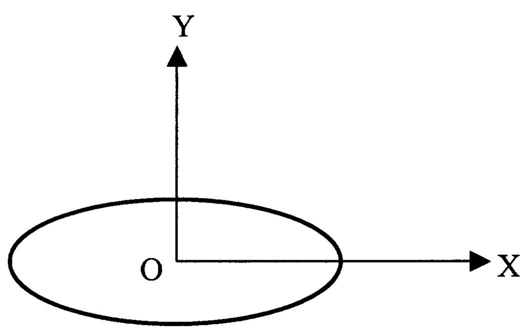


Figure 2.2 Elliptic curve.

In three dimensions, the parametrization for ellipsoids becomes:

$$\begin{bmatrix} X \\ Y \\ Z \\ 1 \end{bmatrix} = \begin{bmatrix} a \cdot \cos\theta \cdot \sin\varphi \\ b \cdot \sin\theta \cdot \sin\varphi \\ c \cdot \cos\varphi \\ 1 \end{bmatrix} \quad \begin{array}{r} \text{For } \theta \in [0, 2\pi) \\ \varphi \in [0, \pi] \end{array} \tag{2.5}$$

2.3 Contact Description

In order to evaluate the contact between particles, it is possible describe the contact using fixed coordinate axes or moving coordinate axes. Figures 2.3 and 2.4 show the fixed coordinate axes and the moving coordinate axes, respectively.

In this thesis, fixed and moving approaches are used to determine the contact between particles [Williams, 1989]. The fixed coordinate axes approach is related to the fluid dynamics concept of Eulerian coordinates. The moving coordinate axes approach is related to the fluid dynamics concept of Lagrangian coordinates.

2.3.1 Fixed Coordinate Axes

The data input or initial conditions can be described with fixed coordinate axes, which is the natural description for physical experiments. In Figure 2.3, “i” and “j” designates the ellipses, while X and Y represent the fixed axes. The notation $\langle \bullet, \bullet \rangle$ is used to denote a vector.

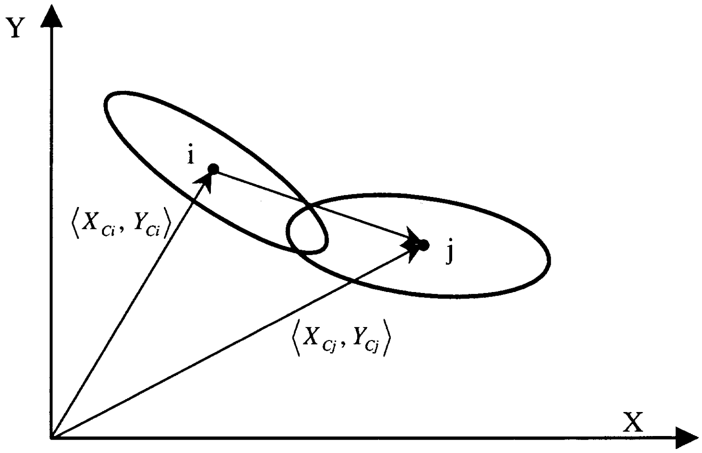


Figure 2.3 Ellipses described with fixed coordinate axes.

The distance between centroids of these ellipses is given by:

$$d = \sqrt{\left(X_{Ci} - X_{Cj}\right)^2 + \left(Y_{Ci} - Y_{Cj}\right)^2} \tag{2.6}$$

and this can be useful to simplify the analysis (Table 2.1). The ellipses are distinguished by subscripts i and j.

Table 2.1 Relationships of Ellipses Intersections and Distance Between Centroids

DISTANCE BETWEEN CENTROIDS	ELLIPSES INTERSECTIONS
$d > (a_i + a_j)$	No Intersection
$d = (a_i + a_j)$	No Intersection or One – Point Intersection
$d < (a_i + a_j)$	No intersection, One – Point Intersection, or More than One – Point Intersection
$d > (b_i + b_j)$	No intersection, One – Point Intersection, or More than One – Point Intersection
$d = (b_i + b_j)$	One – Point Intersection or More than One – Point Intersection
$d < (b_i + b_j)$	More than One – Point Intersection

Note: a_i and a_j are the half of the length of the major axes of the Ellipses i and j respectively. b_i and b_j are the half of the length of the minor axes of the Ellipses i and j, respectively.

2.3.2 Moving Coordinate Axes

The formulations using the moving coordinate axes approach, where the origin is fixed at the centroid of the particle, is depicted in Figure 2.3. The moving coordinate axes approach can reduce the size of the computational domain necessary for the contact detection calculations.

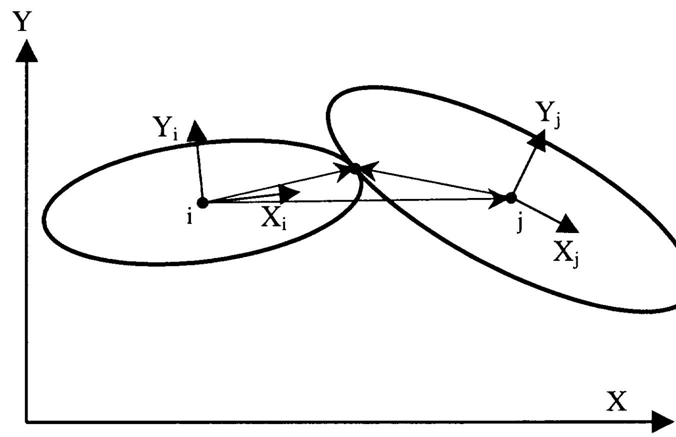


Figure 2.4 Ellipses described with moving coordinate axes.

2.4 Transformation Matrices

Transformation matrices can be used to translate and rotate the axes of the ellipse. The translation matrix is given by:

$$Trans(a,b,c)=\begin{bmatrix} 1 & 0 & 0 & a \\ 0 & 1 & 0 & b \\ 0 & 0 & 1 & c \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{2.7}$$

where a, b and c represent the translation of the coordinate axes. The rotation matrix where z and ϕ are the z-axis of rotation and the angle of rotation (positive in counterclockwise direction), respectively is given by:

$$rot(z,\phi)=\begin{bmatrix}\cos\phi & -\sin\phi & 0 & 0\\ \sin\phi & \cos\phi & 0 & 0\\ 0 & 0 & 1 & 0\\ 0 & 0 & 0 & 1\end{bmatrix} \tag{2.8}$$

Figure 2.5 shows the translation of the elliptic curve from the origin of the fixed coordinates axes to (X_{Ci}, Y_{Ci}). Also depicted is a rotation through angle ϕ.

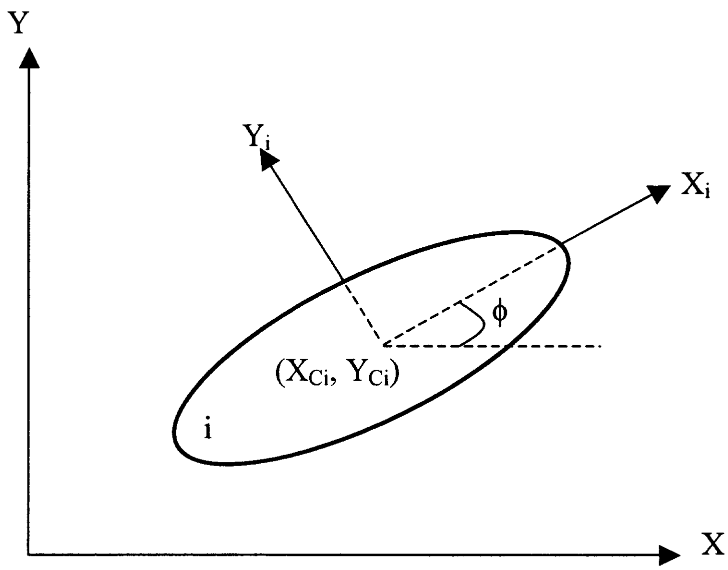


Figure 2.5 Elliptic Curve rotated and translated from the origin of the fixed coordinate axes.

From Equations 2.7, 2.8, and 2.4 the formulation to obtain the equation that defines the elliptic curve in a fixed coordinate found to be:

$$\begin{aligned}\begin{bmatrix}X(\theta_i)\\ Y(\theta_i)\\ Z(\theta_i)\\ 1\end{bmatrix} &= Trans(X_{Ci},Y_{Ci},0,1)\cdot\left(Rot(Z,\phi_i)\cdot\begin{bmatrix}X_i(\theta_i)\\ Y_i(\theta_i)\\ 0\\ 1\end{bmatrix}\right)\\ &= Trans(X_{Ci},Y_{Ci},0,1)\cdot\left(Rot(Z,\phi_i)\cdot\begin{bmatrix}a_i\cdot\cos\theta_i\\ b_i\cdot\sin\theta_i\\ 0\\ 1\end{bmatrix}\right)\end{aligned} \tag{2.9}$$

Thus, the equations that define the elliptic curve with respect to the global coordinate axis are given by:

$$\begin{aligned} X(\theta_i) &= a_i \cdot \cos\theta_i \cdot \cos\phi_i - b_i \cdot \sin\theta_i \cdot \sin\phi_i + X_{Ci} \\ Y(\theta_i) &= a_i \cdot \cos\theta_i \cdot \sin\phi_i + b_i \cdot \sin\theta_i \cdot \cos\phi_i + Y_{Ci} \\ Z(\theta_i) &= 0 \qquad\qquad (0 \le \theta_i \le 2\pi) \end{aligned} \tag{2.10}$$

Further details on the parametric formulations of the elliptic curve and the matrix transformation are explained in references [Lee, 1999; Craig, 1989].

2.5 Superquadratics

Granular materials can be composed of different and complex shapes and sizes. The idea of using superquadratics to describe these complex shapes has been implemented by William et al. [1989] and Mustoe et al. [1993 and 2000].

Superquadratics are an analytical expression that defines the surface of an object [William, 1989]. The superquadratics are extensions of the traditional geometric primitives that can be represent a range of shapes, from ellipsoidal to rectangular. Eighty percent of solids can be represented accurately by superquadratics in higher dimensions or hyperquadratics. The general equation is given by:

$$F(x,y,z) = \left|\frac{x}{a}\right|^{n1} + \left|\frac{y}{b}\right|^{n2} + \left|\frac{z}{c}\right|^{n3} - 1 \tag{2.11}$$

where a, b, and c indicate the half length of the principal axes, and n1, n2 and n3 are real numbers, such that $0 < n_i < \infty$, i = 1, 2, 3. If n1 = n2 = n3 = 2, the function is called an ellipsoid. Moreover, if n1 = n2 = 2 and z = 0, the curve is an ellipse.

