References

[1]Rothe, D. E., "Electron-Beam Studies of Low Reynolds Number Flows Inside a DeLaval Nozzle," AIAA Paper 70-810, June 1970.

[2]Williams, W. D. et al., "Experimental Study of the Plume Characteristics of an Aged Monopropellant Hydrazine Thruster," AEDC-TR-79-2 (AD-A068326), April 1979.

[3]Bird, G. A., "The Nozzle Lip Problem," *Proceedings of the Ninth International Symposium on Rarefied Gas Dynamics*, DFVLR Press, Porz-Wahn, FRG, 1974, Vol. I, pp. A22-1–A22-8..

Calculation of the Volume of a General Hexahedron for Flow Predictions

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Introduction

FOR application of finite volume methods to the solution of conservative partial differential equations the volume of elementary cells must be calculated. The elementary cells are usually general hexahedra with the eight corners of each cell prescribed. The 12 sides of each cell are straight lines joining these corners and therefore the faces are bounded by quadrilaterals, which need not be planar. In previous work (see e.g., Ref. 1) the faces have been defined by two plane triangles obtained after inserting a diagonal in each quadrilateral and then the volume of the cell has been determined. In general, 64 different such cells can be formed, each with a different volume, because there is a choice of two diagonals per face.

A different construction of the cell is to take a face bounded by a quadrilateral to be a doubly-ruled surface. There is one particular doubly-ruled surface that is rather special in that cells with these surfaces can be fitted together to fill the whole space without any consideration of matching of diagonals of the face quadrilaterals. Only one such cell can be constructed once the bounding quadrilaterals have been set up; hence, only one value of volume is obtained. There is no discontinuity of slope or curvature anywhere on the faces of this cell. In this Note an expression for the volume of such a general hexahedral cell is obtained.

Calculation of Pyramid Volume with a Base Formed of a Doubly-Ruled Surface Bounded by a Quadrilateral

The general hexahedron is divided into six pyramids with a common vertex and with one of the faces as the base of each. Consider one of these pyramids with vertex R and base formed of a doubly-ruled surface bounded by the quadrilateral ABCD as shown in Fig. 1. The side-faces RAB, RBC, RCD, and RDA are plane.

Take the vector displacement **RP** of point P from point R when point P lies on the base ABCD of the pyramid to be given by

$$\mathbf{RP} = \mathbf{RA} + \xi\mathbf{AB} + \eta\mathbf{AD} + \xi\eta(\mathbf{AC} - \mathbf{AB} - \mathbf{AD}) \qquad (1)$$

where ξ, η are surface curvilinear coordinates which are such that

$$0 \le \xi \le 1, \qquad 0 \le \eta \le 1 \qquad (2)$$

The surface on which P lies is then a doubly-ruled surface and is the same surface regardless of which corner of the quadrilateral is named A.

If $\boldsymbol{n}_p$ is the unit normal vector at P to the base and dS_p is an elementary element of area of the base about P corresponding to small changes $d\xi$ and $d\eta$ in ξ and η, then by using Eq. (1) we have

$$\begin{aligned} \boldsymbol{n}_p dS_p &= [\mathbf{AB} + \eta(\mathbf{AC} - \mathbf{AB} - \mathbf{AD})] \\ &\quad \times [\mathbf{AD} + \xi(\mathbf{AC} - \mathbf{AB} - \mathbf{AD})] d\xi d\eta \\ &= \{[\mathbf{AB} \times \mathbf{AD}] + \xi[\mathbf{AB} \times \mathbf{DC}] + \eta[\mathbf{BC} \times \mathbf{AD}]\} d\xi d\eta \end{aligned} \qquad (3)$$

The volume V_{RABCD} of the pyramid RABCD is therefore

$$\begin{aligned} V_{\text{RABCD}} &= \frac{1}{3}\int_{\text{ABCD}} \mathbf{RP} \cdot \boldsymbol{n}_p dS_p \\ &= \frac{1}{6}\mathbf{RA} \cdot [\mathbf{DB} \times \mathbf{AC}] + \frac{1}{12}\mathbf{AC} \cdot [\mathbf{AD} \times \mathbf{AB}] \end{aligned} \qquad (4)$$

