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Free-Stream Capturing in Fluid Conservation Law for Moving Coordinates in Three Dimensions

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Introduction

Body-conforming coordinates transformation of a fluid conservation-law form is generally used in computational fluid dynamics. The metrics associated with the coordinates transformation are required to satisfy certain geometric identities to maintain the free stream.¹ These metrics are called free-stream capturing (or preserving) metrics. So far, numerical techniques are known to capture the free-stream on stationary grids.²⁻⁴ However, the extension of the free-stream capturing metrics to moving grids is not straightforward. The error introduced by the time metrics has been overlooked because it is negligible in most cases, but it can be significant in certain applications such as helicopter rotor flow fields.⁵

Rigorous formulations to avoid this error were suggested in Ref. 1, and demonstrated, for example, in Ref. 6. Based on the work in Ref. 1, the present study describes detailed formulas for constructing the free-stream capturing metrics in space and time on both the finite-volume (FV) and finite-difference (FD) framework. The error introduced by the inconsistent time-metric term is also evaluated.

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Finite-Volume Formulation

Geometric Identities and Free-Stream Capturing

Following Ref. 1, the integral form of a conservation law for a given cell can be written as

$$\int_{V(t_2)} Q dV - \int_{V(t_1)} Q dV + \int_{t_1}^{t_2} \oint_{S(t)} \mathbf{n} \cdot \mathbf{F} dS dt = 0 \quad (1)$$

where $V(t)$ is the cell volume and $\mathbf{n} dS(t)$ is a vector element of surface area with outward normal \mathbf{n} . Considering the Euler equations, Q is a vector of conservative variables, *viz.*, density, momentum and energy, and \mathbf{F} is the flux tensor of Q . The flux \mathbf{F} can be decomposed into the flux in the stationary frame, \mathbf{F}_{st} , and the contribution due to surface element velocity, \mathbf{v} as follows

$$\mathbf{F} = \mathbf{F}_{st} - \mathbf{v}Q \quad (2)$$

Let \mathbf{r} , $\mathbf{r}_0(t)$, $\mathbf{v}_0(t)$, and $\Omega(t)$ be the position vectors of a point in space, the origin, velocity and angular velocity of the non-inertial frame relative to the inertial frame, respectively. Then,

$$\mathbf{v} = \mathbf{v}_r + \mathbf{v}_c \quad (3)$$

where

$$\mathbf{v}_r = \mathbf{v}_0(t) + \Omega(t) \times [\mathbf{r} - \mathbf{r}_0(t)] \quad (4)$$

and $\mathbf{v}_c(t)$ is the surface element velocity relative to the non-inertial frame, but expressed in the inertial frame.

The geometric identities given in Ref. 1 are as follows. A mathematical expression of a closed cell is given by

$$\oint_S \mathbf{n} dS = 0 \quad (5)$$

The relative rigid motion of two frames of reference is given by

$$\oint_S \mathbf{n} \cdot \mathbf{v}_r dS = 0 \quad (6)$$

Using Eqs. (4) and (6), one obtains

$$\oint_S \mathbf{r} \times \mathbf{n} dS = 0 \quad (7)$$

The conservation of volume for a time-varying cell is given by

$$V(t_2) - V(t_1) = \int_{t_1}^{t_2} \oint_{S(t)} \mathbf{n} \cdot \mathbf{v}_c dS dt \quad (8)$$

The free-stream preservation due to these geometric identities can be demonstrated by substituting Q_∞ , $\mathbf{F}_{st\infty}$ and Eqs. (2) to (4) to Eq. (1):

$$\begin{aligned} Q_\infty[V(t_2) - V(t_1)] = & - \int_{t_1}^{t_2} [\mathbf{F}_{st\infty} \cdot (\oint_S \mathbf{n} dS) - Q_\infty(\mathbf{v}_0 - \Omega \times \mathbf{r}_0) \cdot (\oint_S \mathbf{n} dS) \\ & - Q_\infty \Omega \cdot (\oint_S \mathbf{r} \times \mathbf{n} dS) - Q_\infty (\oint_S \mathbf{n} \cdot \mathbf{v}_c dS)] dt \end{aligned} \quad (9)$$

The geometric identity, Eq. (5), suffices to capture the free stream in a fixed coordinate system, where most of steady-state computations are carried out, and in a moving coordinate system without rotation ($\Omega = 0$). When the grid is moving with rotation ($\Omega \neq 0$), the second geometric identity, Eq. (7), is to be satisfied. For the general motion of grid with changing cell volume, the third geometric identity, Eq. (8), is also required.