Just as for quadratics, superquadratics can be represented parametrically, defined in Equation 2.12. The superquadratics have latitude (lat) and longitude (long) as the two controlling parameters.

$$\begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} a \cdot sign[\cos(lat) \cdot \cos(long)] \cdot \left|\cos^P(lat) \cdot \cos^Q(long)\right| \\ b \cdot sign[\cos(lat) \cdot \sin(long)] \cdot \left|\cos^P(lat) \cdot \sin^Q(long)\right| \\ c \cdot sign[\sin(lat)] \cdot \left|\sin^P(lat)\right| \end{bmatrix} \tag{2.12}$$

Here, a, b, and c are scaling factors in the X, Y, and Z - coordinate directions. P and Q are exponents that control the squareness / roundness of the shape in the latitude (or north – south) and longitude (or east – west) directions.

$$Note: \quad sign(x) = \begin{Bmatrix} +1, \; x>0 \\ 0, \; x=0 \\ -1, \; x<0 \end{Bmatrix}$$

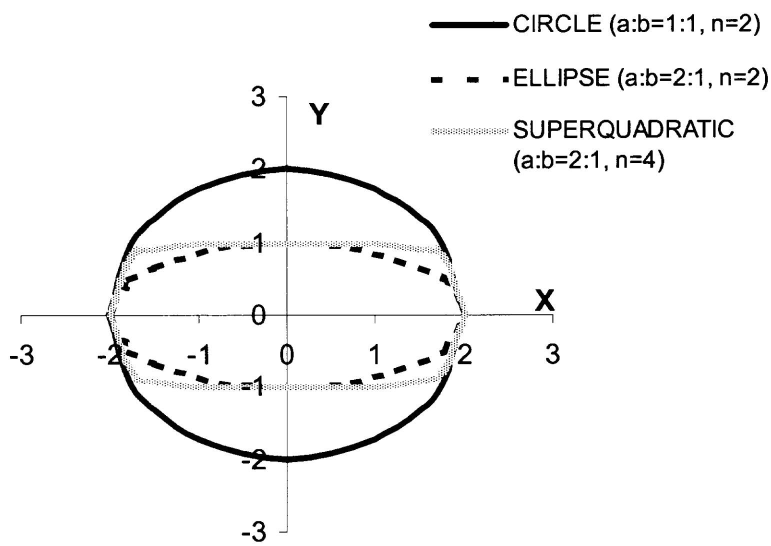


Figure 2.6 Superquadratic representation of a particle (n1 = n2 and z = 0) [Miyata, 2000].

CHAPTER 3

CONTACT DETECTION FOR ELLIPSES

The most time-consuming part of the Discrete Element Method (DEM) is the contact detection. It is extensively time-consuming to check the contact of each particle with the other neighboring particles. This chapter explains a contact detection formulation that uses moving coordinate axes as a main methodology [Mustoe, 1993 and 2000]. A contact detection formulation that uses fixed coordinate axes (Appendix B) was developed as part of the research for this thesis.

This chapter aims to clarify and detail the formulations used by Mustoe et al [1993 and 2000]. The formulation developed through this chapter is the basis for Contact Detection with Penetration Code and Contact Detection without Penetration Code.

3.1 Minimum Overlap Distance Criterion

Mustoe et al [1993 and 2000] introduced the concept of minimum overlap distance. In these Mustoe describes the particles as superquadratics. However, for the purpose of this thesis, attention will be restricted to ellipses.

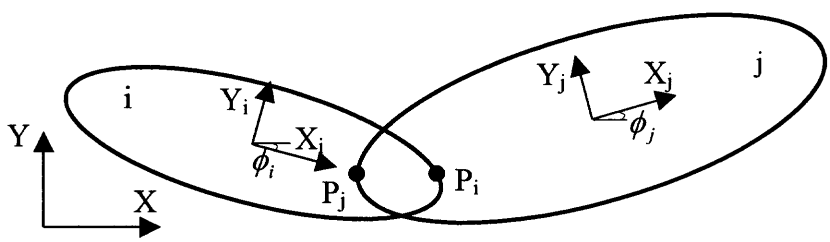


Figure 3.1 Parameters of the ellipses in contact.

The angles ϕ_i and ϕ_j represent the orientations of the elliptical axes with respect to the global system (fixed axes), as shown in Figure 3.1. The position of P_j is the elliptic curve j nearest to the origin of the coordinate axes of Ellipse – i. The (x, y) coordinate of P_j is found by minimizing the function:

$$f_i(X_i, Y_i) \equiv \left(\frac{X_i}{a_i}\right)^2 + \left(\frac{Y_i}{b_i}\right)^2 - 1 \tag{3.1}$$

In order to carry out the necessary minimization, Ellipse – j must be defined with respect to moving coordinate axes that have to be defined with respect to a local coordinate axis of the Ellipse – i. From Figure 3.2, $\Delta X = k + w$ and $\Delta Y = p$ represent the components of the vector between the centers of Ellipse – i and Ellipse – j with respect to the coordinate system attached to Ellipse – i.

$$\left(X_i(\theta_j), Y_i(\theta_j), 0, 1\right)^T = Trans(\Delta X, \Delta Y, 0, 1) \cdot \left[(Rot(z, \Delta\phi))^T \cdot \left(X_j(\theta_j), Y_j(\theta_j), 0, 1\right)^T\right]$$

$$\begin{bmatrix} X_i(\theta_j) \\ Y_i(\theta_j) \\ 0 \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & \Delta X \\ 0 & 1 & 0 & \Delta Y \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \cdot \left\{ \begin{bmatrix} \cos\Delta\phi & \sin\Delta\phi & 0 & 0 \\ -\sin\Delta\phi & \cos\Delta\phi & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} X_j(\theta_j) \\ Y_j(\theta_j) \\ 0 \\ 1 \end{bmatrix} \right\}$$

$$\Rightarrow \quad \begin{bmatrix} X_i(\theta_j) \\ Y_i(\theta_j) \\ 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & \Delta X \\ 0 & 1 & \Delta Y \\ 0 & 0 & 1 \end{bmatrix} \cdot \left\{ \begin{bmatrix} \cos\Delta\phi & \sin\Delta\phi & 0 \\ -\sin\Delta\phi & \cos\Delta\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} X_j(\theta_j) \\ Y_j(\theta_j) \\ 1 \end{bmatrix} \right\}$$

$$\Rightarrow \quad \begin{bmatrix} X_i(\theta_j) \\ Y_i(\theta_j) \\ 1 \end{bmatrix} = \begin{bmatrix} X_j(\theta_j) \cdot \cos\Delta\phi + Y_j(\theta_j) \cdot \sin\Delta\phi + \Delta X \\ -X_j(\theta_j) \cdot \sin\Delta\phi + Y_j(\theta_j) \cdot \cos\Delta\phi + \Delta Y \\ 1 \end{bmatrix}$$

$$\Rightarrow \quad \begin{bmatrix} X_i(\theta_j) \\ Y_i(\theta_j) \end{bmatrix} = \begin{bmatrix} X_j(\theta_j) \cdot \cos\Delta\phi + Y_j(\theta_j) \cdot \sin\Delta\phi \\ -X_j(\theta_j) \cdot \sin\Delta\phi + Y_j(\theta_j) \cdot \cos\Delta\phi \end{bmatrix} + \begin{bmatrix} \Delta X \\ \Delta Y \end{bmatrix} \tag{3.2}$$

where: $X_j(\theta_j) = a_j \cdot \cos\theta_j$, $Y_j(\theta_j) = b_j \cdot \sin\theta_j$, $\Delta\phi = \phi_i - \phi_j$

The next steps are used to generalize the formula for ΔX and ΔY. Mustoe et al. [1993 and 2000] does not provide the generalization of ΔX and ΔY.

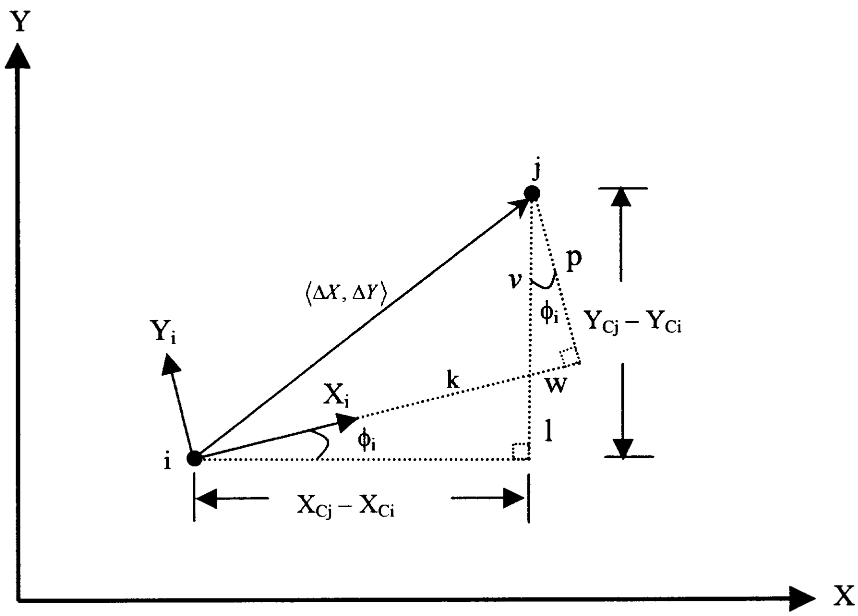


Figure 3.2 Origins' distance of the coordinate axes of Ellipse – j relative to the coordinate axes of Ellipse – i.

The position vector $\langle \Delta X, \Delta Y \rangle = \langle k + w, p \rangle$ describes the position of the coordinate axes of Ellipse – j relative to the coordinate axes of Ellipse – i. Here it is assumed that X_{Ci}, X_{Cj}, Y_{Ci}, Y_{Cj} and ϕ_i are known.

Step 1:

$$\tan\phi_i = \frac{l}{X_{Cj} - X_{Ci}} \Rightarrow l = (X_{Cj} - X_{Ci}) \cdot \tan\phi_i$$

$$v + l = Y_{Cj} - Y_{Ci} \Rightarrow v = (Y_{Cj} - Y_{Ci}) - (X_{Cj} - X_{Ci}) \cdot \tan\phi_i$$

Step 2:

$$\cos\phi_i = \frac{X_{Cj} - X_{Ci}}{k} \Rightarrow k = \frac{X_{Cj} - X_{Ci}}{\cos\phi_i}$$

Step 3:

$$\cos\phi_i = \frac{p}{v} \Rightarrow p = v \cdot \cos\phi_i$$
$$p = \left[\left(Y_{Cj} - Y_{Ci}\right) - \left(X_{Cj} - X_{Ci}\right) \cdot \tan\phi_i\right] \cdot \cos\phi_i$$

Step 4:

$$\sin\phi_i = \frac{w}{v} \Rightarrow w = v \cdot \sin\phi_i$$
$$\Rightarrow w = \left[\left(Y_{Cj} - Y_{Ci}\right) - \left(X_{Cj} - X_{Ci}\right) \cdot \tan\phi_i\right] \cdot \sin\phi_i$$

Then:

$$\Delta X = \frac{X_{Cj} - X_{Ci}}{\cos\phi_i} + \left(Y_{Cj} - Y_{Ci}\right) \cdot \sin\phi_i - \left(X_{Cj} - X_{Ci}\right) \cdot \sin\phi_i \cdot \tan\phi_i$$
$$\Delta Y = \left(Y_{Cj} - Y_{Ci}\right) \cdot \cos\phi_i - \left(X_{Cj} - X_{Ci}\right) \cdot \sin\phi_i$$

Finally:

$$\begin{bmatrix} \Delta X \\ \Delta Y \end{bmatrix} = \begin{bmatrix} \cos\phi_i & \sin\phi_i \\ -\sin\phi_i & \cos\phi_i \end{bmatrix} \cdot \begin{bmatrix} X_{Cj} - X_{Ci} \\ Y_{Cj} - Y_{Ci} \end{bmatrix} \tag{3.3}$$

The subscripts i and j should be inverted on Equations 3.1, 3.2, and 3.3 to find P_i.

The value of θ_j^* is found when Equation 3.1 is minimized. The value θ_j^* is an approximation of the values θ_j that minimize the function. This value defines the point

P_j, in Figure 3.1. Brent's Method to find the minimum of a function is used through this thesis to minimizes the function, as was done by Mustoe et al. [2000]. Brent's Method for finding a minimum is an adaptation of the technique used in Brent's Method to find a root of an equation. In what follows, the phrase "Brent's Method' will be understood to represent his method to minimize a non-linear function. Further details about this method are given in Appendix A.