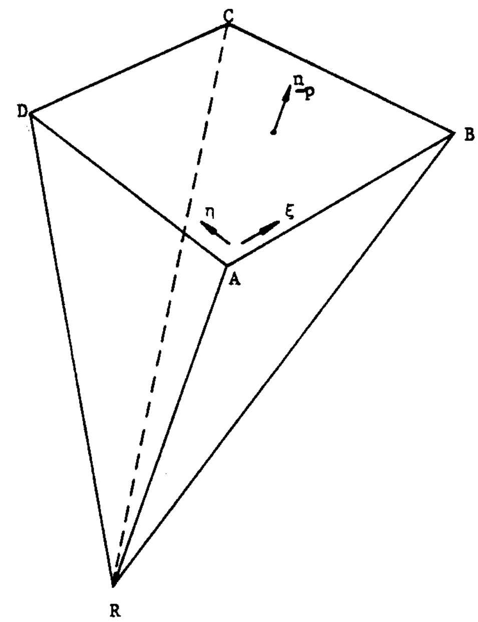

Fig. 1 Pyramid with vertex R and base formed of a doubly-ruled surface bounded by the quadrilateral ABCD.

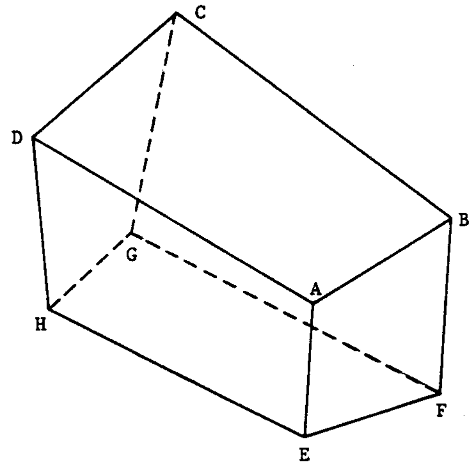

Fig. 2 General hexahedron ABCDEFGH.

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The value of Eq. (4) can be positive or negative according to the position of the point R. If point R is well away from the neighborhood of the quadrilateral ABCD, then the expression is positive if points A,B,C,D are traversed clockwise when viewed from the point R.

Equation (4) may be replaced by a number of equivalent formulas, two of which are

$$V_{\mathrm{RABCD}} = (1/12)\,(\mathbf{RA}+\mathbf{RB})\cdot[\mathbf{DB}\times\mathbf{AC}] \tag{4a}$$

and

$$V_{\mathrm{RABCD}} = (1/24)\,(\mathbf{RA}+\mathbf{RB}+\mathbf{RC}+\mathbf{RD})\cdot[\mathbf{DB}\times\mathbf{AC}] \tag{4b}$$

The quantity $(1/6)\mathbf{RA}\cdot[\mathbf{DB}\times\mathbf{AC}]$ in Eq. (4) is equal to the sum of the volumes of the two tetrahedra RABC and RACD obtained after replacing the doubly-ruled base by the two triangles meeting at the diagonal AC of the quadrilateral ABCD. The quantity $(1/12)\mathbf{AC}\cdot[\mathbf{AD}\times\mathbf{AB}]$ may be regarded as a correction term. There is an equivalent formula to Eq. (4) in which the sum of the volumes of the two tetrahedra RABD and RBCD appears.

Equation (4b) is quite symmetrical, but we shall use Eq. (4a) for calculating the volume of the pyramid RABCD because it is the shortest of the three. It may be written as

$$V_{\mathrm{RABCD}} = (1/6)\,(\mathbf{RA}+\mathbf{RB})\cdot S_{\mathrm{ABCD}} \tag{5}$$

where

$$S_{\mathrm{ABCD}} = \tfrac{1}{2}\,[\mathbf{DB}\times\mathbf{AC}] \tag{6}$$

If the quadrilateral ABCD is planar, then the vector S_{ABCD} is normal to its plane with magnitude equal to its area. If the quadrilateral ABCD is general, then by using Eq. (3), we obtain

$$\int_{\mathrm{ABCD}} n_p \mathrm{d}S_p = S_{\mathrm{ABCD}} = \tfrac{1}{2}\,[\mathbf{DB}\times\mathbf{AC}] \tag{7}$$