The geometric identity, Eq. (5), preserves the free stream at any instance t when $\mathbf{v} = 0$. Thus, the time-differential form of Eq. (1) is often used in the FV formulation. However, if the grid moves, the geometric identities have to be satisfied correctly in the integral form.

Free-Stream Capturing in the Inertial Frame

To preserve the free-stream perfectly with a moving grid, Ref. 1 suggests to consider the rigorous FV formulations in space and time. One of the rigorous FV formulations with a grid velocity expressed in the inertial frame is shown here in detail.

Assuming that \mathbf{v} is given and then by substituting Q_∞ and $\mathbf{F}_{st\infty}$ to Eq. (1), one obtains

$$Q_\infty[V(t_2) - V(t_1)] = -\mathbf{F}_{st\infty} \cdot \int_{t_1}^{t_2} \oint_S \mathbf{n} dS dt + Q_\infty \int_{t_1}^{t_2} \oint_S \mathbf{n} \cdot \mathbf{v} dS dt \quad (10)$$

The first term in the right-hand side of the above equation yields Eq. (5). Then the rest of the equation becomes similar to Eq. (8).

Figure 1 shows a regular hexahedral cell. We assume that all edges are straight lines. Reference 1 describes the formulas for the surface vector \mathbf{S} (note that \mathbf{S} is taken in the positive coordinate direction here) so as to satisfy the geometric identities on the hexahedron:

$$\mathbf{S}_{1562} = \frac{1}{2}(\mathbf{r}_6 - \mathbf{r}_1) \times (\mathbf{r}_5 - \mathbf{r}_2) \quad (11)$$

$$\mathbf{S}_{1562} = (\mathbf{r}_{56} - \mathbf{r}_{12}) \times (\mathbf{r}_{15} - \mathbf{r}_{26}) \quad (12)$$

$$V_{12345678} = \frac{1}{3}(\mathbf{S}_{1485} + \mathbf{S}_{1234} + \mathbf{S}_{1562}) \cdot (\mathbf{r}_7 - \mathbf{r}_1) \quad (13)$$

where $\mathbf{r}_{56} = \frac{1}{2}(\mathbf{r}_5 + \mathbf{r}_6)$, and so on. Note that Eqs. (11) and (12) result in the same expression. In fact, the surface vector is defined uniquely as long as the edges are straight lines. Also note that there are other consistent ways to compute the cell volume instead of Eq. (13). However, Eq. (13) is the simplest form. Let $\mathbf{S}_{1562} = S_{1562}\mathbf{n}$. With either Eq. (11) or (12), one obtains

$$\sum_{cell} S\mathbf{n} = 0 \quad (14)$$

Thus, Eq. (5) is satisfied.

It is essential to compute the second term in the right-hand side of Eq. (10). It can be rewritten as

$$\int_{t_1}^{t_2} \left(\sum_{cell} S\mathbf{n} \cdot \mathbf{v} \right) dt = \sum_{cell} \left(\int_{t_1}^{t_2} S\mathbf{n} \cdot \mathbf{v} dt \right) \quad (15)$$

Let V_S be a volume swept by a surface S between the time interval $[t_1, t_2]$:

$$V_S = \int_{t_1}^{t_2} S\mathbf{n} \cdot \mathbf{v} dt \quad (16)$$

Let $S(t_1) = S_{1562}$ and $S(t_2) = S_{1'5'6'2'}$ (see Fig. 2). The volume V_S can be computed similarly to Eq. (13) as

$$\begin{aligned} V_{S_{1234}} &= V_{122'1'566'5'} \\ &= \frac{1}{3}(\mathbf{S}_{11'5'5} + \mathbf{S}_{122'1'} + \mathbf{S}_{1562}) \cdot (\mathbf{r}_{6'} - \mathbf{r}_1) \end{aligned} \quad (17)$$

where $\mathbf{S}_{11'5'5}$ and $\mathbf{S}_{122'1'}$ are the surface vectors in space and time domain. Note that this formula requires only the difference of the positions of grid points between t_1 and t_2 , not the grid velocity \mathbf{v} itself. Then, instead of Eqs. (6) and (8), one obtains

$$\Delta V = \sum_{cell} V_S \quad (18)$$

This identity does not mean to satisfy Eq. (7) but does satisfy Eq. (6) in the time-integral form. Therefore, Eq. (18) leads to the perfect free-stream capturing with the use of Eq. (11).