Brent's Method always converges for any function to the global minimum, in a given interval, if the function is unimodal. If a function defined in an interval is not unimodal, then it may convergent to a local minimum. In the specific case of contact detection between elliptical particles, convergence to a local minimum is not a problem, because the analysis is for two convex shaped bodies.

The point $P_j = (P_{jX}, P_{jY}) = (X_j(\theta_j^*), Y_j(\theta_j^*)) = (a_j \cdot \cos\theta_j^*, b_j \cdot \sin\theta_j^*)$ is defined in the local coordinate system attached to the centroid of Ellipse – j. To determine if there is contact,

$$f_i\left(X_i\left[X_j(\theta_j^*)\right], Y_i\left[Y_j(\theta_j^*)\right]\right) \equiv \left(\frac{X_i\left[X_j(\theta_j^*)\right]}{a_i}\right)^2 + \left(\frac{Y_i\left[Y_j(\theta_j^*)\right]}{b_i}\right)^2 - 1 \tag{3.4}$$

X_i and Y_i are defined in Equation 3.2.

$$f_i\left(X_i(\theta_j^*), Y_i(\theta_j^*)\right) = \left\{\begin{array}{l} = 0,\ P_j \textit{ is on the surface of} \\ \quad \textit{the body } i \ (\textit{One contact}) \\ < 0,\ P_j \textit{ is inside of the body } i \\ \quad (\textit{Two or more contacts}) \\ > 0,\ P_j \textit{ is outside the surface of} \\ \quad \textit{the body } i \ (\textit{No contact}) \end{array}\right\} \tag{3.5}$$

In order to determine whether there is contact, Equation 3.5 analyze if the Ellipse – j's point P$_j$ = $\left(X_j\left(\theta_j^*\right), Y_j\left(\theta_j^*\right)\right)$ is inside the Ellipse – i. Equation 3.5 with P$_i$ = $\left(X_i\left(\theta_i^*\right), Y_i\left(\theta_i^*\right)\right)$ analyze if the Ellipse – i's point is inside the Ellipse – j.

3.2 Curvature Method

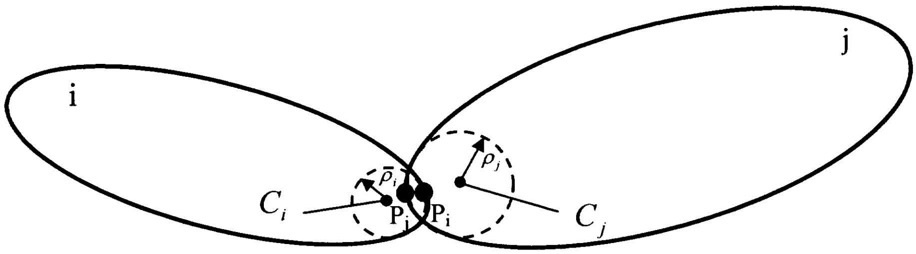


Figure 3.3 Contact Parameters found with the Curvature Method.

After obtaining the points P$_i$ and P$_j$, a circle can be found at the position of the points P$_i$ and P$_j$ in the Ellipse – i and Ellipse – j, respectively. The curvature method is applied to find the radii of curvature (ρ) and the center of curvature (C) of Ellipse – i and Ellipse – j at P$_i$ and P$_j$, respectively, as shown in Figure 3.3. The circular curves will simplify the problem at the interaction between two circular particles.

In what follows, the details of finding these circles is described. The radii of curvature at the two contact points P$_i$ and P$_j$ are given by,

$$\rho_k = \left(1 + \left(\frac{dy_k}{dx_k}\right)^2\right)^{3/2} \Bigg/ \frac{d^2 y_k}{dx_k^2}, \qquad k = i, j \tag{3.6}$$

for a two – dimensional curve defined as y = f(x). Thus, for the elliptical curve:

$$f_k\left(x_k, y_k\right) \equiv \left(\frac{x_k}{a_k}\right)^2 + \left(\frac{y_k}{b_k}\right)^2 - 1 = 0, \qquad k = i, j \tag{3.7}$$

the radii of curvatures are given by,

$$\rho_k = \frac{\left(\left(\frac{\partial f_k}{\partial x_k}\right)^2 + \left(\frac{\partial f_k}{\partial y_k}\right)^2\right)^{3/2}}{\left(\frac{\partial^2 f_k}{\partial x_k^2}\left(\frac{\partial f_k}{\partial y_k}\right)^2 - 2\cdot\frac{\partial^2 f_k}{\partial y_k \cdot \partial x_k}\cdot\frac{\partial f_k}{\partial x_k}\cdot\frac{\partial f_k}{\partial y_k} + \frac{\partial^2 f_k}{\partial y_k^2}\cdot\left(\frac{\partial f_k}{\partial x_k}\right)^2\right)}, \quad k = i, j \tag{3.8}$$

where: $\frac{\partial f_k}{\partial x_k} = \frac{2\cdot x_k}{(a_k)^2}$, $\frac{\partial f_k}{\partial y_k} = \frac{2\cdot y_k}{(b_k)^2}$, $\frac{\partial^2 f_k}{\partial y_k \partial x_k} = 0$, $\frac{\partial^2 f_k}{\partial x_k^2} = \frac{2}{(a_k)^2}$, *and* $\frac{\partial^2 f_k}{\partial y_k^2} = \frac{2}{(b_k)^2}$

The radii of curvature for ellipses can be represented in a simpler manner as shown in Equation 3.9.

$$\rho_k = \frac{\left[\left(\frac{x_k}{(a_k)^2}\right)^2 + \left(\frac{y_k}{(b_k)^2}\right)^2\right]^{3/2}}{\frac{1}{(a_k \cdot b_k)^2}\cdot\left[\left(\frac{x_k}{a_k}\right)^2 + \left(\frac{y_k}{b_k}\right)^2\right]}, \quad k = i, j \tag{3.9}$$

The definition of radii of curvature for superquadratics is given in Appendix C. The position of the center of curvature is the next parameter to be found. First, it is necessary calculate the unit outward normal vector of each ellipse at P_i and P_j. The unit outward normal vector on the surface of Body "k", defined by a ellipse in the local centroidal coordinate system for Body "k", is given by,

$$\hat{n}_k = \begin{bmatrix} n_x \\ n_y \end{bmatrix}_k = \nabla f_k / |\nabla f_k|, \quad k = i, j \tag{3.10}$$

where: $\nabla f_k = \begin{bmatrix} \frac{\partial f_k}{\partial x_k} \\ \frac{\partial f_k}{\partial y_k} \end{bmatrix} = \begin{bmatrix} \frac{2\cdot x_k}{(a_k)^2} \\ \frac{2\cdot y_k}{(b_k)^2} \end{bmatrix}$ and $|\nabla f_k| = \sqrt{\left(\frac{2\cdot x_k}{(a_k)^2}\right)^2 + \left(\frac{2\cdot y_k}{(b_k)^2}\right)^2}$.

The coordinate with respect to centroidal moving axes (local axes) of Ellipse – k for the position of the center of curvature C_k, for the point P_k is given by,

$$\begin{bmatrix} C_x \\ C_y \end{bmatrix}_k = \begin{bmatrix} x_k \\ y_k \end{bmatrix} - \rho_k \cdot \begin{bmatrix} n_x \\ n_y \end{bmatrix}_k , \quad k = i, j \tag{3.11}$$

where: $\begin{bmatrix} x_k \\ y_k \end{bmatrix} = \begin{bmatrix} X_k(\theta_k^*) \\ Y_k(\theta_k^*) \end{bmatrix} = \begin{bmatrix} a_k \cdot \cos(\theta_k^*) \\ b_k \cdot \sin(\theta_k^*) \end{bmatrix}$, from Equation 2.4.

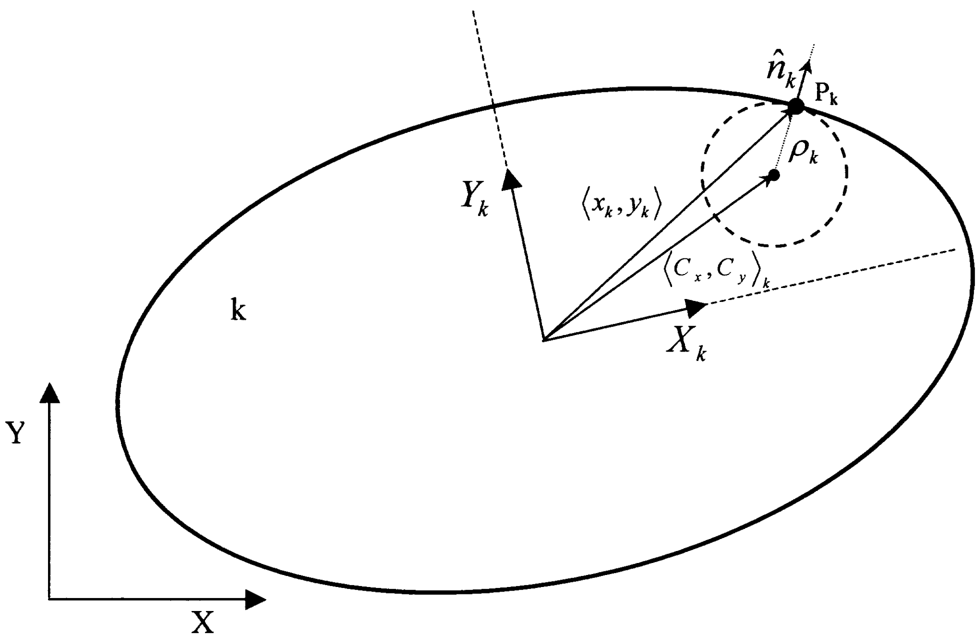


Figure 3.4 Center of curvature's coordinate in the moving coordinate axes.

In Equation 3.11, the center of curvature is defined in the moving coordinate axes of the ellipse. For an easy calculation of distances, it is preferred to have the circles defined in fixed coordinate axes.

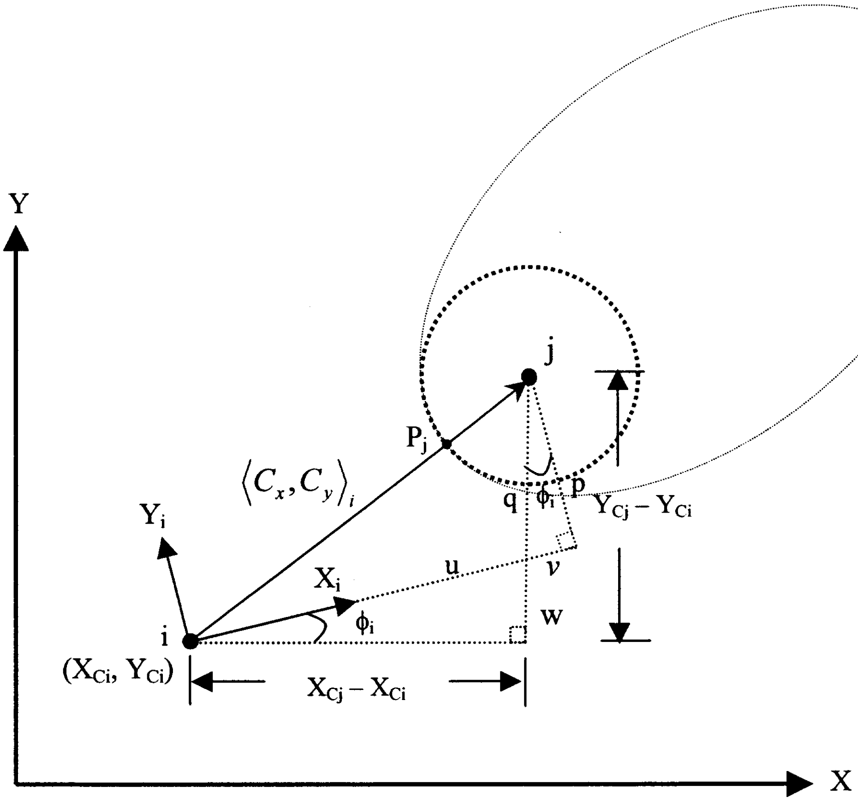


Figure 3.5 Center of curvature defined in a fixed (global) coordinate axes.

