AE/ME 339
Computational Fluid Dynamics (CFD)

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The basic idea behind grid generation is the creation of the transformation laws between the physical space and the computational space.

These laws are known as the *metrics* of the transformation.

We have already performed a simple grid generation without realizing it for the flow over a heated wall when we used the $\tau$, $\xi$, $\eta$ coordinates for the numerical scheme. This was simply a transformation from one rectangular domain to another rectangular domain.
Grid Generation (Chapter 5)

Quality of the CFD solution is strongly dependent on the quality of the grid.
Why is grid generation necessary? Figure 5.1(next slide) can be used to explain.
Note that the standard finite difference methods require a uniformly spaced rectangular grid.
If a rectangular grid is used, few grid points fall on the surface.
Flow close to the surface being very important in terms of forces, heat transfer, etc., a rectangular grid will give poor results in such regions.
Also uniform grid spacing often does not yield accurate solutions.

Typically, the grid will be closely spaced in boundary layers.
FIG. 5.1
An airfoil in a purely rectangular grid.
Figure shows a physical flow domain that surrounds the body and the corresponding rectangular flow domain. Note that if the airfoil is cut and the surface straightened out, it would form the $\xi$-axis. Similarly, the outer boundary would become the top boundary of the computational domain. The left and right boundaries of the computational domain would represent the cut surface. Note the locations of points a, b, and c in the two figures.
Note that in the physical space the cells are not rectangular and the grid is uniformly spaced. There is a one-to-one correspondence between the physical space and the computational space. Each point in the computational space represents a point in the physical space.

The procedure is as follows:

1. Establish the necessary transformation relations between the physical space and the computational space
2. Transform the governing equations and the boundary conditions into the computational space.
3. Solve the equations in the computational space using the uniformly spaced rectangular grid.
4. Perform a reverse transformation to represent the flow properties in the physical space.
General Transformation Relations
Consider a two-dimensional unsteady flow with independent variables
$\tau$, $x$, $y$.

The variables in the computational domain are represented by $\tau$, $\xi$, $\eta$, and

The relations between the two sets of variables can be represented as follows.

\[ \tau = \tau(t) \] \hspace{1cm} (5.1c)

\[ \xi = \xi(x, y, t) \] \hspace{1cm} (5.1a)

\[ \eta = \eta(x, y, t) \] \hspace{1cm} (5.1b)
The derivatives appearing in the governing equations must be transformed using the chain rule of differentiation.

\[
\left( \frac{\partial}{\partial x} \right)_{y,t} = \left( \frac{\partial}{\partial \xi} \right)_{\eta,\tau} \left( \frac{\partial \xi}{\partial x} \right)_{y,t} + \left( \frac{\partial}{\partial \eta} \right)_{\xi,\tau} \left( \frac{\partial \eta}{\partial x} \right)_{y,t} + \left( \frac{\partial}{\partial \tau} \right)_{\xi,\eta} \left( \frac{\partial \tau}{\partial x} \right)_{y,t}
\]

The subscripts are used to emphasize significance of the partial derivatives and they will not be included in the equations that follow.
\[
\left( \frac{\partial}{\partial x} \right) = \left( \frac{\partial}{\partial \xi} \right) \left( \frac{\partial \xi}{\partial x} \right) + \left( \frac{\partial}{\partial \eta} \right) \left( \frac{\partial \eta}{\partial x} \right) \tag{5.2}
\]

\[
\left( \frac{\partial}{\partial y} \right) = \left( \frac{\partial}{\partial \xi} \right) \left( \frac{\partial \xi}{\partial y} \right) + \left( \frac{\partial}{\partial \eta} \right) \left( \frac{\partial \eta}{\partial y} \right) \tag{5.3}
\]

\[
\left( \frac{\partial}{\partial t} \right)_{x,y} = \left( \frac{\partial}{\partial \xi} \right)_{\eta,\tau} \left( \frac{\partial \xi}{\partial t} \right)_{x,y} + \left( \frac{\partial}{\partial \eta} \right)_{\xi,\tau} \left( \frac{\partial \eta}{\partial t} \right)_{x,y} + \left( \frac{\partial}{\partial \tau} \right)_{\xi,\eta} \left( \frac{\partial \tau}{\partial t} \right)_{x,y} \tag{5.4}
\]

