Chapter 2

Particle Finite Element Method in Solid Mechanics

2.1 Introduction

This chapter introduces the general concepts of continuum mechanics theory. The continuum theory and the Finite Element Method (FEM) is the background theory for Particle Finite Element Method (PFEM). Therefore, the general theory for the PFEM is founded in a well known method, the FEM. Next section is a review of the basics principles of continuum solid mechanics that are essential to understand the functioning of the new method.

2.2 Continuum Mechanics

The objective of continuum mechanics is to provide models for the macroscopic behavior of fluids, solids and structures. This chapter summarizes the main equations which govern the deformation of solids.

2.2.1 Motion and Deformation

The motion and deformation of the continua is described by kinematic relations of spatial variables. A body \( \mathcal{B} \) can be defined for a certain number of points which are in a region of the Euclidean space. Taking into account the motion of the body, the configuration \( \varphi \) has time dependence. The position of a particle \( X \) at time \( t \) in the configuration \( \varphi \) will be:

\[
x = \varphi_t (X) = \varphi (X, t)
\]  

(2.1)

\( \varphi_t \) is called the mapping form between configurations. From now on the notation is: capital letters in indices and tensors will denote reference configuration and small letters will be used to denote current configuration.
Let us define now the displacement of a material point as the difference between its current position and its original position. The displacement vector \( u(X,t) \) can be written as

\[
u(X,t) = \varphi(X,t) - X \tag{2.2}\]

This is shown in Figure II-1.

![Figure II-1. Reference and current configurations](image)

**Time derivatives**

Most nonlinear problems are time dependent. There are complete time-dependent processes, like a contact problem, but also nonlinear problems where the constitutive relations are time-dependent or history-dependent, such as in the case of friction between solid materials.

Computing the material time derivatives of the kinematical quantities the velocity and acceleration of a material point are obtained

\[
\begin{align*}
\dot{u}(X,t) &= v(X,t) = \frac{\partial \varphi}{\partial t}(X,t) = \dot{\varphi}(X,t) \\
\ddot{u}_0(X,t) &= a(X,t) = \ddot{\varphi}(X,t) = \ddot{v}(X,t)
\end{align*}
\tag{2.3}
\tag{2.4}
\]

**Description of the deformation**

The description of the deformation is an essential part of nonlinear mechanics. To describe the deformation process locally the deformation gradient \( F \) is introduced. The deformation gradient is the tensor that associates to a material line element \( dX \) in \( B \) the line element \( dx \) in \( \varphi(B) \)

\[
dx = F dX \tag{2.5}
\]
In the terminology of mathematics, the deformation gradient $F$ is the Jacobian matrix of the motion $\varphi (X,t)$.

To preserve the continuous structure of $\mathcal{B}$ during the deformation, the mapping has to be one-to-one; this means that $F$ cannot be singular. This is equivalent to the condition

$$J = \det F \neq 0$$

where $J$ is the Jacobian determinant.

2.2.2 Strain measures

Different strain measures are used in non linear continuum mechanics. In this section the more usual measures of strain will be explained. One of the most common ones of the right Cauchy-Green tensor $\mathcal{C}$, defined in the initial configuration $\mathcal{B}$ as

$$\mathcal{C} = F^T F$$

(2.7)

In the initial state $F = 1$ then this strain measure is $\mathcal{C} = 1$, to denote the strain in the initial configuration it is convenient to introduce the Green-Lagrange strain tensor $E$

$$E = \frac{1}{2} (F^T F - 1) = E = \frac{1}{2} (\mathcal{C} - 1)$$

(2.8)

With respect to the current configuration the Almansi strain tensor is often used. This is defined as

$$e = \frac{1}{2} (1 - b^{-1})$$

(2.9)

Where tensor $b$ is denoted as the left Cauchy-Green tensor

$$b = F^T F$$

(2.10)

The Almansi strain tensor is connected with the Green-Lagrange strain tensor via the following transformation

$$E = F^T e F$$

(2.11)
Vector and tensor transformations

Two operations must be defined: the pull back operation, that means the transformation between the differential elements from the current to the reference configuration, and the push forward operation which is the transformation in the opposite direction, from the initial to the current configuration.