The position vector $\langle C_x, C_y \rangle_i = \langle u + v, p \rangle$ describes the position of the center of curvature j in a frame with moving coordinate axes. The values $X_{Cj} - X_{Ci}$ and $Y_{Cj} - Y_{Ci}$ describe the position of the center of curvature j with respect to the origin of the coordinate axes in a fixed coordinate frame. The given values are C_x, C_y, and ϕ_i.

Step 1:

$$\cos \phi_i = \frac{C_y}{q} \Rightarrow q = \frac{C_y}{\cos \phi_i}$$

Step 2:

$$\tan \phi_i = \frac{v}{C_y} \Rightarrow v = C_y \cdot \tan \phi_i$$

$$u + v = C_x \Rightarrow u = C_x - v = C_x - C_y \cdot \tan \phi_i$$

Step 3:

$$\cos \phi_i = \frac{X_{Cj} - X_{Ci}}{u} \Rightarrow X_{Cj} - X_{Ci} = \left[C_x - C_y \cdot \tan \phi_i\right] \cdot \cos \phi_i$$

$$X_{Cj} - X_{Ci} = C_x \cdot \cos \phi_i - C_y \cdot \sin \phi_i$$

Step 4:

$$\sin \phi_i = \frac{w}{u} \Rightarrow w = u \cdot \sin \phi_i = \left[C_x - C_y \cdot \tan \phi_i\right] \cdot \sin \phi_i$$

$$Y_{Cj} - Y_{Ci} = w + q = \left[C_x - C_y \cdot \tan \phi_i\right] \cdot \sin \phi_i + \frac{C_y}{\cos \phi_i}$$

Finally:

$$\begin{bmatrix} X_{Cj} - X_{Ci} \\ Y_{Cj} - Y_{Ci} \end{bmatrix} = \begin{bmatrix} \cos \phi_i & -\sin \phi_i \\ \sin \phi_i & \cos \phi_i \end{bmatrix} \cdot \begin{bmatrix} C_x \\ C_y \end{bmatrix} \tag{3.12}$$

Hence $X_{Cj} - X_{Ci}$ and $Y_{Cj} - Y_{Ci}$ can be computed from Equation 3.12. Thus, the center of curvature in the fixed coordinate axes is now given by,

$$\begin{bmatrix} G_x \\ G_y \end{bmatrix}_k = \begin{bmatrix} \cos \phi_k & -\sin \phi_k \\ \sin \phi_k & \cos \phi_k \end{bmatrix} \cdot \begin{bmatrix} C_x \\ C_y \end{bmatrix}_k + \begin{bmatrix} X_C \\ Y_C \end{bmatrix}_k, \quad k = i, j \tag{3.13}$$

From the above expressions, the penetration can be computed between two contacting Ellipses "i" and "j". The normal overlap penetration distance is defined by,

$$h = \rho_i + \rho_j - d \tag{3.14}$$

where d is the distance between the center of curvatures C_i and C_j, that is, defined in the fixed coordinate axes (G_x, G_y). The distance between centers of curvature is defined as:

$$d = \sqrt{\left(G_{xi} - G_{xj}\right)^2 + \left(G_{yi} - G_{yj}\right)^2} \tag{3.15}$$

The contact between bodies "i" and "j" exists just when $h \geq 0$. However at $h > 0$, this condition can be used to determine the particles' interaction force.

3.3 Code Documentation

This section discusses in detail the Contact Detection With Penetration Code, since it is more useful than Contact Detection Without Penetration Code. Both codes use different formulations, but they have the same givens and can detect contact between two particles. The calculation of the penetration distance is a great advance, because the code can be easily expanded to analyze contact force, displacement and to perform time integration.

3.3.1 Problem Description

These codes come from the necessity of an automatic detection mechanism that describes the interacting particles. The penetration in the Contact Detection With Penetration Code describes and quantifies the interaction. The contact detection formulas are given in Equations 3.6 – 3.11. These general formulas can be used for different ellipses.

Table 3.1 Nomenclature of Given Values for Contact Detection With Penetration Code

aA, bA	Ellipse A half length in the x-axis and y-axis
aB, bB	Ellipse B half length in the x-axis and y-axis
pA, pB	Angle in z-axis, for Ellipses A and B respectively, that define the orientation of moving coordinate axes with respect to fixed coordinate axes.
Xoa, Yoa	Position of the center of the elliptic curve A in fixed coordinate axes
Xob, Yob	Position of the center of the elliptic curve B in fixed coordinate axes
TOL	Length of the interval of uncertainty in the output values

Table 3.2 Nomenclature of Unknowns for Contact Detection With Penetration Code.

del	Penetration Distance
Y1, Y2	Angle that minimizes the Ellipse – B in the coordinate axes of Ellipse – A and vice versa respectively

3.3.2 Solution Methodology

In order to find the penetration distance, the first step is to write a program that minimizes the elliptic curve with respect to a defined coordinate axes. These coordinate axes represent another ellipse (particle). Equations 3.1 – 3.3 redefine the curve equations in other coordinate axes.

Moreover, when the minimum points for both ellipses are determined, the next step is to implement the curvature method. The curvature method is derived in Equations 3.6 – 3.11. The curvature method is used to find penetration distance.

CHAPTER 4

VALIDATION OF CONTACT DETECTION WITH ELLIPTICAL PARTICLES

This chapter shows some representative results, which were classified into four separate types. The classification helps to understand the codes' advantages and disadvantages. The discussion analyzes the data.

4.1 Contact Detection Results

This section validates the Contact Detection Without Penetration Code. Each subsection has a general type of results that can be obtained by the code. The four general types are no contact point, one contact point, two contact points, and special cases.

4.1.1 No-Contact Cases

In these cases, the code should output "no contact points" two times. The contact detection is defined two times because each ellipse calculates the contact. The function at the minimum point ($f(\theta^*)$) is assumed for no-contact case's detection is higher or equal than 0.1. Examples 4.1 and 4.2 are given at tolerance 1E-5 and 1E-7. The results are in agreement with physical reality. The contact detection is practically not changed at all when the tolerance is decreased from 1E-5 to 1E-7. However, at tolerance 1E-7 the running time is higher than at tolerance 1E-5. In Example 4.1 the times for running code [Paciorek, 2002] are 6 and 334 at tolerances 1E-5 and 1E-7, respectively. In Example 4.2 the times for running code are 6 and 305 at tolerances 1E-5 and 1E-7, respectively.

Visually and analytically the simulation can recreate particles moving. Numerically, the particles are static and the axes that define the particles may move. Example 4.1 is a case for two ellipses. Ellipse A has a length of 8 and 10 in X axis and Y axis respectively. The center of the ellipse is the coordinate (1, 1). The angle of rotation of ellipse A is 45 degrees.

Ellipse B has a length of 4 and 6 in the X axis and Y axis, respectively. The center of the ellipse is at the coordinate (4, 8). The angle of rotation of ellipse B is 45 degrees. Figure 4.1 shows the case in Example 4.1.

<u>Example 4.1.a</u>: Two ellipses.

Description of Ellipse A
Half Length in the X and Y Axis are: 4, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 2, 3
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (4, 8)

Input data given in a fixed coordindate axes

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 198.961 degrees
Then the f(198.961) = 0.814199
The point is outside of the body, [NO CONTACT POINT]

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 14.9372 degrees
Then the f(14.9372) = 1.83336
The point is outside of the body, [NO CONTACT POINT]

Output data given in moving coordindate axes

Note: Time for running code: 4

Example 4.1.b: Two ellipses.

Description of Ellipse A
Half Length in the X and Y Axis are: 4, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 2, 3
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (4, 8)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-007
The value of ZB that minimizes the function is: 198.961 degrees
Then the f(198.961) = 0.814199
The point is outside of the body, [NO CONTACT POINT]

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-007
The value of ZA that minimizes the function is: 14.9373 degrees
Then the f(14.9373) = 1.83336
The point is outside of the body, [NO CONTACT POINT]

Note: Time for running code: 334

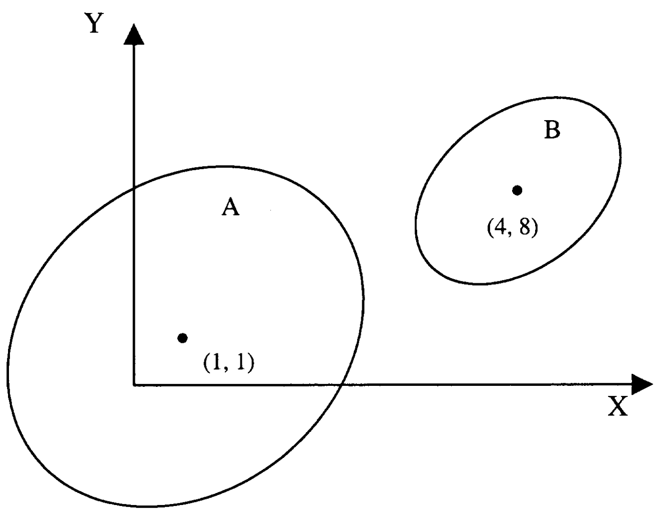


Figure 4.1 A non-contact case with two ellipses.

Example 4.2 is a case for one ellipse and one circle at tolerances of 1E-5 and 1E-7. Ellipse A has a length of 8 and 10 in the X axis and Y axis respectively. The center of the ellipse is the coordinate (1, 1). The angle of rotation of ellipse A is 45 degrees.

Ellipse B has a length of 6 and 6 in the X axis and Y axis, respectively. Since the lengths in the X axis and Y axis are the same, ellipse B can be considered as a circle. The diameter of this circle is equal to 6. The center of the ellipse is in the coordinate (4, 8). The angle of rotation of ellipse B is 45 degrees. Figure 4.2 shows the case in Example 4.2.

<u>Example 4.2.a</u>: One ellipse and one circle.

Description of Ellipse A
Half Length in the X and Y Axis are: 4, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 3, 3
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (4, 8)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 196.693 degrees
Then the f(196.693) = 0.255901
The point is outside of the body, [NO CONTACT POINT]

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 21.0835 degrees
Then the f(21.0835) = 0.356479
The point is outside of the body, [NO CONTACT POINT]

Note: Time for running code: 4

Example 4.2.b: One ellipse and one circle.