\[
\left( \frac{\partial}{\partial t} \right) = \left( \frac{\partial}{\partial \xi} \right) \left( \frac{\partial \xi}{\partial t} \right) + \left( \frac{\partial}{\partial \eta} \right) \left( \frac{\partial \eta}{\partial t} \right) + \left( \frac{\partial}{\partial \tau} \right) \left( \frac{\partial \tau}{\partial t} \right) \tag{5.5}
\]
The first derivatives in the governing equations can be transformed using Eqs. (5.2), (5.3) and (5.5).

The coefficients of the transformed derivatives such as the ones given below are known *metrics*.

\[
\frac{\partial \xi}{\partial x}, \frac{\partial \xi}{\partial y}, \frac{\partial \eta}{\partial x}, \frac{\partial \eta}{\partial y}
\]

Similarly, chain rule should be used to transform higher order derivatives. Example:

\[
\frac{\partial^2}{\partial x^2} = \left( \frac{\partial}{\partial \xi} \right) \left( \frac{\partial^2 \xi}{\partial x^2} \right) + \left( \frac{\partial}{\partial \eta} \right) \left( \frac{\partial^2 \eta}{\partial x^2} \right) + \left( \frac{\partial^2}{\partial \xi^2} \right) \left( \frac{\partial \xi}{\partial x} \right)^2 \\
\quad + \left( \frac{\partial^2}{\partial \eta^2} \right) \left( \frac{\partial \eta}{\partial x} \right)^2 + 2 \left( \frac{\partial^2}{\partial \eta \partial \xi} \right) \left( \frac{\partial \eta}{\partial x} \right) \left( \frac{\partial \xi}{\partial x} \right)
\]

\[\text{...........................................(5.9)}\]
Metrics and Jacobian (5.3)
In CFD the metric terms are not often available as analytical expressions.
Instead they are often represented numerically.
The following inverse transformation is often more convenient to use than the original transformation

\[ x = x(\xi, \eta, \tau) \] \hspace{1cm} (5.18a)
\[ y = y(\xi, \eta, \tau) \] \hspace{1cm} (5.18b)
\[ t = t(\tau) \] \hspace{1cm} (5.18c)
Let \( x = x(\xi, \eta) \), \( y = y(\xi, \eta) \) and \( u = u(x, y) \). then we can write

\[
du = \frac{\partial u}{\partial x} dx + \frac{\partial u}{\partial y} dy \tag{5.19}
\]

\[
\frac{\partial u}{\partial \eta} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial \eta} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial \eta} \tag{5.21}
\]

\[
\frac{\partial u}{\partial \xi} = \frac{\partial u}{\partial x} \frac{\partial x}{\partial \xi} + \frac{\partial u}{\partial y} \frac{\partial y}{\partial \xi} \tag{5.20}
\]

Eqs. (5.21) and (5.22) are two equations for the two unknown derivatives.
Solving for the partial derivative w. r. t. x gives, using Cramer’s rule

\[
\frac{\partial u}{\partial x} = \frac{1}{J} \left[ \frac{\partial u}{\partial \xi} \frac{\partial y}{\partial \eta} - \frac{\partial u}{\partial \eta} \frac{\partial y}{\partial \xi} \right]
\]  

(5.23a)

Eq. (5.22) can now be written in terms of \( J \).