The vector S_{ABCD} is exactly the same as the surface vector S_{5678} of Kordulla and Vinokur,[1] which is to be expected because, if we form the scalar product of Eq. (7) with an arbitrary constant vector and apply the divergence theorem in the space enclosed by any two surfaces bounded by the nonplanar quadrilateral ABCD, we find that the surface integrals are independent of the surface. The result that S_{ABCD} is independent of what surface is bounded by the nonplanar quadrilateral ABCD then follows because the multiplying vector was arbitrary.

Calculation of the Volume of a General Hexahedron

The volume V_{ABCDEFGH} of the hexahedron ABCDEFGH is now obtained as the sum of the volumes of six pyramids with any point R taken as common vertex. Thus

$$V_{\mathrm{ABCDEFGH}} = V_{\mathrm{RABCD}} + V_{\mathrm{RAEFB}} + V_{\mathrm{RADHE}} + V_{\mathrm{RGFEH}} + V_{\mathrm{RGHDC}} + V_{\mathrm{RGCBF}} \tag{8}$$

If point R is within the hexahedron, all the quantities on the right-hand side of Eq. (8) are positive because the points on the bases of the relevant pyramids are then traversed clockwise when viewed from R. The bases of the first three pyramids meet at point A and the bases of the second three pyramids at point G.

By using Eq. (5) for the base ABCD and its analog for the other bases, we get

$$\begin{aligned} V_{\mathrm{ABCDEFGH}} = (1/6)\{ &(\mathbf{RA}+\mathbf{RB})\cdot S_{\mathrm{ABCD}} + (\mathbf{RA}+\mathbf{RE})\cdot S_{\mathrm{AEFB}} \\ &+ (\mathbf{RA}+\mathbf{RD})\cdot S_{\mathrm{ADHE}} + (\mathbf{RG}+\mathbf{RF})\cdot S_{\mathrm{GFEH}} \\ &+ (\mathbf{RG}+\mathbf{RH})\cdot S_{\mathrm{GHDC}} + (\mathbf{RG}+\mathbf{RC})\cdot S_{\mathrm{GCBF}}\} \end{aligned} \tag{9}$$

Now if F is an arbitrary constant vector then

$$\int_{\mathrm{ABCDEFGH}} \nabla F \mathrm{d}V = 0 \tag{10}$$

where $\mathrm{d}V$ is an elementary element of volume within the hexahedron ABCDEFGH. By aplying the divergence theorem to the integral on the left-hand side of Eq. (10) and taking account of the fact that F is arbitrary, we get, by using Eq. (7) for the base ABCD and its analog for the other bases

$$S_{\mathrm{ABCD}} + S_{\mathrm{AEFB}} + S_{\mathrm{ADHE}} + S_{\mathrm{GFEH}} + S_{\mathrm{GHDC}} + S_{\mathrm{GCBF}} = 0 \tag{11}$$

By using Eq. (11) in Eq. (9) we see immediately that the volume V_{ABCDEFGH} does not depend upon the position of the common vortex point R, as is to be expected. However, the actual form of the expression on the right-hand side of Eq. (9) does depend upon the position of the point R. If the volumes of a large number of hexahedral cells are to be evaluated it may be sensible to take point R to be the same for all cells, and it could be the origin of coordinates. In that case we would write Eq. (6) as

$$\begin{aligned} S_{\mathrm{ABCD}} &= \tfrac{1}{2}[(\mathbf{RB}-\mathbf{RD})\times(\mathbf{RC}-\mathbf{RA})] \\ &= \tfrac{1}{2}\{[\mathbf{RA}\times\mathbf{RB}] + [\mathbf{RB}\times\mathbf{RC}] + [\mathbf{RC}\times\mathbf{RD}] \\ &\quad + [\mathbf{RD}\times\mathbf{RA}]\} \end{aligned} \tag{12}$$

and then

$$\begin{aligned} (1/6)(\mathbf{RA}+\mathbf{RB})\cdot S_{\mathrm{ABCD}} = (1/12)\{&(\mathbf{RA}+\mathbf{RB})\cdot[\mathbf{RC}\times\mathbf{RD}] \\ &+ (\mathbf{RC}+\mathbf{RD})\cdot[\mathbf{RA}\times\mathbf{RB}]\} \end{aligned} \tag{13}$$