Description of Ellipse A
Half Length in the X and Y Axis are: 4, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 3, 3
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (4, 8)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-007
The value of ZB that minimizes the function is: 196.692 degrees
Then the f(196.692) = 0.255901
The point is outside of the body, [NO CONTACT POINT]

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-007
The value of ZA that minimizes the function is: 21.0834 degrees
Then the f(21.0834) = 0.356479
The point is outside of the body, [NO CONTACT POINT]

Note: Time for running code: 305

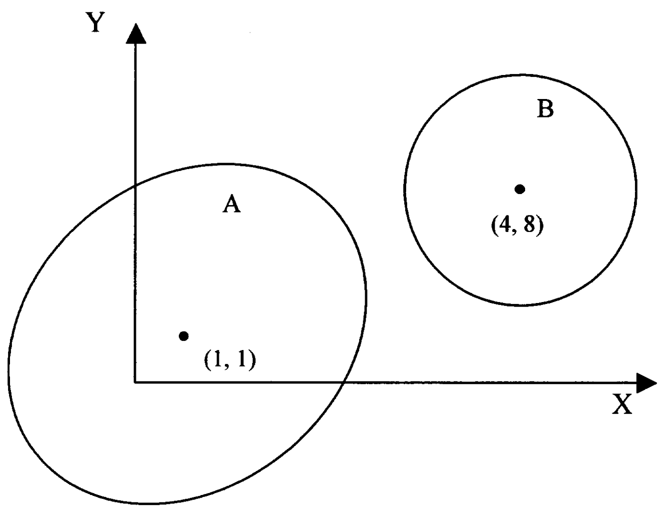


Figure 4.2 A non-contact case with one ellipse and one circle.

4.1.2 One-Contact Case

Contact Detection Without Penetration Code includes the option of a one contact case. Example 4.3, in Figure 4.3, has one contact case for two circles at 1E-5 of tolerance. These cases are very rare for the exactitude required. In an instance of zero f(θ^*), the function at the minimum point is assumed for one contact case's detection is between ± 0.1. Figure 4.3 shows the case in Example 4.3.

<u>Example 4.3</u>: Two circles, TOL = 1E-5

Description of Ellipse A
Half Length in the X and Y Axis are: 5, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 5, 5
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (7, 9)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 188.13 degrees
Then the f(188.13) = 7.90035e-013
The point is on the surface of both bodies [ONE CONTACT POINT]

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 8.13012 degrees
Then the f(8.13012) = 2.01394e-013
The point is on the surface of both bodies [ONE CONTACT POINT]

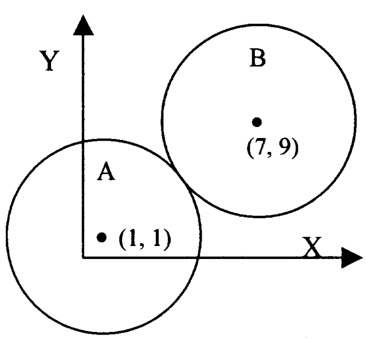


Figure 4.3 A one-point contact case with two circles.

4.1.3 Two-Contact Cases

Examples 4.4 and 4.5 are two contact point cases. In the Contact Detection Without Penetration code, two contact points are the maximum number of contact points. The function at the minimum point (f(θ^*)) is assumed for two-contact case's detection is less or equal than -0.1. Specifically, example 4.4 is the basic case with two circles. Both circles have a radius of 2 and an angle of rotation of 45 degrees. The centers of the circle A and B are in the coordinates (1, 1) and (3, 3), respectively and the tolerance is 1E-5.

<u>Example 4.4</u>: Two circles.

Description of Ellipse A
Half Length in the X and Y Axis are: 2, 2
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 2, 2
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (3, 3)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 180 degrees
Then the f(180) = -0.828427
The point is inside of the body, [TWO CONTACT POINTS]

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 0.00031842 degrees
Then the f(0.00031842) = -0.828427
The point is inside of the body, [TWO CONTACT POINTS]

Example 4.5 provides a more “complicated” case than Example 4.4. The case is for one ellipse and one circle at 1E-5 of tolerance.

<u>Example 4.5</u>: Two ellipses.

Description of Ellipse A
Half Length in the X and Y Axis are: 3, 5
Angle of Rotation of Ellipse A: 30 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 4, 3
Angle of Rotation of Ellipse B: 60 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (5, 6)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 164.701 degrees
Then the f(164.701) = -0.401732
The point is inside of the body, [TWO CONTACT POINTS]

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 15.4105 degrees
Then the f(15.4105) = -0.325772
The point is inside of the body, [TWO CONTACT POINTS]

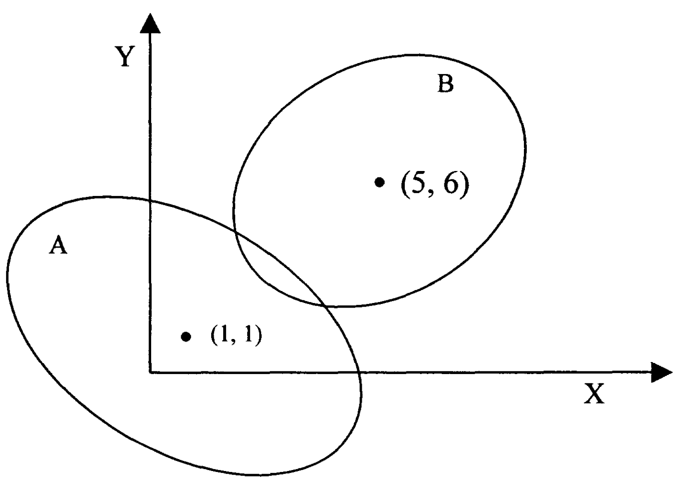


Figure 4.4 A two-contact case with two ellipses.

4.1.4 Special Cases

A special case occurs when the code output is "no contact" for one ellipse and "two contacts" for another ellipse. The special case is caused by the short distance of the ellipses' center relative to the major and minor axes. In these cases, it is correct to assume that the ellipses have two contact points (as maximum points of contact). The code displays no contact and two contacts because the points in the curves will be farther from the centers. These cases should not happen when the code is implemented with force-penetration simulation because they avoid the penetration conditions that generate these cases.

Example 4.6 has a two circles case. Circles A and B have a diameter of 10 and 4 respectively. Ellipse A is a circle with an angle of rotation of 45 degrees and the position of the center is (1, 1) defined in the fixed coordinate axes. Ellipse B is a circle with an angle of rotation of 45 degrees and the position of the center is (3, 3) defined in the fixed coordinate axes. The equations are defined at 1E-5 of tolerance.

<u>Example 4.6</u>: Two circles.

Description of Ellipse A
Half Length in the X and Y Axis are: 5, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 2, 2
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (3, 3)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 180 degrees
Then the f(180) = -0.972548
The point is inside of the body, [TWO CONTACT POINTS]

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 0.00031842 degrees
Then the f(0.00031842) = 0.178932
The point is outside of the body, [NO CONTACT POINT]

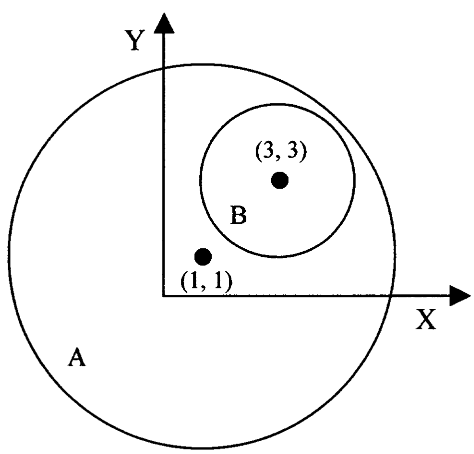


Figure 4.5 A special case with two circles.

Example 4.7 displays the results for a special case with two ellipses at a tolerance of 1E-5. In this case the overlap is big, relative with the distance between centers. Ellipse A has a length of 6 in the X axis and 10 in the Y axis. The angle of rotation is 45 degrees and the position of the center is (1, 1) in the fixed coordinate axes. Ellipse B has a length of 10 in the X axis and 6 in the Y axis. The angle of rotation is 45 degrees and the position of the center is (3, 4) in the fixed coordinate axes.

Example 4.7: Two ellipses.

Description of Ellipse A
Half Length in the X and Y Axis are: 3, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 5, 3
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (3, 4)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 219.643 degrees
Then the f(219.643) = -0.930736
The point is inside of the body, [TWO CONTACT POINTS]

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 168.585 degrees
Then the f(168.585) = 0.686508
The point is outside of the body, [NO CONTACT POINT]

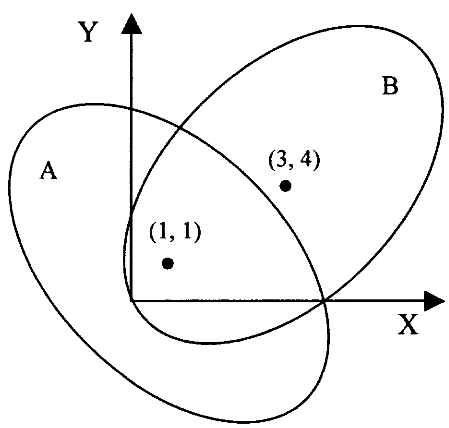


Figure 4.6 A special case with two ellipses.

4.2 Contact Detection with Penetration Distance Results

This section validates the Contact Detection With Penetration Code. Contact Detection With Penetration code uses a different method for contact detection. This method has as an advantage the easy calculation of penetration distance. Also, this method has fewer propensities to fail in unrealistic situations and does not fail at small penetration. The penetration distance is an important quantity that is needed to calculate the interacting forces.

4.2.1 No-Contact Cases

Example 4.8 shows the results for a no contact case with one ellipse and one circle at a tolerance of 1E-5. Ellipse A has a length of 8 in the X axis and 10 in the Y axis. The angle of rotation is 45 degrees and the position of the center is (1, 1) in the fixed coordinate axes. The circle has a radius of 3. The angle of rotation is 45 degrees and the position of the center is (20, 20) in the fixed coordinate axes. The penetration distance is negative which means no contact exists.

Example 4.8: One circle and one ellipse (Figure 4.2).

Description of Ellipse A
Half Length in the X and Y Axis are: 4, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 3, 3
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (20, 20)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 180 degrees
Then the f(180) = 34.6112

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 0.00031842 degrees
Then the f(0.00031842) = 57.1155

The Penetration Distance is: -19.8701
NO CONTACT EXISTS

Example 4.9 gives the results for a no contact case with two ellipses at a tolerance of 1E-5. Ellipse A has a length of 8 in the X axis and 10 in the Y axis. The angle of rotation is 45 degrees and the position of the center is (1, 1) in the fixed coordinate axes. Ellipse B has a length of 4 in the X axis and 6 in the Y axis. The angle of rotation is 45 degrees and the position of the center is (4, 8) in the fixed coordinate axes.

Example 4.9: Two ellipses.

Description of Ellipse A
Half Length in the X and Y Axis are: 4, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 2, 3
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (4, 8)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 198.961 degrees
Then the f(198.961) = 0.814199

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 14.9372 degrees
Then the f(14.9372) = 1.83336

The Penetration Distance is: -1.40822
NO CONTACT EXISTS

4.2.2 Two Contact Cases

Example 4.10 gives the results for a two contact case with two ellipses at tolerances of 1E-5 and 1E-7. These ellipses can be classified as circles. Both circles have a radius of 2 and angle of rotation of 45 degrees. The position of the center of ellipse A and ellipse B are (1, 1) and (3, 3) in a fixed coordinate axes, respectively. The penetration distance is positive (1.1716) which means contact exists.

<u>Example 4.10.a</u>: Two circles.

```
Description of Ellipse A
Half Length in the X and Y Axis are: 2, 2
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 2, 2
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (3, 3)


Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 180 degrees
Then the f(180) = -0.828427

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 0.00031842 degrees
Then the f(0.00031842) = -0.828427

The Penetration Distance is: 1.17157
CONTACT EXISTS
```

Note: Time for running code: 5

Example 4.10.b: Two circles.