Define the Jacobian \( J \) as

\[
J = \frac{\partial (x, y)}{\partial (\xi, \eta)} = \begin{vmatrix} \frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\ \frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta} \end{vmatrix}
\]

(5.22a)
Similarly we can write the derivative w.r.t \( y \) as

\[
\frac{\partial u}{\partial y} = \frac{1}{J} \left[ \left( \frac{\partial u}{\partial \eta} \right) \left( \frac{\partial x}{\partial \xi} \right) - \left( \frac{\partial u}{\partial \xi} \right) \left( \frac{\partial x}{\partial \eta} \right) \right] \tag{5.23b}
\]

and we can define the following

\[
\frac{\partial}{\partial x} = \frac{1}{J} \left[ \left( \frac{\partial u}{\partial \xi} \right) \left( \frac{\partial y}{\partial \eta} \right) - \left( \frac{\partial}{\partial \eta} \right) \left( \frac{\partial y}{\partial \xi} \right) \right] \tag{5.24a}
\]

\[
\frac{\partial}{\partial y} = \frac{1}{J} \left[ \left( \frac{\partial}{\partial \eta} \right) \left( \frac{\partial x}{\partial \xi} \right) - \left( \frac{\partial}{\partial \xi} \right) \left( \frac{\partial x}{\partial \eta} \right) \right] \tag{5.24b}
\]
The above equations can be easily extended to three space dimensions 
(x, y an z).
The above equations can also be obtained formally as follows

\[ \xi = \xi(x, y) \] ........................(5.25a)

\[ d\xi = \frac{\partial \xi}{\partial x} dx + \frac{\partial \xi}{\partial y} dy \] ..........................(5.26a)

\[ \eta = \eta(x, y) \] ..........................(5.25b)

\[ d\eta = \frac{\partial \eta}{\partial x} dx + \frac{\partial \eta}{\partial y} dy \] ..........................(5.26b)

\[
\begin{bmatrix}
\frac{d\xi}{dx} & \frac{d\xi}{dy} \\
\frac{d\eta}{dx} & \frac{d\eta}{dy}
\end{bmatrix}
\begin{bmatrix}
dx \\
dy
\end{bmatrix} \] ..........................(5.27)
Similarly

\[ x = x(\xi, \eta) \]..............................................(5.28a)

\[ y = y(\xi, \eta) \]..............................................(5.28b)

\[ dx = \frac{\partial x}{\partial \xi} d\xi + \frac{\partial x}{\partial \eta} d\eta \]..............................................(5.29a)

\[ dy = \frac{\partial y}{\partial \xi} d\xi + \frac{\partial y}{\partial \eta} d\eta \]..............................................(5.29b)

\[
\begin{bmatrix}
dx \\
dy \\
\end{bmatrix} = 
\begin{bmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\
\frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta} \\
\end{bmatrix} 
\begin{bmatrix}
d\xi \\
d\eta \\
\end{bmatrix} \]..............................................(5.30)
Eq. (5.30) can be solved for $d\xi$, $d\eta$

$$
\begin{bmatrix}
    d\xi \\
    d\eta
\end{bmatrix} = \begin{bmatrix}
    \frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\
    \frac{\partial y}{\partial \xi} & \frac{\partial x}{\partial \eta}
\end{bmatrix}^{-1} \begin{bmatrix}
    dx \\
    dy
\end{bmatrix}\tag{5.31}
$$

Consider the conservation form 2D flow with no source term

$$
\frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0\tag{5.37}
$$
Using results from matrix algebra for inversion of matrices, RHS can be written as follows

\[
\begin{bmatrix}
\frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} \\
\frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} \\
\frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y}
\end{bmatrix}
\begin{bmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\
\frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta}
\end{bmatrix}^{-1}
\] 

\[\text{.............................(5.32)}\]
Since the determinant of a matrix and its transpose are the same we can write

\[
\begin{vmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial x}{\partial \eta} \\
\frac{\partial y}{\partial \xi} & \frac{\partial y}{\partial \eta}
\end{vmatrix}
= \begin{vmatrix}
\frac{\partial x}{\partial \xi} & \frac{\partial y}{\partial \xi} \\
\frac{\partial x}{\partial \eta} & \frac{\partial y}{\partial \eta}
\end{vmatrix}
\equiv J...........................(5.34)
\]