2.2.3 Stress measures

The most known stress tensor is the Cauchy stress tensor that is denoted by $\sigma$. It is a magnitude expressed in the current configuration $\varphi (B)$. The Cauchy theorem defines the meaning of the stresses. The relation between the traction vector $t$ and the surface normal vector $n$ is

$$
t = \sigma^T n,
$$

\begin{bmatrix}
t_1 \\
t_2 \\
t_3
\end{bmatrix} =
\begin{bmatrix}
\sigma_{11} & \sigma_{12} & \sigma_{13} \\
\sigma_{21} & \sigma_{22} & \sigma_{23} \\
\sigma_{31} & \sigma_{32} & \sigma_{33}
\end{bmatrix} \begin{bmatrix}
 n_1 \\
n_2 \\
n_3
\end{bmatrix}
\tag{2.12}

From the local balance of angular momentum we obtain

$$
\sigma = \sigma^T
$$
\tag{2.13}

i.e. $\sigma$ is a symmetric tensor. There are other stress measures equivalent to the Cauchy stress tensor and expressed in the initial configuration $B$. To define them, an equivalence of a force defined in $B$ and $\varphi (B)$ is done. A pull back of the stress measures is written as

$$
\int_{\partial B(r)} \sigma n \, dA = \int_{\partial B} \sigma J F^{-T} N \, dA = \int_{\partial B} P N \, dA
$$
\tag{2.14}

Last relation defines the first Piola-Kirchhoff stress tensor $P$

There is a symmetric stress tensor which is defined with regard to the reference configuration. This is the second Piola-Kirchhoff stress tensor $S$

$$
S = F^{-1} P = J F^{-1} \sigma F^{-T}
\tag{2.15}$$
\(\mathbf{S}\) does not denote an experimentally measurable stress but it is an essential stress measure that plays an important role in the constitutive theory. First, it is the complete pull back of the Cauchy stress tensor to the reference configuration \(\mathcal{B}\). Second, and most important property, it is “work conjugate” (duality paired) with the Green-Lagrange strain tensor of equation (2.8).

Instead of the Cauchy stress tensor \(\sigma\), the Kirchhoff stress tensor \(\tau\) is often employed. It is defined as the pushes forward of the second Piola-Kirchhoff stress tensor \(\mathbf{S}\) to the current configuration.

\[
\tau = F \mathbf{S} F^T, \quad \tau = J \sigma
\]  

(2.16)

2.3 Lagrangian formulation

2.3.1 Balance laws

The physical system must satisfy a group of fundamental laws. The equations that describe the mechanical behavior of the continuum arise from this group of laws. They are called balance laws or conservation laws usually expressed as partial differential equations.

Mass conservation

The mass conservation principle requires that the mass of any material domain remains constant. There is no material flow through the boundaries of a material domain and there is no mass loss to energy conversion. The balance of the mass \(m\) of a body is given by the equation

\[
m = \int_{\partial B} \rho_0 dV = \int_{\partial \mathcal{B}} \rho dV = \text{const.}
\]  

(2.17)

Where \(\rho_0\) is the density in the initial configuration and \(\rho\) the density in the current configuration. With a Langragian description and assuming sufficient smoothness, the next equation can be given for mass conservation

\[
\rho (X,t) J (X,t) = \rho_0 (X,t)
\]  

(2.18)
Local balance of momentum and angular momentum

The balance of momentum principle is the equivalent of Newton’s second law of motion, which relates the forces acting on a body to its acceleration. The equation of local balance of momentum with respect to a volume in the current configuration $\varphi (B)$ can be written as

$$\frac{\partial \sigma}{\partial t} + \rho b = \rho \ddot{u} \tag{2.19}$$

where $\sigma$ is the Cauchy stress tensor, $\rho b$ define the volume or body forces (e.g. gravitational force), and $\rho \ddot{u}$ is the inertial force term. For the static analysis, where the loads are applied slowly, the inertial forces can be neglected. The resulting equation is called the equilibrium equation

$$\nabla \sigma + \rho b = 0 \tag{2.20}$$

The local balance of angular momentum in the absence of micro polar stresses, which is usually the case in non-magnetic materials, yields to

$$\sigma = \sigma^T \tag{2.21}$$

This equation re-expresses the symmetry of the Cauchy stress tensor.