Equations similar to Eq. (13) may be obtained easily for each group of terms on the right-hand side of Eq. (9) and the terms added together give a symmetrical expression for V_{ABCDEFGH}. Such an expression may be the most economical to evaluate in terms of Cartesian coordinates of points, when point R is taken at the origin, but the resulting value of the expression can be the difference of quantities of similar size when the hexahedral cell is far away from point R. We prefer to take point R to be in the region of the hexahedron and here we take it to coincide with the corner G of the hexahedron ABCDEFGH. Equation (9) then becomes, upon using Eq. (6) and its analog,

$$\begin{aligned} V_{\mathrm{ABCDEFGH}} &= (1/12)\{(\mathbf{GA}+\mathbf{GB})\cdot[\mathbf{DB}\times\mathbf{AC}] \\ &\quad + (\mathbf{GA}+\mathbf{GE})\cdot[\mathbf{BE}\times\mathbf{AF}] + (\mathbf{GA}+\mathbf{GD})\cdot[\mathbf{ED}\times\mathbf{AH}] \\ &\quad + \mathbf{GF}\cdot[\mathbf{HF}\times\mathbf{GE}] + \mathbf{GH}\cdot[\mathbf{CH}\times\mathbf{GD}] + \mathbf{GC}\cdot[\mathbf{FC}\times\mathbf{GB}]\} \\ &= (1/12)\mathbf{GA}\cdot\{[\mathbf{DB}\times\mathbf{AC}] \\ &\quad + [\mathbf{BE}\times\mathbf{AF}] + [\mathbf{ED}\times\mathbf{AH}]\} \\ &\quad + (1/12)\boldsymbol{GB}\cdot\{[\mathbf{DB}\times\mathbf{AC}] + [\mathbf{GC}\times\mathbf{FC}]\} \\ &\quad + (1/12)\mathbf{GE}\cdot\{[\mathbf{BE}\times\mathbf{AF}] + [\mathbf{GF}\times\mathbf{HF}]\} \\ &\quad + (1/12)\mathbf{GD}\cdot\{[\mathbf{ED}\times\mathbf{AH}] + [\mathbf{GH}\times\mathbf{CH}]\} \end{aligned} \tag{14}$$

The value of V_{ABCDEFGH} obtained from Eq. (14) is positive provided that the ordering of the corners A, B, C, D, E, F, G, H is as shown in Fig. 2. The corner points of any such hexahedron can be named in the way indicated in Fig. 2. The corner points A and B are first named so that AB is any side. Points D and E are then chosen so that AD and AE are sides and are such that AE turns towards AD when the hexahedron experiences a right hand rotation about the line AB. Points C, F, and H complete the three faces through A and the remaining point is G.

Addendum

The authors' attention has been drawn by J. H. B. Smith to the fact that the surface defined in Eq. (1) is a member of a one-parameter family of doubly-ruled quadric surfaces containing the quadrilateral ABCD. The pair of plane surfaces intersecting in the diagonal AC and the pair of plane surfaces intersecting in the diagonal DB are degenerate members of this family. The equation of a general member of the family is

$$[2p\xi\eta+(1-p)]\,(\mathbf{RP}-\mathbf{RA})=(1-p)\xi(1-\eta)\mathbf{AB}$$
$$+(1-p)\eta(1-\xi)\mathbf{AD}+(1+p)\xi\eta\mathbf{AC} \qquad (15)$$

where p is the parameter and ξ,η are surface curvilinear coordinates.