Substitute Eq. (5.34) into Eq. (5.33)

\[
\begin{bmatrix}
\frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} \\
\frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y}
\end{bmatrix}
= \frac{1}{J}
\begin{bmatrix}
\frac{\partial y}{\partial \eta} & -\frac{\partial x}{\partial \eta} \\
-\frac{\partial y}{\partial \xi} & \frac{\partial x}{\partial \xi}
\end{bmatrix}
\]..........................(5.35)
Comparing corresponding elements of the two matrices on the LHS and the RHS gives the following relations.

\[
\frac{\partial \xi}{\partial x} = \frac{1}{J} \frac{\partial y}{\partial \eta} \tag{5.36a}
\]

\[
\frac{\partial \eta}{\partial x} = -\frac{1}{J} \frac{\partial y}{\partial \xi} \tag{5.36b}
\]

\[
\frac{\partial \xi}{\partial y} = -\frac{1}{J} \frac{\partial x}{\partial \eta} \tag{5.36c}
\]

\[
\frac{\partial \eta}{\partial y} = \frac{1}{J} \frac{\partial x}{\partial \xi} \tag{5.36d}
\]
Consider the conservation form 2D flow with no source term

\[ \frac{\partial U}{\partial t} + \frac{\partial F}{\partial x} + \frac{\partial G}{\partial y} = 0 \] (5.37)
The above equation can be transformed to (see section 5.4)

\[
\frac{\partial U_1}{\partial t} + \frac{\partial F_1}{\partial \xi} + \frac{\partial G_1}{\partial \eta} = 0 \tag{5.38}
\]

Where the \( U_1, F_1, \) and \( G_1 \) are as follows

\[
U_1 = JU \tag{5.48a}
\]

\[
F_1 = JF \frac{\partial \xi}{\partial x} + JG \frac{\partial \xi}{\partial y} \tag{5.48b}
\]

\[
G_1 = JF \frac{\partial \eta}{\partial x} + JG \frac{\partial \eta}{\partial y} \tag{5.48c}
\]
Algebraic Methods

Known functions are used to map irregular physical domain into rectangular computational domains.
Example: Grid stretching may be necessary for some problems such as flow with boundary layers. Let us consider the transformation:

\[ \xi = x \quad \text{....}(5.50a) \]

\[ \eta = \ln(y + 1) \quad \text{....}(5.50b) \]

Inverse transformation

\[ x = \xi \quad \text{....}(5.51a) \]

\[ y = \exp(\eta) - 1 \quad \text{....}(5.51b) \]
The following relation (Eq. 5.52) hold between increments $\Delta y$ and $\Delta \eta$

\[
\frac{dy}{d\eta} = e^\eta \\
\int dy = e^\eta d\eta \\
\Delta y = e^\eta \Delta \eta \text{..........................}(5.52)
\]
Therefore as \( \eta \) increases, \( \Delta y \) increases exponentially. Thus we can choose \( \Delta \eta \) constant and still have an exponential stretching of the grid in the y-direction.

\[
\frac{\partial (\rho u)}{\partial (x)} + \frac{\partial (\rho v)}{\partial (y)} = 0 \quad \text{(5.53)}
\]

\[
\frac{\partial (\rho u)}{\partial \xi} \frac{\partial \xi}{\partial (x)} + \frac{\partial (\rho u)}{\partial \eta} \frac{\partial \eta}{\partial (x)} + \frac{\partial (\rho v)}{\partial \xi} \frac{\partial \xi}{\partial (y)} + \frac{\partial (\rho v)}{\partial \eta} \frac{\partial \eta}{\partial (y)} = 0 \quad \text{(5.54)}
\]

\[
\frac{\partial \xi}{\partial (x)} = 1 \quad \frac{\partial \xi}{\partial (y)} = 0 \quad \frac{\partial \eta}{\partial (x)} = 0 \quad \frac{\partial \eta}{\partial (y)} = \frac{1}{1 + y} \quad \text{……(5.55)}
\]
Substitute in Eq. (5.54) to get

\[
\frac{\partial (\rho u)}{\partial \xi} + \frac{1}{1 + y} \frac{\partial (\rho v)}{\partial \eta} = 0 \quad \text{......(5.56)}
\]

\[
\frac{\partial (\rho u)}{\partial \xi} + \frac{1}{e^n} \frac{\partial (\rho v)}{\partial \eta} = 0 \quad \text{......(5.57)}
\]

\[
e^n \frac{\partial (\rho u)}{\partial \xi} + \frac{\partial (\rho v)}{\partial \eta} = 0
\]

Eq. (5.57) is the continuity equation in the computational domain. Thus we have transformed the continuity equation from the physical space to the computational space.
The metrics carry the specifics of a particular transformation.