Free-Stream Capturing in the Non-Inertial Frame

It is convenient to use the non-inertial frame for certain applications. Thus, the FV formulation with a grid velocity expressed in the non-inertial frame is shown next. The analysis also provides a deep insight for the free-stream capturing because it considers three types of motion given in Eqs. (3) and (4) separately. The discretized forms of the geometric identities in the FV method can be expressed as

$$\sum_{cell} S \mathbf{n} = 0 \quad (19)$$

$$\sum_{cell} S \mathbf{r} \times \mathbf{n} = 0 \quad (20)$$

$$\Delta V = \sum_{cell} V_{S_c} \quad (21)$$

where V_{S_c} is obtained from Eq. (16) by replacing \mathbf{v} with \mathbf{v}_c (see Ref. 1 for more details).

Reference 1 introduces the area moment $\mathbf{M} = \int_S \mathbf{r} \times \mathbf{n} dS$ so as to satisfy the discretized geometric identity, Eq. (7), on the hexahedron:

$$\mathbf{M}_{1562} = \mathbf{r}_{165} \times \mathbf{S}_{165} + \mathbf{r}_{126} \times \mathbf{S}_{126} \quad (22)$$

where $\mathbf{r}_{165} = \frac{1}{3}(\mathbf{r}_1 + \mathbf{r}_6 + \mathbf{r}_5)$, $\mathbf{S}_{165} = \frac{1}{2}(\mathbf{r}_6 - \mathbf{r}_1) \times (\mathbf{r}_5 - \mathbf{r}_1)$, and so on. Note that $\mathbf{M}_{1562} \neq \mathbf{r}_{1562} \times \mathbf{S}_{1562}$. The expression, $\mathbf{r}_{1562} \times \mathbf{S}_{1562}$, is not well-defined for computing area moment. In contrast, Eq. (22) is well-defined. To see these, let \mathbf{r}_\diamond , \mathbf{r}_Δ , \mathbf{S}_\diamond and \mathbf{S}_Δ be \mathbf{r}_{1562} , \mathbf{r}_{165} , $|\mathbf{S}_{1562}|\mathbf{n}$ and $|\mathbf{S}_{165}|\mathbf{n}$, respectively. After simple algebraic manipulation, one

obtains

$$\sum_{cell} \mathbf{r}_{\diamond} \times \mathbf{S}_{\diamond} \neq 0 \quad (23)$$

in contrast,

$$\sum_{cell} \mathbf{r}_{\Delta} \times \mathbf{S}_{\Delta} = 0 \quad (24)$$

Therefore, in addition to Eq. (21), the free-stream capturing can be shown as

$$[\mathbf{F}_{st\infty} - (\mathbf{v}_0 - \Omega \times \mathbf{r}_0)Q_{\infty}] \cdot \left(\sum_{cell} \mathbf{S}_{\diamond} \right) - Q_{\infty} \Omega \cdot \left(\sum_{cell} \mathbf{M} \right) = 0 \quad (25)$$

The inconsistency of Eqs. (23) and (24) was pointed out in Ref. 1 and had been overlooked for constructing the free-stream capturing metrics in space and time. In other words, surface vectors and moments have to be computed to satisfy Eqs. (5) and (7), respectively.