First law of thermodynamics

This law expresses the principle of conservation of the energy of a thermodynamical process. The first law of thermodynamics postulates that the rate of change of total energy $\dot{E}$ is induced by the work done by body forces and surface forces, the mechanical power $P$ and the heat transfer $Q$ into the system. The statement of the conservation of the energy is

$$\dot{E} = P + Q \tag{2.22}$$

Where the mechanical power $P$ is defined by

$$P = \frac{d}{dt} \left[ \int_{\varphi(B)} \frac{1}{2} \rho \boldsymbol{v} \cdot \boldsymbol{v} \, dV + \int_{\varphi(B)} \sigma \cdot \mathbf{d} \right] \tag{2.23}$$
The first integral expresses is the material time derivate of the kinetic energy and the second one of the work performed by the Cauchy stress tensor over the symmetrical spatial velocity gradient $d$. The term $\sigma \cdot d$ contributes to the internal energy.

The heat transfer input into the system has the expression

$$ Q = - \int_{\partial B} \mathbf{q} \cdot \mathbf{n} \, da + \int_B \rho \mathbf{r} \, dv $$

(2.24)

The integrals represent two sources of energy. The first one is the heat transfer through the surface of the body, described by the heat flux vector $\mathbf{q}$ and the surface normal $\mathbf{n}$. The second integral is the heat induced by the internal heat source $\mathbf{r}$.

2.4 Discretization of the continuum

The discrete equations for the updated lagrangian formulation are obtained with a finite element model, which uses interpolations for the test and trial functions. The domain $\varphi (B)$ is subdivided into elements $e$ from 1 to $n_e$. The domain in each element is denoted by $\varphi(\Omega_e)$.

$$ \varphi(B) = \bigcup_{e=1}^{n_e} \varphi(\Omega_e) $$

(2.25)

Each element $\varphi(\Omega_e)$ has a certain number of nodes $n_n$. Each node has a spatial position in the current configuration $x_I$, where $I = 1$ to $n_n$. Nodes define the connection between elements for the assembly of the domain. Most boundary conditions are imposed on nodes.

2.4.1 Isoparametric concept

The interpolation of any variable $u$ is written in term of the nodal values of the shape functions $N_I$ in the studied manner

$$ u(X,t) = \sum_{I=1}^{n_n} N_I(X)u_I(t) $$

(2.26)

$N_I(X)$ are $C^0$ interpolants which satisfy the condition

$$ N_I(X,J) = \delta_{IJ} $$

(2.27)

where $\delta_{IJ}$ is the Kronecker delta.
The finite element model uses the isoparametric concept for the geometry. That means that shape functions are expressed in the parent configuration instead of the current configuration. The parent configuration is an elemental configuration defined with the natural coordinates of the element. The natural coordinates define the geometry of the element by an orthogonal base that normalizes the shape functions. The coordinates in the current configuration are defined as

$$x_c = \sum_{i=1}^{n_n} N_I(\xi) x_i$$

(2.28)

This equation is the basis for transforming the geometry from a configuration to another following standard transformation rules.

Figure II-2. Isoparametric description of deformation

**Derivatives of the functions**

The spatial derivatives are obtained by implicit differentiation because the functions are usually not explicitly invertible respect to the natural coordinates of the parent configuration. The chain rule is used in this case for computing the derivatives

$$\nabla_{\xi} N_I = \frac{\partial N_I}{\partial \xi} = \frac{\partial N_I}{\partial x} \frac{\partial x}{\partial \xi}$$

(2.29)
where

\[
\frac{\partial \mathbf{x}}{\partial \xi} = \sum_{j=1}^{n_n} N_{I, \xi}(\xi) \mathbf{x}_I \otimes \mathbf{E}_\xi
\]  

(2.30)

being \( \frac{\partial \mathbf{x}}{\partial \xi} \) the Jacobian of the map between the current configuration of the element and the parent element configuration. It is denoted as

\[
\mathbf{J}_e = \text{Grad}_\xi \mathbf{x}_e = \frac{\partial \mathbf{x}}{\partial \xi} = \sum_{j=1}^{n_n} \mathbf{x}_I \otimes N_{I, \xi}(\xi) \mathbf{E}_\xi
\]  

(2.31)

The derivatives of the functions between configurations can be written as

\[
\nabla_\xi \mathbf{N}_I = \mathbf{J}_e^T \nabla_\mathbf{x} \mathbf{N}_I
\]  

(2.32)

