Resolution of Geometrical Configurations by a
3-D Staggered Mesh System

by

H. M. Domanus

William T. Sha, Principal Investigator

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Components Technology Division
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Resolution of Geometrical Configurations by a Three Dimensional Staggered Mesh System

I. Introduction

Any computer program development of thermal hydraulic analyses must begin with a relationship between the grid system and the geometric configuration. The relationship chosen sets the limits of possible applications and affects virtually all programming details of the code. In the COMMIX code^[1] development, a staggered mesh system is being employed in finite differencing the governing differential equations. A methodology has been developed to extend applications of the staggered mesh system to complicated three-dimensional geometrical configurations.

The methodology presented here employs x-y-z cartesian coordinates and modifies the finite differencing equations^[2] to resolve irregular three-dimensional geometrical configurations in a staggered mesh system. More important, it lends itself to a consistent approach to handle various types of boundary conditions.

II. Geometric Configuration Specification

The geometrical configuration is specified by considering a collection of bounded finite surfaces. The collection of surfaces forms a closed finite volume referred to as the region of interest.

Each component surface is defined by the following specifications:

1. A three-dimensional rectangular box defining a closed subregion containing the surface.
2. A function $f(x,y,z) = 0$ defining the coordinates of a surface point.
3. A function $g(x,y,z) \geq 0$ or both functions $g(x,y,z) \geq 0$ and $h(x,y,z) \geq 0$ to further define the extent of the surface $f(x,y,z)$.

The location of the origin of a cartesian coordinate system is chosen such that all coordinates in the region of interest are positive. Once the origin has been established, coordinates and functions defining surfaces can

be determined. The total number of surfaces, NSURF, used to characterize the region of interest is then determined. Consider the pipe section shown in Fig. 1. The pipe is of radius 2 meters and is 5 meters long. It can be characterized by three surfaces as indicated. A box containing surface 1 is specified by

$$\begin{aligned} \text{XMIN (1)} &= 0.0 & \text{XMAX (1)} &= 6.0 \\ \text{YMIN (1)} &= 0.0 & \text{YMAX (1)} &= 6.0 \\ \text{ZMIN (1)} &= 4.0 & \text{ZMAX (1)} &= 6.0 \end{aligned}$$

Because surface 1 may be uniquely defined using the f & g function definitions, the coarseness of the three-dimensional rectangular box is irrelevant.

The $f(x,y,z)$ function defines the surface. In addition to relating coordinates of a surface point, $f(x,y,z)$ also carries surface normal information. If point B = (XB,YB,ZB) is located on the surface then $f(XB,YB,ZB) = 0.0$, and a unit normal vector $\hat{n}(XB,YB,ZB) = (XN,YN,ZN)$ is pointing from point B into the region of interest. The coordinates of the unit normal vector are given by

$$XN = \frac{1}{\|N\|} \frac{\partial f}{\partial x} (XB,YB,ZB)$$

$$YN = \frac{1}{\|N\|} \frac{\partial f}{\partial y} (XB,YB,ZB)$$

$$ZN = \frac{1}{\|N\|} \frac{\partial f}{\partial z} (XB,YB,ZB)$$

where $\|N\|$ is:

$$\|N\| = \sqrt{\left(\frac{\partial f}{\partial x}\right)^2 + \left(\frac{\partial f}{\partial y}\right)^2 + \left(\frac{\partial f}{\partial z}\right)^2}$$

The functional form of $f(x,y,z)$ is defined as:

$$\begin{aligned} f(x,y,z) &= (FX2) x^2 + (FX) x + (FY2) y^2 + (FY) y \\ &+ (FZ2) z^2 + (FZ) z + (FXI) xy + (FXZ) xz \\ &+ (FYZ) yz + FC = 0. \end{aligned}$$

This functional form appears adequate for defining surfaces of current interest (i.e., cylinders, hexagonal fuel assembly can wall, planes, piping tees, elbows, etc.). However, more complicated functions such as cubic polynomials in x, y and z can readily be incorporated, if it is found to be necessary.

Fig. 1. Geometric Specification of a Pipe Section.

