APPENDIX I

METHOD OF LEAST SQUARE

*The Method of Least Square can be used to Approximately Solve a Set of **N** Equations with **M** Unknowns*

I.1 SIMPLE EXAMPLE

In experimental mechanics, it is very common to obtain a large amount of data that cannot be exactly defined by a simple analytical function. For example, consider the following four (N) data points:

Table I.1 Four Data Points

x	y
0.00	1.0
0.75	0.6
1.50	0.3
2.00	0.0

Now let us approximate the data with the following linear function with two *(M)* unknown constants:

$$c_1 + c_2 x = y(x) \tag{I.1}$$

If this equation is evaluated at the four data points, the following ***observational equations*** are obtained:

$$\begin{aligned} c_1 &= 1.0 \\ c_1 + 0.75\,c_2 &= 0.6 \\ c_1 + 1.50\,c_2 &= 0.3 \\ c_1 + 2.00\,c_2 &= 0.0 \end{aligned} \tag{I.2}$$

These four equations can be written as the following matrix equation:

$$\begin{bmatrix} 1.0 & 0.00 \\ 1.0 & 0.75 \\ 1.0 & 1.50 \\ 1.0 & 2.00 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 1.0 \\ 0.6 \\ 0.3 \\ 0.0 \end{bmatrix} \quad \text{Or, symbolically as} \quad \mathbf{Ac} = \mathbf{b} \tag{I.3}$$

Equation I.3 cannot be solved exactly because the four equations have two unknowns. However, both sides of the equation can be multiplied by $\mathbf{A}^{\mathbf{T}}$ and the following two equations in terms of two unknowns are produced:

$$\mathbf{A}^{\mathbf{T}}\mathbf{Ac} = \mathbf{A}^{\mathbf{T}}\mathbf{b} \qquad \text{Or,} \quad \begin{bmatrix} 4.00 & 4.25 \\ 4.25 & 6.81 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 1.9 \\ 0.9 \end{bmatrix} \tag{I.4}$$

The solution of this symmetric set of equations is:

$$\begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} 0.992 \\ -0.487 \end{bmatrix} \tag{I.5}$$

It is apparent that the error, which is the difference between the values at the data points and the values produced by the approximate equation, can be calculated from:

$$\mathbf{e} = \mathbf{Ac} - \mathbf{b} \quad = \begin{bmatrix} -.008 \\ +.035 \\ -.030 \\ -.018 \end{bmatrix} \tag{I.6}$$

I.2 GENERAL FORMULATION

It will be shown in this section that the ad hoc approach, presented in the previous section, produces results in which ***the sum of the square of the errors at the data points*** is a minimum. The error vector can be written as:

$$\mathbf{e} = \mathbf{Ac} - \mathbf{b} \quad \text{or,} \quad \mathbf{e}^{\mathbf{T}} = \mathbf{c}^{\mathbf{T}}\mathbf{A}^{\mathbf{T}} - \mathbf{b}^{\mathbf{T}} \tag{I.7}$$

It is now possible to calculate the sum of the square of the errors, a scalar value S, from the following matrix equation:

$$S = \mathbf{e}^{\mathbf{T}}\mathbf{e} = \mathbf{c}^{\mathbf{T}}\mathbf{A}^{\mathbf{T}}\mathbf{A}\,\mathbf{c} - \mathbf{b}^{\mathbf{T}}\mathbf{Ac} - \mathbf{c}^{\mathbf{T}}\mathbf{A}^{\mathbf{T}}\mathbf{b} + \mathbf{b}^{\mathbf{T}}\mathbf{b} = \mathbf{c}^{\mathbf{T}}\mathbf{H}\,\mathbf{c} - 2\mathbf{c}^{\mathbf{T}}\mathbf{B}^{\mathbf{T}} + \mathbf{b}^{\mathbf{T}}\mathbf{b} \tag{I.8}$$

From basic mathematical theory, the minimum value S must satisfy the following M equations:

$$\frac{\partial S}{\partial c_m} = 0 \quad \text{where} \, m = 1 - - - - M \tag{I.9}$$

Application of Equation (I.9) to Equation (I.8) yields the following typical matrix equation in which each term is a scalar:

$$\frac{\partial S}{\partial c_m} = \begin{bmatrix} 0 & 0 & - & 1 & - & 0 \end{bmatrix} \mathbf{Hc} + \mathbf{c}^{\mathbf{T}} \mathbf{H}^{\mathbf{T}} \begin{bmatrix} 0 \\ 0 \\ - \\ 1 \\ - \\ 0 \end{bmatrix} + \tag{I.10}$$

$$2\begin{bmatrix} 0 & 0 & - & 1 & - & 0 \end{bmatrix} \mathbf{B} = 2\begin{bmatrix} 0 & 0 & - & 1 & - & 0 \end{bmatrix} [\mathbf{Hc} - \mathbf{B}] = 0$$

Hence, all M equations can be written as the following matrix equation:

$$\begin{bmatrix} \frac{\partial S\Omega}{\partial c_1} \\ \frac{\partial S\Omega}{\partial c_2} \\ - \\ \frac{\partial S\Omega}{\partial c_m} \\ - \\ \frac{\partial S\Omega}{\partial c_M} \end{bmatrix} = \begin{bmatrix} \mathbf{1} & \mathbf{0} & - & \mathbf{0} & - & \mathbf{0} \\ \mathbf{0} & \mathbf{1} & - & \mathbf{0} & - & \mathbf{0} \\ - & - & - & - & - & - \\ \mathbf{0} & \mathbf{0} & - & \mathbf{1} & - & \mathbf{0} \\ - & - & - & - & - & - \\ \mathbf{0} & \mathbf{0} & - & \mathbf{0} & - & \mathbf{1} \end{bmatrix} [2\mathbf{Hc} - 2\mathbf{B}] = 2\mathbf{I}[\mathbf{Hc} - \mathbf{B}] = [\mathbf{0}] \tag{I.11}$$

Therefore, the vector of constants $\mathbf{c}$ can be determined from the solution of the following matrix equation:

$$\mathbf{Hc} = \mathbf{B} \tag{I.12}$$

Because the positive-definite symmetric matrix $\mathbf{H} = \mathbf{A}^{\mathbf{T}}\mathbf{A}$ and $\mathbf{B} = \mathbf{A}^{\mathbf{T}}\mathbf{b}$, the multiplication of the observational equations by $\mathbf{A}^{\mathbf{T}}$ produces the same set of equations. Therefore, it is not necessary to perform the formal minimization procedure each time one uses the least square method.