**Boundary Fitted Coordinate System (5.7)**

Here we consider the flow through a divergent duct as given in Figure 5.6 (next slide). $de$ is the curved upper wall and $fg$ is the centerline. Let $y_s = f(x)$ be the function that represents the upper wall. The following transformation will give rise to a rectangular grid.

\[
\xi = x \quad (5.65) \\
\eta = y/y_s \quad (5.66)
\]

To test this choose $y_s = 1.5x$ and let $x$ vary from 1 to 5.
At $x = 1$, $\xi = 1$, $\eta_{max} = y_{max}/y_s = 1$, and $x = 5$, $\xi = 5$, $\eta_{max} = y_{max}/y_s = 1$.

Thus the irregular domain is transformed into into a rectangular domain.
Consider a second case where the Nozzle wall is curved
\[ y_{\text{max}} = x^2 \quad \ldots \quad 1 \leq x \leq 2 \]

\[ \xi = x \]

\[ \eta = \frac{y}{y_{\text{max}}} = \frac{y}{x^2} \]

\[ \frac{\partial \xi}{\partial x} = 1, \quad \frac{\partial \xi}{\partial y} = 0 \]

\[ \frac{\partial \eta}{\partial x} = -2 \frac{y}{x^3} = -2 \frac{\eta}{x} = -2 \frac{\eta}{\xi} \]

\[ \frac{\partial \eta}{\partial y} = \frac{1}{x^2} = \frac{1}{\xi^2} \]
The above formulation is analytic

\[ \xi_x, \xi_y, \eta_x, \eta_y \]

Could also be obtained using central differencing.

The Jacobian is defined as

\[ J \equiv \frac{\partial (\xi, \eta)}{\partial (x, y)} \equiv \begin{vmatrix} \frac{\partial \xi}{\partial x} & \frac{\partial \xi}{\partial y} \\ \frac{\partial \eta}{\partial x} & \frac{\partial \eta}{\partial y} \end{vmatrix} \equiv \xi_x \eta_y - \xi_y \eta_x \]
Consider a point in the domain where we have \( \xi = 1.75, \eta = 0.75 \). Let us calculate \( \eta_x \) analytically and numerically.

At this point:

\[
x = 1.75
\]

\[
y = \eta x^2 = 0.75 \times (1.75)^2 = 2.29688
\]

\[
\eta_x = -2 \frac{\eta}{\xi} = -2 \times \frac{0.75}{1.75} = -0.85715
\]

\[
x_\xi = 1.0, \ y_\xi = 0
\]
We can also numerically calculate the derivatives using CD

\[
y_{\eta} = \frac{\Delta y}{\Delta \eta} = \frac{3.0625 - 1.53125}{2 \times 0.25} = 3.0625
\]

\[
I = J^{-1} = x_{\xi}y_{\eta} - y_{\xi}x_{\eta} = 1 \times 3.0625 - 0 \times 0 = 3.0625
\]

\[
\xi = 1.5: y = y_{\text{max}} \eta = 2.25 \times 0.75 = 1.6875
\]

\[
\xi = 2: y = y_{\text{max}} \eta = 4 \times 0.75 = 3.0
\]

\[
y_{\xi} = \frac{\Delta y}{\Delta \xi} = \frac{3.0 - 1.6875}{2.0 - 1.5} = 2.625
\]

\[
\eta_{x} = -\frac{y_{\xi}}{I} = -\frac{2.625}{3.0625} = -0.85714
\]