Description of Ellipse A
Half Length in the X and Y Axis are: 2, 2
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 2, 2
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (3, 3)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-007
The value of ZB that minimizes the function is: 180 degrees
Then the f(180) = -0.828427

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-007
The value of ZA that minimizes the function is: 3.09413e-006 degrees
Then the f(3.09413e-006) = -0.828427

The Penetration Distance is: 1.17157
CONTACT EXISTS

Note: Time for running code: 433

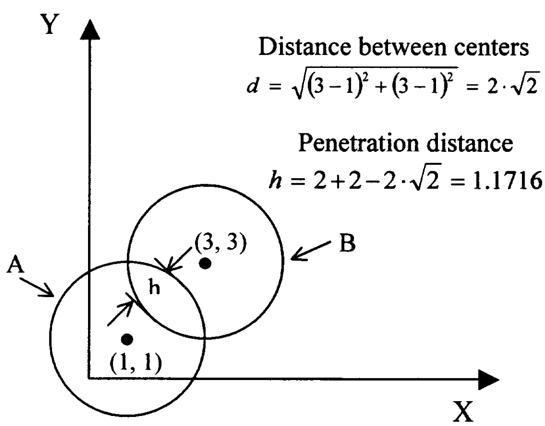


Figure 4.7 A contact case with two circles.

Example 4.11 gives the results for a two contact case with circles at a tolerance of 1E-5. Ellipse A is circle with a radius of 5 and angle of rotation of 45 degrees. The position of the center of ellipse A is (1, 1) in a fixed coordinate axes. Ellipse B is a circle with a radius of 2 and an angle of rotation of 45 degrees. The position of the center of ellipse B is (3, 3) in a fixed coordinate axes. This case is classified as special case in section 4.1.4. In this example the code is used to compute the penetration distance. Here one circle encloses the other. The penetration distance is positive (4.17157) which means contact exists.

<u>Example 4.11</u>: Two circles.

Description of Ellipse A
Half Length in the X and Y Axis are: 5, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 2, 2
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (3, 3)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 180 degrees
Then the f(180) = -0.972548

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 0.00031842 degrees
Then the f(0.00031842) = 0.178932

The Penetration Distance is: 4.17157
CONTACT EXISTS

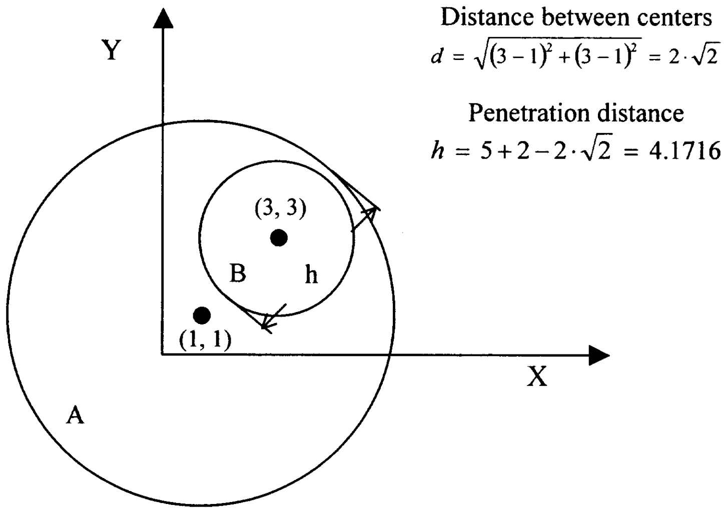


Figure 4.8 A special case of contact with two circles.

4.2.3 Special Case

Example 4.12 gives the results for a two contact case with circles at tolerances of 1E-5 and 1E-7. Ellipse A is circle with a radius of 5 and an angle of rotation of 45 degrees. The position of the center of ellipse A is (1, 1) in a fixed coordinate axes. Ellipse B is a circle with a radius of 2 and an angle of rotation of 45 degrees. The position of the center of ellipse B is (12, 12) in a fixed coordinate axes. This case is classified as special case in section 4.1.4.

Example 4.12.a: Two ellipses.

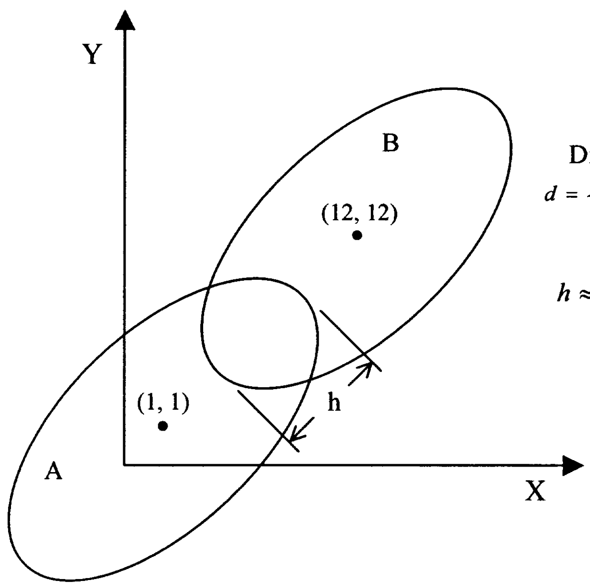
Description of Ellipse A
Half Length in the X and Y Axis are: 10, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 10, 5
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (12, 12)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 180 degrees
Then the f(180) = -0.69127

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 0.00031842 degrees
Then the f(0.00031842) = -0.69127

The Penetration Distance is: 4.44365
CONTACT EXISTS



Distance between centers

$$d = \sqrt{(12-1)^2+(12-1)^2} = 11\cdot\sqrt{2}$$

Penetration distance

$$h \approx 10+10-11\cdot\sqrt{2} = 4.4437$$

Figure 4.9 A contact case with two ellipses at 45 degrees.

Example 4.12.b: Two ellipses. Note: The ellipses have the same dimensions but in this case the distance between centers is smaller than 4.12.a. The value is not correct. It is due to the center of curvature's position, in Ellipse – B, changes in the local coordinate axes. The position is not at the end as Example 4.12.b.

```
Description of Ellipse A
Half Length in the X and Y Axis are: 10, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 10, 5
Angle of Rotation of Ellipse B: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (7, 7)


Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 180 degrees
Then the f(180) = -0.977056

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 0.00031842 degrees
Then the f(0.00031842) = -0.977056

The Penetration Distance is: -1.51472
NO CONTACT EXISTS
```

Example 4.13 gives the results for a two contact case with circles at a tolerance of 1E-5. Ellipse A has a radius of 5 and an angle of rotation of 45 degrees. The position of the center of ellipse A is (1, 1) in a fixed coordinate axes. Ellipse B has a radius of 2 and an angle of rotation of 45 degrees. The position of the center of ellipse B is (3, 3) in a fixed coordinate axes. This case is classified as special case in section 4.1.4. The same procedure is applied in Example 4.14 – 4.17 at different positions. In its the code is validated at characteristic cases.

Example 4.13: Two ellipses.

Description of Ellipse A
Half Length in the X and Y Axis are: 10, 5
Angle of Rotation of Ellipse A: 135 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (-1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 10, 5
Angle of Rotation of Ellipse B: 135 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (-12, 12)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 180 degrees
Then the f(180) = -0.69127

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 0.00031842 degrees
Then the f(0.00031842) = -0.69127

The Penetration Distance is: 4.44365
CONTACT EXISTS

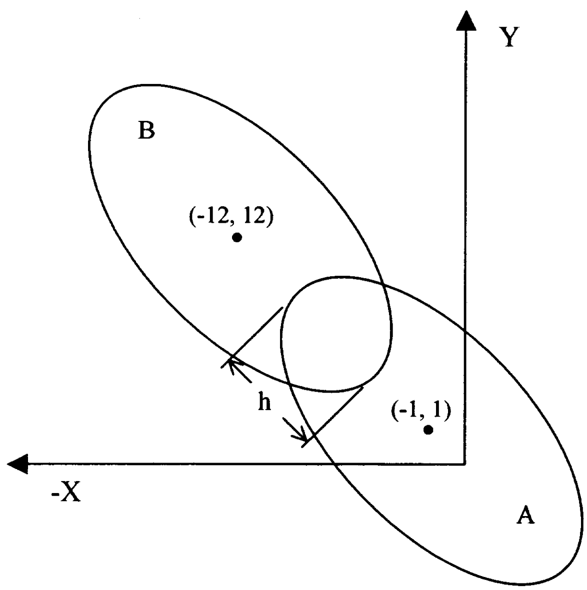


Figure 4.10 A contact case with two ellipses at 135 degrees in which centers are on the second quadrant.

Example 4.14: Two ellipses.

Description of Ellipse A
Half Length in the X and Y Axis are: 5, 3
Angle of Rotation of Ellipse A: 90 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 5, 3
Angle of Rotation of Ellipse B: 90 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 8)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 180 degrees
Then the f(180) = -0.84

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 0.00031842 degrees
Then the f(0.00031842) = -0.84

The Penetration Distance is: 3
CONTACT EXISTS

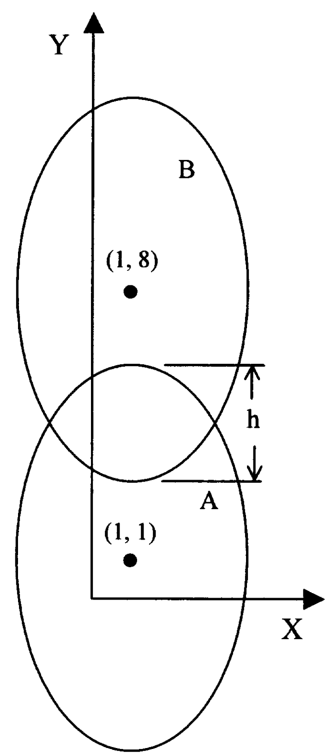


Figure 4.11 A contact case with two ellipses at 90 degrees.

Example 4.15: Two ellipses.

Description of Ellipse A
Half Length in the X and Y Axis are: 10, 5
Angle of Rotation of Ellipse A: 135 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 10,5
Angle of Rotation of Ellipse B: 135 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (4, 4)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 90 degrees
Then the f(90) = -0.977056

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 270 degrees
Then the f(270) = -0.977056

The Penetration Distance is: 5.75736
CONTACT EXISTS

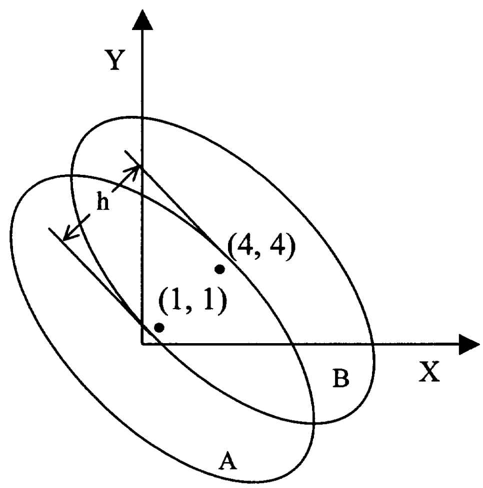


Figure 4.12 A contact case with two ellipses at 135 degrees in which centers are on the first quadrant.

<u>Example 4.16</u>: Two ellipses.