The appropriate f function to define surface 1 of Fig. 1 is

$$f(x,y,z) = -z+5 = 0 \text{ or equivalently}$$

$$FZ(1) = -1 \text{ and } FC(1) = 5, \text{ other } f \text{ coefficients} = 0.$$

The unit surface normal is $\hat{n} = (0,0,-1)$ indicating the region of interest is located below the plane $z=5$.

The $g(x,y,z)$ function definition limits the extent of the surface.

$$\begin{aligned} \text{The functional form used is } g(x,y,z) = & (GX2) x^2 + (GX) x + (GY2) y^2 + (GY) y \\ & + (GZ2) z^2 + (GZ) z + (GXY) xy + (GXZ) xz \\ & + (GYZ) yz + GC \geq 0.0. \end{aligned}$$

The appropriate g function to complete the definition of surface 1 in Fig. 1 is $g(x,y,z) = -x^2 + 6x - y^2 + 6y - 14 \geq 0$ or

$$GX2(1) = -1, GX(1) = 6,$$

$$GY2(1) = -1, GY(1) = 6, GC(1) = -14, \text{ other } g \text{ coefficients} = 0.$$

The g function definition gives surface 1 its circular shape, since every point $B = (XB,YB,ZB)$ on the surface $f(XB,YB,ZB) = 0$ must satisfy

$$g(XB,YB,ZB) \geq 0.0$$

The function $h(x,y,z)$ also imposes a restriction on the extent of the surface. The functional form is:

$$\begin{aligned} h(x,y,z) = & (HX2) x^2 + (HX) x + (HY2) y^2 + (HY) y \\ & + (HZ2) z^2 + (HZ) z + (HXY) xy + (HXZ) xz \\ & + (HYZ) yz + HC \geq 0.0. \end{aligned}$$

Use of the g and h functions is optional, but when irregularly shaped surfaces are required these functions are needed. The $h(x,y,z)$ function limitation is not needed in the example specification of surface 1 in Fig. 1. Therefore, all h coefficients are set equal to zero. Similarly, surfaces 2 and 3 of Fig. 1 are specified by:

$$XMIN(2) = 0, \quad XMAX(2) = 6$$

$$YMIN(2) = 0, \quad YMAX(2) = 6$$

$$ZMIN(2) = -1, \quad ZMAX(2) = 1$$

$$FZ(2) = 1, \text{ other } f \text{ coefficients} = 0$$

$$GX2(2) = -1, GX(2) = 6,$$

$$GY2(2) = -1, GY(2) = 6, GC(2) = -14, \text{ other } g \text{ coefficients} = 0$$

and

$XMIN(3) = 0, XMAX(3) = 6$
 $YMIN(3) = 0, YMAX(3) = 6$
 $ZMIN(3) = 0, ZMAX(3) = 5$
 $FX2(3) = -1, FX(3) = 6,$
 $FY2(3) = -1, FY(3) = 6, FC(3) = -14,$ other f coefficients = 0
 all g and h coefficients = 0.

III. Grid Definition

Once the geometrical configuration has been defined in detail as outlined in Sect. II, a grid is imposed to approximately resolve the region of interest. The grid is a staggered mesh system.

After determining the dimensions of a rectangular box completely enclosing the region of interest, a partitioning of each of the three sides of the box in the x, y and z directions is chosen. There are IMAX, JMAX and KMAX number of partitions in the x, y and z directions, respectively. The length of the Ith partition in the x direction is specified by DX(I). Similarly, DY(J) and DZ(K) are the lengths of the Jth and Kth partitions in the y and z directions, respectively. The overall dimensions of the box are:

$$\begin{aligned}
 \text{length in x dimension} &= \sum_{I=1}^{IMAX} DX(I) \\
 \text{length in y dimension} &= \sum_{J=1}^{JMAX} DY(J) \quad \text{and} \\
 \text{length in z dimension} &= \sum_{K=1}^{KMAX} DZ(K).
 \end{aligned}$$

From this partitioning, four different grids are considered for a staggered mesh system. Each grid may be viewed as the intersection points of three orthogonal line systems, parallel to the x, y and z axes, respectively. The four grids are referred to as the field points or grid, U points, V points or W points.