I.3 CALCULATION OF STRESSES WITHIN FINITE ELEMENTS

The basic equilibrium equation of a finite element system, as produced by the application of the principle of minimum potential energy, can be written as a summation of element contributions in the following form:

$$\mathbf{R} = \sum_{i=1}^{\#elements} \mathbf{k}_i \mathbf{u} = \sum_{i=1}^{\#elements} \mathbf{f}_i \tag{I.13}$$

where $\mathbf{k}_i$ is a typical element stiffness, $\mathbf{u}$ is the element node displacements and $\mathbf{f}_i$ is the element nodal forces, or stress resultants. The external node loads $\mathbf{R}$ are the specified point loads, the body forces that are integrated over the element volume, the consistent nodal loads associated with surface tractions and thermal loads. Those external nodal loads are in exact equilibrium with the sum of the forces acting on the elements.

The original development of the finite element method was presented as an extension of structural analysis in which node point equilibrium was the fundamental starting point. Therefore, the accuracy of the element nodal forces was apparent. Unfortunately, the use of abstract variational methods in modern computational mechanics has tended to make this very important equilibrium property obscure. Hence, using virtual work and the method of least square, one can calculate element stresses directly from nodal forces.

The consistent stresses within a finite element, developed using displacement functions, normally do not satisfy the fundamental equilibrium equations. From Equation (2.1), the three-dimensional equilibrium equations, written in a global x, y, and z reference system, are:

$$\begin{aligned}
&\frac{\partial \sigma_x}{\partial x} + \frac{\partial \tau_{xy}}{\partial y} + \frac{\partial \tau_{xz}}{\partial z} = 0 \\
&\frac{\partial \tau_{yx}}{\partial x} + \frac{\partial \sigma_y}{\partial y} + \frac{\partial \tau_{yz}}{\partial z} = 0 \\
&\frac{\partial \tau_{zx}}{\partial x} + \frac{\partial \tau_{zy}}{\partial y} + \frac{\partial \sigma_z}{\partial z} = 0
\end{aligned} \tag{I.14}$$

Those equations, which are fundamental laws of physics, are always exactly satisfied within a real structure; therefore, it is very important that the stress distribution calculated within elements of a finite element system satisfy those equations. To accomplish that objective for three-dimensional solids, the assumed stress distribution satisfies those equations and is of the following form:

$$\begin{aligned}
\sigma_x &= c_1 - (c_{12} + c_{17})x + c_3 y + c_3 z \\
\sigma_y &= c_4 + c_5 x - (c_{11} + c_{21})y + c_3 y + c_6 z \\
\sigma_x &= c_7 + c_8 x + c_9 y - (c_{15} + c_{20})z \\
\tau_{xy} &= c_{10} + c_{11} x + c_{12} y + c_{13} z \\
\tau_{xz} &= c_{14} + c_{15} x + c_{16} y + c_{17} z \\
\tau_{yz} &= c_{18} + c_{19} x + c_{20} y + c_{21} z
\end{aligned} \qquad \text{or, } \mathbf{s} = \mathbf{Pc} \tag{I.15}$$

where $\mathbf{P}$ is a 6 by 21 array that is a function of the global x, y and z reference system.
The element node forces can be expressed in terms of the assumed stress distribution by the direct application of the principle of virtual work in which the virtual displacements $\bar{\mathbf{d}}$ are of the same form as the basic displacement approximation. Or, from Equation (6.3), the virtual displacements, including incompatible modes, are:

$$\bar{\mathbf{d}} = \begin{bmatrix} \mathbf{B_C} & \mathbf{B_I} \end{bmatrix} \begin{bmatrix} \bar{\mathbf{u}} \\ \overline{\alpha} \end{bmatrix} \tag{I.16}$$

If the virtual and incompatible displacements are all set to one, the following equation can be used to calculate node forces for an eight-node solid element:

$$\mathbf{f} = \begin{bmatrix} \mathbf{f_i} \\ \mathbf{0} \end{bmatrix} = \int_{Vol} \bar{\mathbf{d}}^{\mathbf{T}} \mathbf{s} \, dV = \left[\int_{Vol} \begin{bmatrix} \mathbf{B_C^T} \\ \mathbf{B_I^T} \end{bmatrix} \mathbf{P} \, dV \right] \mathbf{c} = \mathbf{Q}\mathbf{c} \tag{I.17}$$

The 33 by 21 matrix $\mathbf{Q}$ is calculated using standard numerical integration. The forces associated with the nine incompatible modes are zero.
The system of equations is approximately solved by the least square method, which involves the solution of:

$$\mathbf{Q}^T\mathbf{Q}\mathbf{c} = \mathbf{Q}^T\mathbf{f} \quad \text{or} \quad \mathbf{H}\mathbf{c} = \mathbf{B} \tag{I.18}$$

After $\mathbf{c}$ is evaluated for each load condition, the six components of stress at any point (x,y,z) within the element can be evaluated from Equation (I.15).