The pair of plane surfaces intersecting in the diagonal AC are obtained when $p=+1$; the pair of plane surfaces intersecting in the diagonal BD are obtained when $p=-1$. The surface that is the same regardless of which corner of the quadrilateral is named A is obtained when $p=0$ and this is the case we have used in our Eq. (1) and is the case that we want in order that the hexahedral cells can be fitted together without any consideration of matching of diagonals of the face quadrilaterals.

Conclusions

An expression for the volume of a general hexahedron has been obtained. The faces of the hexahedron had first to be defined as doubly-ruled surfaces, but once that was done the actual volume, for a given set of eight corner points, is unique. Hexahedral cells so defined have the practical merit that they can be fitted together to fill the whole space without any consideration of matching of diagonals of the face quadrilaterals. Moreover the cell faces are completely smooth. The expression obtained is longer than that of Kordulla and Vinokur, but it need be evaluated only once for each cell in a finite volume method and the result stored. The penalty for evaluating the longer expression is tolerable when it is set against the advantage of the ease of fitting the cells together.

Acknowledgment

The authors acknowledge helpful discussions with C. C. Lytton about the form of presentation of results.

References

[1]Kordulla, W. and Vinokur, M., "Efficient Computation of Volume in Flow Predictions," *AIAA Journal*, Vol. 21, June 1983, pp. 917-918.

The Position of Laminar Separation Lines on Smooth Inclined Bodies

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Nomenclature

i,j,λ	= integers
J	= number of vortex filaments starting from separation line
$K_\lambda(\xi)$	= coefficient in the equation of the vortex sheet [Eq. (1)]
$\bar{K}_\lambda(\xi)$	$=K_\lambda(2\lvert K_4\rvert)^{(2-\lambda)/2}$
$k_{\lambda,i}$	= coefficients in the expansions of $\bar{K}_\lambda(\xi)$, $\lambda=3,5$ [Eq. (2)]
L	= number of terms in the expansions of $\bar{K}_\lambda(\xi)$, $\lambda=3,5,-1$ [Eq. (2)]
ℓ_1	= x component of $\underset{\sim}{\sigma}_1$
ℓ_R	= longitudinal reference length
$\underset{\sim}{n}_0,\underset{\sim}{n}_1$	= unit upstream normal vectors to parabolic cylinder and vortex sheet, respectively (Fig. 2)
$\underset{\sim}{n}_2$	= unit vector, normal to vortex line and tangential to vortex sheet at P′, pointing downstream [Eq. (7) and Fig. 2]
δn_2	= infinitesimal length measured from P′ in the direction of $\underset{\sim}{n}_2$
P	= typical point on separation line, on left-hand side facing upstream, with $x=\xi$ (Figs. 1 and 2)
P′	= typical point on sheet vortex line originating at P (Fig. 2)
Q	= general field point near vortex sheet (Fig. 1)
$\underset{\sim}{r}_P,\underset{\sim}{r}_Q$	= position vectors of P and Q, respectively, measured from origin of x, y, and z
x,y,z	= body Cartesian coordinates (Fig. 1)
y',z'	= local coordinates in plane normal to separation line at P, with origin at P (Fig. 1)
$\bar{y}',\bar{z}'$	= nondimensional coordinates $2\lvert K_4\rvert y'$ and $2\lvert K_4\rvert z'$, respectively
$\xi,\eta(\xi),\zeta(\xi)$	= x,y,z coordinates of P
$\underset{\sim}{\sigma}_1,\underset{\sim}{\sigma}_2,\underset{\sim}{\sigma}_3$	= unit vectors parallel to separation line downstream tangent at P, Py', and Pz', respectively (Fig. 1)
$\underset{\sim}{\tau}$	= unit downstream tangent to vortex line at P′ (Fig. 2)
$\psi(\xi)$	= vorticity flux function on vortex line originating at P
ω	= ± magnitude of surface vorticity vector on sheet at P′

Introduction

MANY calculations of separated flow from smooth elongated bodies have been made using inviscid potential-flow models (see for example, Refs. 1-4). Except for Ref. 4, all of these methods require prior specification of the separation lines.

Calculations of the laminar separation line itself have been made using boundary-layer calculations driven by unseparated

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