Discrete locations are defined in terms of

$$\begin{aligned}
 X(1) &= 1/2 DX(1) \\
 X(I) &= X(I-1) + 1/2 [DX(I-1) + DX(I)], \quad I = 2, IMAX \\
 Y(1) &= 1/2 DY(1) \\
 Y(J) &= Y(J-1) + 1/2 [DY(J-1) + DY(J)], \quad J = 2, JMAX
 \end{aligned}$$

and

$$Z(1) = 1/2 \text{ DZ}(1)$$

$$Z(K) = Z(K-1) + 1/2 [\text{DZ}(K-1) + \text{DZ}(K)], K = 2, \text{ KMAX}.$$

Field points have coordinates

$$(X(I), Y(J), Z(K)),$$

U points have coordinates

$$(X(I) + 1/2 \text{ DX}(I), Y(J), Z(K)),$$

V points have coordinates

$$(X(I), Y(J) + 1/2 \text{ DY}(J), Z(K)) \text{ and}$$

W points have coordinates

$$(X(I), Y(J), Z(K) + 1/2 \text{ DZ}(K)), I = 1, \text{ IMAX}, J = 1, \text{ JMAX}, K = 1, \text{ KMAX}.$$

For example, consider field points with y and z fixed. These field points all lie on a line referred to as a CX line, parallel to the x axis. (The set of CX lines is defined for a given J and K where $J = 1, \text{ JMAX}$ and $K = 1, \text{ KMAX}$.) Similarly, CY and CZ lines are defined, respectively, parallel to the y and z axes. Intersections of CX, CY and CZ lines define field points.

A similar system is considered for U points with UX, UY and UZ lines. Intersections of these lines define U points. Similarly, VX, VY and VZ lines for V points and WX, WY and WZ lines for W points are considered. The field grid locates discrete points of the field variables (i.e., pressure, temperature, density). The U, V and W grids, respectively, locate discrete points of velocity components. Because of the relationship between field and velocity points in the staggered mesh system, some of these lines are redundant. In particular,

CX lines = UX lines

CY lines = VY lines and

CZ lines = WZ lines.

IV. Identification of Internal and Surface Intersection Grid Points

The rectangular box completely enclosing the region of interest has been partitioned and resolved by $\text{IMAX} * \text{JMAX} * \text{KMAX}$ number grid points as described in

Sect. III. These grid points (i.e., $IMAX * JMAX * KMAX$) may be more than the number needed to resolve the internal region of interest. Only points inside the region of interest need be considered. Because of the potentially large computer storage requirements in three dimensional finite difference calculations, it is desirable to eliminate all grid points outside the region of interest. This is accomplished by identifying and labeling grid points inside the region of interest with a counter M. Each point M has a $IJK(M)$ position identifier associated with it as

$$IJK(M) = iijjkk$$

so that I,J,K can be recovered by the relations

$$I = IJK(M)/10000$$

$$J = (IJK(M) - 10000 * I)/100$$

$$K = IJK(M) - 10000 * I - 100 * J$$

using FORTRAN fixed point arithmetic. The spacial position of point M can be obtained from the I, J, K set as

field point: $(X(I), Y(J), Z(K))$

U point: $(X(I) + 1/2 DX(I), Y(J), Z(K))$

V point: $(X(I), Y(J) + 1/2 DY(J), Z(K))$

W point: $(X(I), Y(J), Z(K) + 1/2 DZ(K)).$

All internal field points are identified and numbered from $M = 1, NM$. It may happen that a velocity point is inside the region of interest while the related field point is not. Such points are identified and labeled $M=NM + 1, NM1$. If the region of interest deviates from the enclosing rectangular box, $(IMAX * JMAX * KMAX - NM)$ number of storage locations will have been eliminated from further considerations.

In addition to identifying internal points, points of surface intersection with CX, CY, CZ, UY, UZ, VX, VZ, WX and WY lines are identified and labeled with counter L, where $L = 1, NL$. Each point L is located at coordinates $(XB(L), YB(L), ZB(L))$ and has local surface nominal $\hat{n} = (XN(L), YN(L), ZN(L))$. Surface intersection points are classified as to the type of line generating it as well as being associated with the particular intersecting surface, N. This information is summarized and stored by the $LCX(N), LCY(N), LCZ(N), LUY(N), LUZ(N), LVX(N), LVZ(N), LWX(N)$ and $LWY(N)$, $N = 1, NSURF$ arrays as indicated by Table 1.