Description of Ellipse A
Half Length in the X and Y Axis are: 10, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 10, 5
Angle of Rotation of Ellipse B: 135 degrees
Position of the Ellipse Center in Fixed Coordinate Axes: (8, 8)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 90 degrees
Then the f(90) = -0.759949

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 0.00031842 degrees
Then the f(0.00031842) = -0.999596

The Penetration Distance is: 5.10051
CONTACT EXISTS

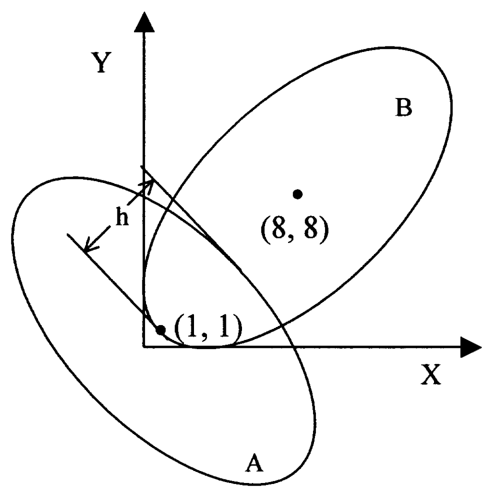


Figure 4.13 A two contact points case with two ellipse at different angles (45 degrees and 135 degrees).

Example 4.17: Two ellipses.

Description of Ellipse A
Half Length in the X and Y Axis are: 10, 5
Angle of Rotation of Ellipse A: 45 degrees
Position of the Ellipse Center in Global Coordinate Axes: (1, 1)

Description of Ellipse B
Half Length in the X and Y Axis are: 10, 5
Angle of Rotation of Ellipse B: 30 degrees
Position of the Ellipse Center in Global Coordinate Axes: (14, 15)

Function: f(XA) = (XA/aA)*(XA/aA)+(YA/bA)*(YA/bA)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZB that minimizes the function is: 203.322 degrees
Then the f(203.322) = -0.00233079

Function: f(XB) = (XB/aB)*(XB/aB)+(YB/bB)*(YB/bB)-1
Evaluated in the interval:[0, 6.28319]
Tolerance: 1e-005
The value of ZA that minimizes the function is: 13.5606 degrees
Then the f(13.5606) = -0.0026179

The Penetration Distance is: 0.0108018
CONTACT EXIST

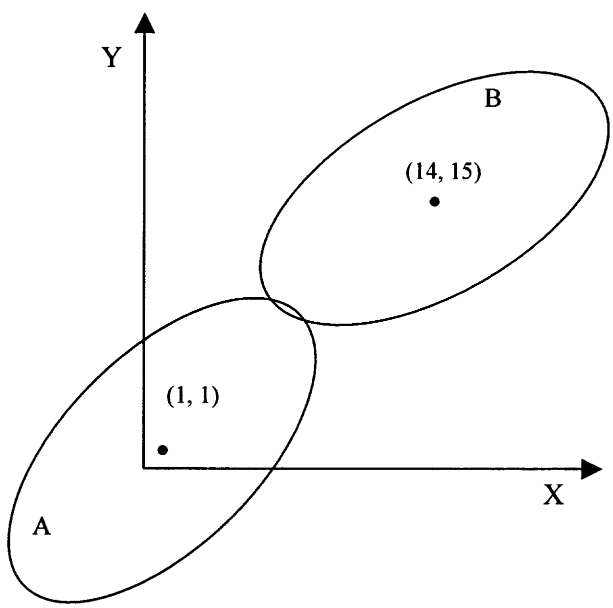


Figure 4.14 A contact case with two ellipse at different angles (45 degrees and 30 degrees).

4.3 Discussion

Both codes, Contact Detection With and Without Penetration, identified the nearest point of one elliptic curve to the center of another elliptic curve and vice versa. These two points, in the Contact Detection Without Penetration Code, are used to determine the position of the points with respect to the curves. Contact Detection With Penetration uses these two points to calculate the penetration distance. Contact Detection With Penetration Code is more robust and has more applications than that of Contact Detection Without Penetration.

The results, in Contact Detection Without Penetration, classify a special case when one ellipse is inside another ellipse. In this case, Contact Detection Without Penetration indicates as expected for one curve no contact and for the other curve two contacts. The special case can be eliminated if the code assumes automatically two contact points. Both codes do not describe the cases of ellipses that contact in more than two points. If the curves contact in more than two points, the code will indicate just two contact points. However, more than two contact points is an unrealistic physical case.

CHAPTER 5

CONCLUSIONS

In summary, the formulations in Mustoe et al. [1993 and 2000] were successfully implemented for contact detection and penetration distance. However, the formulations provided by Mustoe are incomplete. Derivation of some formulations was necessary to implement computer codes. The Contact Detection Without Penetration Code determines the contact points for realistic cases. However, the Contact Detection Without Penetration Code cannot be easily expanded to other applications. The algorithms are based on the discussed mathematical analysis proof reliability for contact detection.

The Contact Detection With Penetration Code successfully calculates the penetration distance in real cases. The penetration distance is an important value because it can be used to determine the contact points, as well as to expand the code to include the contact force.

The Contact Detection With Penetration Code is composed of eight functions, which simplify the understanding, reusability, and expansion of the code. Substantial changes in the code structure need to be performed to include many particles. Also, the application of some optimization mechanism is of importance. The formulation and the general concepts developed in this thesis will serve as the foundation for such an undertaking.

APPENDIX A

BRENT'S METHOD

This section is aimed at understanding the Brent's Method for finding a minimum. A general problem is to determine the maximum or minimum of real – valued functions. The objective is to minimize the function, but the same concept can be converted to maximization because the minimum of f (x) is the maximum of –f (x).

A.1 Unimodal Function

A Unimodal Function is a function that only has one minimum or maximum on a defined interval. The mathematical definition of unimodal [Johnson, 2002] is:

The value x^* minimizes the function f(x) which is defined in the interval [a, b]. Let x_1 and $x_2 \in [a, b]$ be such that $x_1 < x_2$, then the function is unimodal when:

- if $x_2 < x^*$ then $f(x_2) < f(x_1)$, and
- if $x_1 > x^*$ then $f(x_1) < f(x_2)$.

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- if $x_1 > x^*$ then $f(x_1) > f(x_2)$.

The unimodal assumption provides the logic for eliminating portions of [a, b] that do not contain the optimal solution. It is possible to have three cases:

Case 1: $f(x_1) > f(x_2)$. Since f(x) is unimodal, the solution cannot occur in the interval $[x_2, b]$. The solution must lie in the interval $[a, x_2)$.

Case 2: $f(x_1) < f(x_2)$. Since f(x) is unimodal, the solution cannot occur in the interval $[a, x_1)$. The solution must be in the interval $[x_1, b]$.

Case 3: $f(x_1) = f(x_2)$. The solution must lie somewhere in the interval (x_1, x_2).

A.2 Golden Section in One Dimension

The functions have to be bracketed for the interval (a, b). The function is evaluated at intermediate point x, then a new smaller interval, either (a, x) or (x, b) is found. The minimum is bracketed only when there is a triplet of points, a < b < c (or c < b < a), such that f(b) is less than f(a) and f(c). If f(b) < f(x), then the new bracketing triplet is (b, x, c). The process continues until the interval is small enough, with respect to the tolerance.

The way that the new point is selected is called golden mean or golden section. The optimal bracketing interval (a, b, c) has its middle point b a fraction distance 0.38197 from a, and 0.61803 from c. A Golden Section does not require the derivative of the function.

A.3 Parabolic Interpolation

Lagrange Polynomial to fit the three points (a, f(a)), (b, f(b)), and (c, f(c)).

$$f(x) = f(a)\cdot\frac{(x-b)\cdot(x-c)}{(a-b)\cdot(a-c)} + f(b)\cdot\frac{(x-c)\cdot(x-a)}{(b-c)\cdot(b-a)} + f(c)\cdot\frac{(x-a)\cdot(x-b)}{(c-a)\cdot(c-b)} \qquad \text{(A.1)}$$

The conditions for a minimum are $f'(x) = 0$ and $f''(x) \neq 0$.

$$f'(x) = f(a)\cdot\frac{(x-b)+(x-c)}{(a-b)\cdot(a-c)} + f(b)\cdot\frac{(x-c)+(x-a)}{(b-c)\cdot(b-a)} + f(c)\cdot\frac{(x-a)+(x-b)}{(c-a)\cdot(c-b)} = 0 \qquad \text{(A.2)}$$

Multiply by $(a-b)\cdot(b-c)\cdot(c-a)$ then is found:

$$0 = f(a)\cdot(c-b)\cdot(2x-b-c)+f(b)\cdot(a-c)\cdot(2x-c-a)+f(c)\cdot(b-a)\cdot(2x-a-b)$$

Hence, the Inverse Parabolic function that defines the abscissa x is:

$$x = b - \frac{1}{2}\cdot\frac{(b-a)^2\cdot[f(b)-f(c)]-(b-c)^2\cdot[f(b)-f(a)]}{(b-a)\cdot[f(b)-f(c)]-(b-a)\cdot[f(b)-f(a)]} \tag{A.3}$$

A.4 Brent's Method formulation in One – Dimension

Brent's Method uses a Golden Section search, switching when it is possible to successive parabolic interpolation. It uses parabolic interpolation when the process is convergent and does not leave the interval (a, b). If the function is nicely parabolic near minimum, then the parabola fitted through any three points ought to more in a single step to the minimum, or at least near it. Since the goal is the abscissa rather than the ordinate, the procedure is called inverse parabolic interpolation. The abscissa x is the minimum of a parabola through three points f(a), f(b), and f(c) as defined in Equation A.3. The formula fails only when the three points are collinear, in which case the denominator is zero.

A Golden Section search is designed to handle the worst possible case of the function minimization. In the worst possible case, the parabolic steps are acceptable but useless. The Brent's Method will alternate between parabolic steps and Golden Section. If the function F has a continuous second derivative that is positive at the minimum, then the convergence is superlinear.

A.5 Examples

Examples are provided to demonstrate the efficacy of Brent's Method at different conditions. Example A.1 and Example A.3 demonstrate the Brent's Method in unimodal and not unimodal sections of the function. Example A.2 demonstrates the Brent's Method in not unimodal sections with (1) one maximum and one minimum, and (2) two maximums and minimum.

Example A.1: Function $f(x)=x^3-2\cdot x-5$

Not Unimodal:
One maximum
One minimum

Function: f(x) = x^3 - 2*x -5
Evaluated in the interval:[-1.7, 0.816497]
Tolerance: 1e-005
The value of x that minimizes the function is: 0.81649
Then the f(0.81649) = -6.08866

Unimodal:
One minimum

Function: f(x) = x^3 - 2*x -5
Evaluated in the interval:[0, 1]
Tolerance: 1e-005
The value of x that minimizes the function is: 0.816497
Then the f(0.816497) = -6.08866

Not Unimodal:

Function: f(x) = x^3 - 2*x -5
Evaluated in the interval:[-15, 15]
Tolerance: 1e-005
The value of x that minimizes the function is: -15
Then the f(-15) = -3350

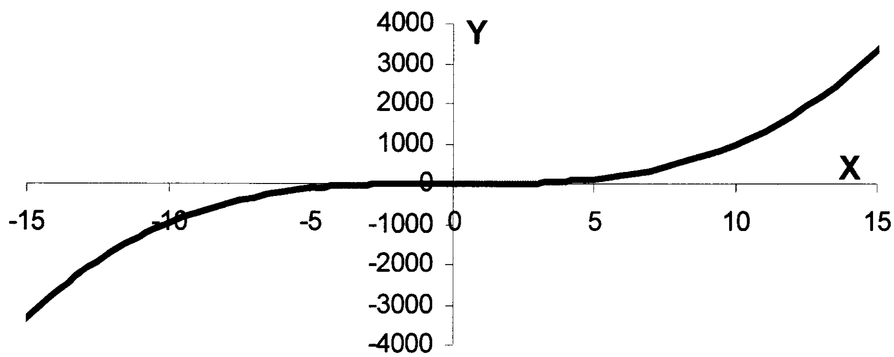

Figure A.1 Function: $f(x)=x^3-2\cdot x-5$.