The gradient of a vector field \( \mathbf{u}_e \) respect to the current configuration \( \mathbf{x} \) will be expressed as

\[
\text{grad} \mathbf{u}_e = \sum_{j=1}^{n_n} \mathbf{u}_I \otimes \mathbf{J}_e^{-T} \nabla_\xi \mathbf{N}_I
\]  

(2.33)

Note that in all cases \( \mathbf{J}_e \) is the Jacobian between the parent and the current configuration. The transformation also can be made from the parent to the reference configuration. The Jacobian in this case is expressed as

\[
\mathbf{J}_e = \text{Grad}_\xi \mathbf{X}_e = \frac{\partial \mathbf{X}}{\partial \xi} = \sum_{j=1}^{n_n} \mathbf{X}_I \otimes N_{I, \xi}(\xi) \mathbf{E}_\xi
\]  

(2.34)

The gradient of vector field \( \mathbf{u}_e \) respect to the reference configuration \( \mathbf{X} \) has the form
\[
\text{Grad } u_e = \sum_{I=1}^{n_e} u_I \otimes J_e^{-T} \nabla_\xi N_I
\]

(2.35)

where

\[
\nabla_\xi N_I = J_e^{T} \nabla_x N_I
\]

(2.36)

The deformation gradient of an element can be expressed as a function of the transformation jacobians between the parent and the spatial configurations

\[
F_e = J_e \cdot J_e^{-1} \quad J_e = \text{det } F_e = \frac{\text{det } J_e}{\text{det } J_e}
\]

(2.37)

2.4.2 Shape Functions

Vector fields in the discretization with finite elements are approximated with the shape functions. The shape functions or interpolation functions are related to the dimension of the problem and the characteristics of the used element. The most simple and common element in two dimensions is the linear triangle. On the other hand, in three dimensions the simplest element is the linear tetrahedral.

Linear Triangle (2D)

The linear triangle has three nodes. Figure II-3 shows the element at the \( \xi \) and \( \eta \) natural coordinates in the present configuration \( \Omega_{ij} \).

![Figure II-3. Linear triangle, 3 nodes](image-url)
The shape functions for the linear triangle are
\[ N_1 = 1 - \xi - \eta, \quad N_2 = \xi, \quad N_3 = \eta \]  
(2.38)

The computation of the derivatives of the shape functions respect or the current configuration for an element \( \Omega_e \) is expressed by
\[ \nabla_x N_I = \begin{pmatrix} N_I,1 \\ N_I,2 \\ N_I,3 \\ N_I,\xi \\ N_I,\eta \\ N_I,\zeta \end{pmatrix} = j_e^{-T} \begin{pmatrix} N_I,1 \\ N_I,2 \\ N_I,3 \\ N_I,\xi \\ N_I,\eta \\ N_I,\zeta \end{pmatrix} \]
(2.39)

with \( j_e \) the jacobian matrix for the transformation between the current and the parent configurations.

**Linear Tetrahedra (3D)**

The linear tetrahedra has four nodes. Natural coordinates of the linear tetrahedral are shown in Figure II-4.

![Figure II-4. Linear Tetrahedra, 4 nodes](image)

The shape functions for the linear tetrahedral are
\[ N_1 = 1 - \xi - \eta - \zeta, \quad N_2 = \xi, \quad N_3 = \eta, \quad N_4 = \zeta \]  
(2.40)

The computation of the derivatives of the shape functions respect to the current configuration is given by
\[ \nabla_x N_I = \begin{pmatrix} N_I,1 \\ N_I,2 \\ N_I,3 \\ N_I,\xi \\ N_I,\eta \\ N_I,\zeta \end{pmatrix} = j_e^{-T} \begin{pmatrix} N_I,1 \\ N_I,2 \\ N_I,3 \\ N_I,\xi \\ N_I,\eta \\ N_I,\zeta \end{pmatrix} \]
(2.41)
In three dimensions the jacobian matrix has the expression

\[
J_e = \sum_{I=1}^{n_n} x_I \otimes \nabla_{x^I} N_I = \begin{bmatrix}
    x_{1,\xi} & x_{1,\eta} & x_{1,\zeta} \\
    x_{2,\xi} & x_{2,\eta} & x_{2,\zeta} \\
    x_{3,\xi} & x_{3,\eta} & x_{3,\zeta}
\end{bmatrix}
\]  

(2.42)