TABLE 1. Associated Surface Points with L Counter

Line Type	Surface No.	Beginning	L Value	Ending
CX	1	1		LCX(1)
CY	1	LCX(1) + 1		LCY(1)
CZ	1	LCY(1) + 1		LCZ(1)
CX	2	LCZ(1) + 1		LCX(2)
CZ	2	LCX(2) + 1		LCY(2)
.	.	.		.
.	.	.		.
.	.	.		.
CZ	NSURF	LCY(NSURF) + 1		LCZ(NSURF)
UY	1	LCZ(NSURF) + 1		LUY(1)
UZ	1	LUY(1) + 1		LUZ(1)
VX	1	LUZ(1) + 1		LVX(1)
VZ	1	LVX(1) + 1		LVZ(1)
WX	1	LVZ(1) + 1		LWX(1)
WY	1	LWX(1) + 1		LWY(1)
UY	2	LWY(1) + 1		LUY(2)
UZ	2	LUY(2) + 1		LUZ(2)
.	.	.		.
.	.	.		.
.	.	.		.
WX	NSURF	LVZ(NSURF) + 1		LWX(NSURF)
WY	NSURF	LWX(NSURF) + 1		LWY(NSURF) = NL

V. Positional Relationships between Internal and Surface Points

In addition to identifying and locating internal and surface points, positional relationships between one internal point and its neighbors (either internal or surface) are determined. Some arbitrary conventions are introduced to communicate this information within the computer code. Positional relationships among field points are summarized by the 6 arrays MIM(M), MIP(M), MJM(M), MJP(M), MKM(M) and MKP(M). The MIM(M) array refers to the adjacent field point in the minus x direction along a CX line. Similarly, MIP(M) refers to the adjacent field point in the positive x direction along a CX line. The other arrays have similar meanings along minus and plus CY and CZ lines, respectively. Figures 2 and 3 show the relationships between field points F(M) and their corresponding spatial locations. Values of these arrays indicate whether the adjacent field point is inside, outside or a surface point, as well as the particular M or L value of the adjacent field or surface point.

While the MIM, MIP, MJM, etc., arrays also indicate positional relationships between internal U, V and W points, they do not carry information of surface points derived from UY, UZ, VX, VZ, WX or WY line intersections. To accommodate this information, the JU(M), KU(M), IV(M), KV(M), IW(M) and JW(M) arrays are, respectively, introduced. These arrays indicate whether the U, V or W point, M, is inside, outside or adjacent to a surface point, and if adjacent to a surface point, the particular L value the surface point is labeled.

Adjacent internal field, U, V or W points from a surface point, L, along the appropriate CX, CY, CZ, UY, UZ, VX, VZ, WX or WY line are contained in the MB(L) array. This information is useful in boundary condition calculations in which surface values are related to internal values.

VI. Conclusion

The methodology presented in this report has the following unique features:

1. Optimizing the computer storage utilization.
2. Providing flexibility of describing the complicated three-dimensional configurations (such as cylinder, hexagonal

Fig. 2. Positional Relationship Between Internal Points in x-y Plane.

Fig. 3. Positional Relationship Between Internal Points in y-z plane.

fuel assembly duct wall, planes, piping, tee, elbow etc.)
encountered in engineering applications within the xyz
cartesian coordinates.

Appendix A

As a further example of the methodology presented in this report, consider the configuration of a piping system with two bends shown in Fig. A1. Each of the two 90° bends is approximated by two intermediate cylindrical sections. The pipes are of radius 2 and go through two 90° turns of radius 5. Detailed projections of the bends are shown in Figs. A2 and A3. A summary of the surface specifications used to model this piping system is included in Table A1. Note that there is considerable flexibility in the methodology of specifying these surfaces. The XMIN, XMAX, YMIN, YMAX, ZMIN, ZMAX specification is not necessary for any of these surfaces. However, this specification is useful for other surface types.

The methodology presented in this report significantly tightens up the storage requirements from considering a 20X20X20 box. Only points inside the piping system need be considered. There is approximately a 90% savings of computer storage in the number of internal computational points used for this example.

Fig. A1. Geometry of a Piping System with Two 90° bends.