<u>Example A.2</u>: Function f(x) = sin(x). This function has more than one time the same minimum value.

One maximum and one minimum:

Function: f(x) = sin(x)
Evaluated in the interval:[1, 5]
Tolerance: 1e-005
The value of x that minimizes the function is: 4.71239
Then the f(4.71239) = -1

Two maximums and two minimums:

Function: f(x) = sin(x)
Evaluated in the interval:[-5, 5]
Tolerance: 1e-005
The value of x that minimizes the function is: -1.5708
Then the f(-1.5708) = -1

Function: f(x) = sin(x)
Evaluated in the interval:[-5, 5]
Tolerance: 1e-009
The value of x that minimizes the function is: -1.5708
Then the f(-1.5708) = -1

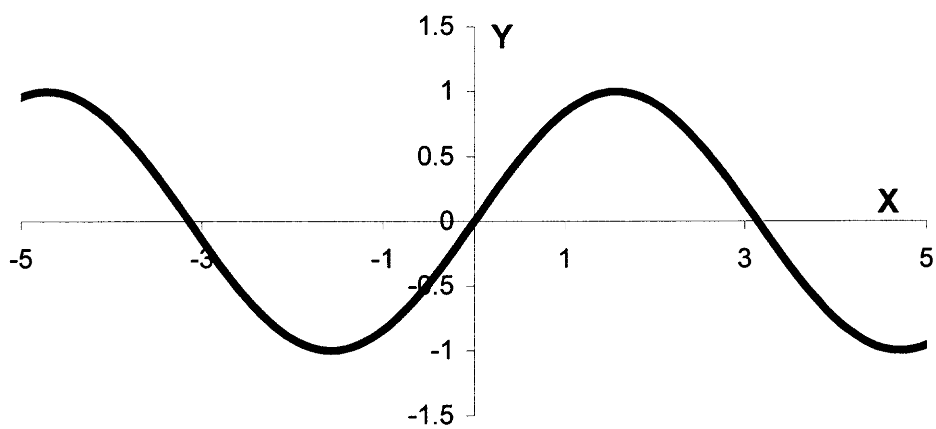

Figure A.2 Function: $f(x) = \sin x$.

Example A.3: Function $f(x)=x^4+x^3-x^2+5$

Unimodals:

Function: f(x) = x^4+x^3-x^2+5
Evaluated in the interval:[-2, -0.75]
Tolerance: 1e-005
The value of x that minimizes the function is: -1.17539
Then the f(-1.17539) = 3.90327

Function: f(x) = x^4+x^3-x^2+5
Evaluated in the interval:[0.1, 1]
Tolerance: 1e-005
The value of x that minimizes the function is: 0.425391
Then the f(0.425391) = 4.92877

Not Unimodals:

Function: f(x) = x^4+x^3-x^2+5
Evaluated in the interval:[-10, 10]
Tolerance: 1e-005
The value of x that minimizes the function is: -1.17539
Then the f(-1.17539) = 3.90327

Function: f(x) = x^4+x^3-x^2+5
Evaluated in the interval:[-20, 20]
Tolerance: 1e-005
The value of x that minimizes the function is: -0.72136
Then the f(-0.72136) = 4.37505

Function: f(x) = x^4+x^3-x^2+5
Evaluated in the interval:[-20, 20]
Tolerance: 1e-020
The value of x that minimizes the function is: -0.72136
Then the f(-0.72136) = 4.37505

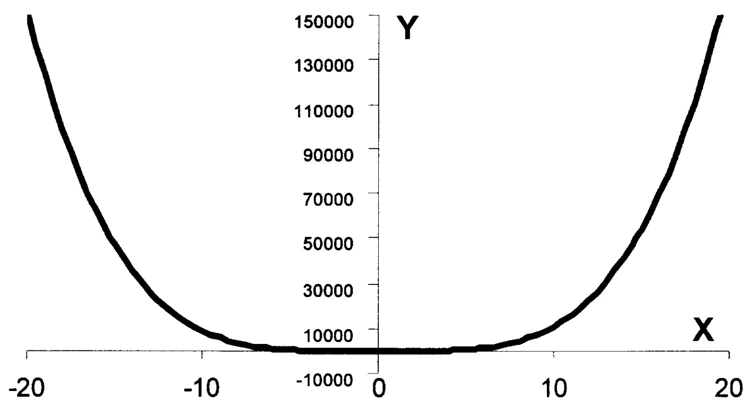

Figure A.3 Function: $f(x)=x^4+x^3-x^2+5$.

APPENDIX B

CONTACT DETECTION WITH FIXED COORDINATE AXES

This thesis uses moving coordinate axes to detect contact. This appendix aims to give another option. This option is used just the fixed coordinate axes design a formulation to detect contacts. The formulation developed has not been proved yet. First, the necessary conditions for n – intersection in a specific positions are:

$$X\left[X_i\left(\theta_i^{(1)}\right)\right] = X\left[X_j\left(\theta_j^{(1)}\right)\right],\ X\left[X_i\left(\theta_i^{(2)}\right)\right] = X\left[X_j\left(\theta_j^{(2)}\right)\right],\ \ldots, X\left[X_i\left(\theta_i^{(n)}\right)\right] = X\left[X_j\left(\theta_j^{(n)}\right)\right] \quad \text{(B.1 a)}$$

and

$$Y\left[Y_i\left(\theta_i^{(1)}\right)\right] = Y\left[Y_j\left(\theta_j^{(1)}\right)\right],\ Y\left[Y_i\left(\theta_i^{(2)}\right)\right] = Y\left[Y_j\left(\theta_j^{(2)}\right)\right],\ \ldots, Y\left[Y_i\left(\theta_i^{(n)}\right)\right] = Y\left[Y_j\left(\theta_j^{(n)}\right)\right] \quad \text{(B.1 b)}$$

These conditions can be reformulated in the next equations (Eq. B.2).

$$X\,[X_i(\theta_i)] = X\,[X_j(\theta_j)] \quad \Rightarrow \quad X\,[X_i(\theta_i)] - X\,[X_j(\theta_j)] = 0 \quad \text{(B.2 a)}$$

$$Y\,[Y_i(\theta_i)] = Y\,[Y_j(\theta_j)] \quad \Rightarrow \quad Y\,[Y_i(\theta_i)] - Y\,[Y_j(\theta_j)] = 0 \quad \text{(B.2 b)}$$

The Equations B.3 shows a representation as a function of the conditions in Equations B.2. In other to find the intersection, a root or zero finding can be implemented in the Equations B.3.

$$F\,[X_i(\theta_i), X_j(\theta_j)] \equiv X\,[X_i(\theta_i)] - X\,[X_j(\theta_j)] \quad \text{(B.3 a)}$$

$$G\,[Y_i(\theta_i), Y_j(\theta_j)] \equiv Y\,[Y_i(\theta_i)] - Y\,[Y_j(\theta_j)] \quad \text{(B.3 b)}$$

From the combination of Equations B.1, B.4, and 2.10:

$$F(\theta_i,\theta_j) \equiv \left(a_i \cdot \cos\,\theta_i \cdot \cos\,\phi_i - b_i \cdot \sin\,\theta_i \cdot \sin\,\phi_i\right) - \left(a_j \cdot \cos\,\theta_j \cdot \cos\,\phi_j - b_j \cdot \sin\,\theta_j \cdot \sin\,\phi_j\right) + \Delta X \tag{B.4 a}$$

$$G(\theta_i,\theta_j) \equiv \left(a_i \cdot \cos\,\theta_i \cdot \sin\,\phi_i + b_i \cdot \sin\,\theta_i \cdot \cos\,\phi_i\right) - \left(a_B \cdot \cos\,\theta_B \cdot \sin\,\phi_B + b_B \cdot \sin\,\theta_B \cdot \cos\,\phi_B\right) + \Delta Y \tag{B.4 b}$$

Where:

$$\Delta X = X_{Ci} - X_{Cj} \tag{B.4 c}$$

$$\Delta Y = Y_{Ci} - Y_{Cj} \tag{B.4 d}$$

These two nonlinear equations (Eq. B.4 a – b) can be solved with Newton's Method for non-linear equation. The initial guesses have to be in the range [0, 2π).

APPENDIX C

RADII OF CURVATURE FOR SUPERQUADRATICS

This appendix aims to formulate an algebraic expression for the superquadratic's radii of curvature. The definition of the superquadratic's radii of curvature should help to understand the concept and expand the program to simulate general shaped bodies. The superquadratic curve is defined as:

$$f_k \equiv \left(\frac{|x_k|}{a_k}\right)^{n_k} + \left(\frac{|y_k|}{b_k}\right)^{n_k} - 1 = 0, \quad k=i,j \tag{C.1}$$

The radii of curvatures at the two contact points P_i and P_j is given by:

$$\rho_k = \frac{\left(\left(\frac{\partial f_k}{\partial x_k}\right)^2 + \left(\frac{\partial f_k}{\partial y_k}\right)^2\right)^{3/2}}{\left(\frac{\partial^2 f_k}{\partial x_k^2}\left(\frac{\partial f_k}{\partial y_k}\right)^2 - 2\cdot\frac{\partial^2 f_k}{\partial y_k \cdot \partial x_k}\cdot\frac{\partial f_k}{\partial x_k}\cdot\frac{\partial f_k}{\partial y_k} + \frac{\partial^2 f_k}{\partial y_k^2}\cdot\left(\frac{\partial f_k}{\partial x_k}\right)^2\right)}, \quad k = i,j \tag{C.2}$$

where: $\frac{\partial f_k}{\partial x_k} = \frac{n_k \cdot |x_k|^{(n_k-1)}}{a_k^{n_k}}$, $\frac{\partial f_k}{\partial y_k} = \frac{n_k \cdot |y_k|^{(n_k-1)}}{b_k^{n_k}}$, $\frac{\partial^2 f}{\partial y\, \partial x} = 0$,

$$\frac{\partial^2 f}{\partial x^2} = n_k \cdot (n_k - 1)\cdot\frac{|x_k|^{(n_k-2)}}{a_k^{n_k}}, \quad \frac{\partial^2 f}{\partial y^2} = n_k \cdot (n_k - 1)\cdot\frac{|y_k|^{(n_k-2)}}{b_k^{n_k}}.$$

Then the radii can be represented in a simple way as shown in Equation C.3. Equation C.3 can be used to calculate the radii of curvature in a general shape particle.

$$\rho_k = \frac{\left[\frac{1}{x_k^2}\cdot\left(\frac{x_k}{a_k}\right)^{2\cdot n_k} + \frac{1}{y_k^2}\cdot\left(\frac{y_k}{b_k}\right)^{2\cdot n_k}\right]^{3/2}}{\frac{(n_k - 1)}{(a_k \cdot b_k)^{n_k}\cdot(x_k \cdot y_k)^2}\cdot\left[\left(\frac{|x_k|\cdot y_k^2}{b_k}\right)^{n_k} + \left(\frac{x_k^2 \cdot |y_k|}{a_k}\right)^{n_k}\right]}, \quad k=i,j \tag{C.3}$$

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