Fig. A2. Section of First Pipe Bend in Plane $x = 18$.

Fig. A3. Section of Second Pipe Bend in Plane $z = 18$.

TABLE A1: Summary of Piping System Geometry

<u>Surface</u>	<u>Description</u>
#1	<p>Circular region radius = 2 in plane $z = 0$, $\bar{v} = (0,0,1)$ centered at (18,2,0).</p> <p> $XMIN(1) = 15$ $XMAX(1) = 21$ $YMIN(1) = -1$ $YMAX(1) = 5$ $ZMIN(1) = -1$ $ZMAX(1) = +1$ </p> <p>$FZ(1) = 1$ Other f coeffs. = 0.</p> <p> $GX2(1) = -1$, $GX(1) = 36$, $GY2(1) = -1$, $GY(1) = 4$, $GC(1) = -324$, Other g coeffs. = 0. All h coeffs. = 0. </p>
#2	<p>Cylindrical surface bounded by planes $z=0$, and $SIN(15)(y-7) + COS(15)(z-13) = 0$,</p> <p> $XMIN(2) = 15$ $XMAX(2) = 21$ $YMIN(2) = -1$ $YMAX(2) = 5$ $ZMIN(2) = 0$ $ZMAX(2) = 20$ </p> <p> $FX2(2) = -1$ $FX(2) = 36$, $FY2(2) = -1$ $FY(2) = 4$, $FC(2) = -324$ Other f coeffs. = 0. $GY(2) = -.259$ $GZ(2) = -.966$ $GC(2) = 14.369$ Other g coeffs. = 0. All h coeffs. = 0. </p>
#3	<p>Cylindrical surface of radius - 2 approximating part of first pipe bend between plane $SIN(15)(y-7) + COS(15)(z-13) = 0$, and plane $SIN(45)(y-7) + COS(45)(z-13) = 0$,</p> <p> $XMIN(3) = 15$ $XMAX(3) = 21$ $YMIN(3) = 0$ $YMAX(3) = 7$ $ZMIN(3) = 13$ $ZMAX(3) = 20$ </p> <p> $FX2(3) = -1$ $FX(3) = 36$ $FY2(3) = -.750$ $FY(3) = -9.419$ $FZ2(3) = -.250$ $FZ(3) = +5.438$ $FYZ(3) = .866$ $FC(3) = -349.569$ Other f coeffs. = 0. </p> <p> $GY(3) = +.259$ $GZ(3) = +.966$ $GC(3) = -14.369$ Other g coeffs. = 0. </p>

HY(3) = - .707 HZ(3) = - .707
 HC(3) = 14.142
 Other h coeffs. = 0.

#4

Cylindrical surface of radius = 2
 approximating part of first pipe bend between
 plane $\text{SIN}(45)(y-7) + \text{COS}(45)(z-13) = 0$, and
 plane $\text{COS}(15)(y-7) + \text{SIN}(15)(z-13) = 0$.

XMIN(4) = 15 XMAX(4) = 21
 YMIN(4) = 0 YMAX(4) = 7
 ZMIN(4) = 13 ZMAX(4) = 20

 FX2(4) = - 1 FX(4) = 36.
 FY2(4) = - .250 FY(4) = - 12.758
 FZ2(4) = - .750 FZ(4) = 22.098
 FYZ(4) = .866 FC(4) = - 482.775
 Other f coeffs. = 0.

GY(4) = .707 GZ(4) = .707
 GC(4) = - 14.142
 Other g coeffs. = 0.

HY(4) = - .966 HZ(4) = - .259
 HC(4) = 10.126
 Other h coeffs. = 0.

#5

Straight middle section of pipe between
 plane $\text{COS}(15)(y-7) + \text{SIN}(15)(z-13) = 0$, and
 plane $-\text{SIN}(15)(x-13) + \text{COS}(15)(y-13) = 0$.

XMIN(5) = 15 XMAX(5) = 21
 YMIN(5) = 0 YMAX(5) = 20
 ZMIN(5) = 13 ZMAX(5) = 20

 FX2(5) = - 1. FX(5) = 36
 FZ2(5) = - 1. FZ(5) = 36
 FC(5) = 644.0
 Other f coeffs. = 0.

GY(5) = .966 GZ(5) = .259
 GC(5) = - 10.126
 Other g coeffs. = 0.

HX(5) = .259 HY(5) = - .966
 HC(5) = 9.192
 Other h coeffs. = 0.

#6

Cylindrical surface of radius = 2
 approximating part of second pipe bend between
 plane - $\text{SIN}(15)(x-13) + \text{COS}(15)(y-13) = 0.0$ and
 plane - $\text{SIN}(45)(x-13) + \text{COS}(45)(y-13) = 0.0$.

$\text{XMIN}(6) = 0$ $\text{XMAX}(6) = 20$
 $\text{YMIN}(6) = 0$ $\text{YMAX}(6) = 20$
 $\text{ZMIN}(6) = 0$ $\text{ZMAX}(6) = 20$

$\text{FX2}(6) = - .750$ $\text{FX}(6) = 39.419$
 $\text{FY2}(6) = - .250$ $\text{FY}(6) = 22.758$
 $\text{FZ2}(6) = - 1.0$ $\text{FZ}(6) = 36.000$
 $\text{FGY}(6) = - .866$ $\text{FC}(6) = - 837.941$
 Other f coeffs. = 0.

$\text{GX}(6) = - .259$ $\text{GY}(6) = .966$
 $\text{GC}(6) = - 9.192$
 Other g coeffs. = 0.

$\text{HX}(6) = .707$ $\text{HY}(6) = - .707$
 Other h coeffs. = 0.

#7

Cylindrical surface of radius = 2
 approximating part of second pipe bend between
 plane - $\text{SIN}(45)(x-13) + \text{COS}(45)(y-13) = 0.0$ and
 plane - $\text{COS}(15)(x-13) + \text{SIN}(15)(y-13) = 0.0$.

$\text{XMIN}(7) = 0$ $\text{XMAX}(7) = 20$
 $\text{YMIN}(7) = 0$ $\text{YMAX}(7) = 20$
 $\text{ZMIN}(7) = 0$ $\text{ZMAX}(7) = 20$

$\text{FX2}(7) = - .250$ $\text{FX}(7) = 22.758$
 $\text{FY2}(7) = - .750$ $\text{FY}(7) = 39.419$
 $\text{FZ2}(7) = - 1.000$ $\text{FZ}(7) = 36.000$
 $\text{FGY}(7) = - .866$ $\text{FC}(7) = - 837.941$
 Other f coeffs. = 0.

$\text{GX}(7) = - .707$ $\text{GY}(7) = .707$
 Other g coeffs. = 0.

$\text{HX}(7) = .966$ $\text{HY}(7) = - .259$
 $\text{HC}(7) = - 9.192$
 Other h coeffs. = 0.

#8

Final straight section of pipe between
 plane - $\text{COS}(15)(x-13) + \text{SIN}(15)(y-13) = 0.0$ and
 plane $x=0$.

$\text{XMIN}(8) = 0$ $\text{XMAX}(8) = 20$
 $\text{YMIN}(8) = 0$ $\text{YMAX}(8) = 20$
 $\text{ZMIN}(8) = 0$ $\text{ZMAX}(8) = 20$

FY2(8) = - 1.000 FY(8) = 36.000
FZ2(8) = - 1.000 FZ(8) = 36.000
FC(8) = 644.000
Other f coeffs. = 0.

GX(8) = - .966 GY(8) = .259
GC(8) = 9.192
Other g coeffs. = 0.

All h coeffs. = 0.

#9

Circular region in plane x=0

XMIN(9) = 0 XMAX(9) = 20
YMIN(9) = 0 YMAX(9) = 20
ZMIN(9) = 0 ZMAX(9) = 20

FX(9) = 1.000 Other f coeffs. = 0.

GY2(9) = - 1.000 GY(9) = 36.000
GZ2(9) = - 1.000 GZ(9) = 36.000
GC(9) = 644.000
Other g coeffs. = 0.

All h coeffs. = 0.

References

1. Sha, W. T., Domanus, H. M. and Schmitt, R. C., "COMMIX-Three-Dimensional, Time-Dependent, Two-Phase Flow with Non-Equilibrium Velocity and Temperature Computer Program," to be published in 1978.
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