The error introduced by the use of the inconsistent area moment has a unique feature. Let the cell surface be a parallelogram ($\mathbf{S}_{\diamond} = \mathbf{S}_{\Delta} + \mathbf{S}_{\nabla} = 2\mathbf{S}_{\Delta}$ and $\mathbf{r}_{\diamond} = \frac{1}{2}(\mathbf{r}_{\Delta} + \mathbf{r}_{\nabla})$). Now the difference between Eqs. (23) and (24) can be shown as

$$\sum_{cell} (\mathbf{r}_{\diamond} \times \mathbf{S}_{\diamond} - \mathbf{r}_{\Delta} \times \mathbf{S}_{\Delta} - \mathbf{r}_{\nabla} \times \mathbf{S}_{\nabla}) = \sum_{cell} ([(\mathbf{r}_{\diamond} - \mathbf{r}_{\Delta}) + (\mathbf{r}_{\diamond} - \mathbf{r}_{\nabla})] \times \mathbf{S}_{\Delta}) = 0 \quad (26)$$

Thus the error disappears, for example, on the Cartesian grid. For a hexahedron having arbitrary quadrilateral surfaces, the error can be written as

$$\frac{1}{V} \left| \sum_{cell} (\mathbf{r}_{\diamond} - \mathbf{r}_{\Delta}) \times \mathbf{S}_{\Delta} \right| = O(1) \quad (27)$$

where $|\mathbf{r}_{\diamond} - \mathbf{r}_{\Delta}| = O(h)$, $|\mathbf{S}_{\Delta}| = O(h^2)$ and $V = O(h^3)$. This error may be ignored as long as the effect of Coriolis force is negligible in the flow field.

Alternate Ways of Free-Stream Capturing

There are two other ideas to preserve the free stream. The simple way, especially for the rigid motion of a grid, is to use the free-stream subtraction technique,² when the free stream is uniform. One can obtain the equation by replacing Q and \mathbf{F} in Eq. (1) with $Q - Q_{\infty}$ and $\mathbf{F} - \mathbf{F}_{\infty}$, respectively.

The other conceptually different way is to use \mathbf{S}_Δ always; that is, to regard the hexahedral cell as dodecahedron or to divide the hexahedral cell into tetrahedron. Then, instead of Eq. (14), one will obtain

$$\sum_{cell} \mathbf{S}_\Delta = 0 \quad (28)$$

for either dodecahedron or tetrahedron in addition to Eq. (24). The resulting metric terms will preserve the free stream. The use of the tetrahedral cell allows the most compact and consistent metric formulation. Note, however, that the use of the tetrahedron results in unstructured-grid formulations.

Finite-Difference Formulation

Geometric Identities in the Finite-Difference Formulation

The analysis of the FD method can be simplified with the aid of the above discussion of the FV method. The FD formulation has to be derived from the integral form, Eq. (1). Again from Ref. 1, the differential form for Eq. (1) can be written with a generalized coordinate transformation,

$$\mathbf{r} = \mathbf{r}(\xi, \eta, \zeta, \tau), \quad t = \tau \quad (29)$$

as follows:

$$\hat{Q}_\tau + \hat{E}_\xi + \hat{F}_\eta + \hat{G}_\zeta = 0 \quad (30)$$

where subscripts indicate partial differentiation,

$$\hat{Q} = QV, \quad \hat{E} = \mathbf{S}^\xi \cdot \mathbf{F}, \quad \hat{F} = \mathbf{S}^\eta \cdot \mathbf{F}, \quad \hat{G} = \mathbf{S}^\zeta \cdot \mathbf{F}$$

and where

$$\mathbf{S}^\xi = \mathbf{r}_\eta \times \mathbf{r}_\zeta, \quad \mathbf{S}^\eta = \mathbf{r}_\zeta \times \mathbf{r}_\xi, \quad \mathbf{S}^\zeta = \mathbf{r}_\xi \times \mathbf{r}_\eta \quad (31)$$

and

$$V = \mathbf{r}_\xi \cdot \mathbf{r}_\eta \times \mathbf{r}_\zeta \quad (32)$$

These metrics are related with the usual FD notations as

$$\frac{\nabla \xi}{J} = \frac{1}{J}(\xi_x, \xi_y, \xi_z)^T = \mathbf{S}^\xi \quad (33)$$

and

$$\frac{\xi_t}{J} = -\mathbf{S}^\xi \cdot \mathbf{r}_\tau \quad (34)$$

where $\mathbf{r}_\tau = \mathbf{v}$ and J is the transformation Jacobian, $J = 1/V$. Analogous definitions can be derived for the other directions. The differential forms of the geometric identities are known as

$$(\mathbf{S}^\xi)_\xi + (\mathbf{S}^\eta)_\eta + (\mathbf{S}^\zeta)_\zeta = 0 \quad (35)$$

and

$$V_\tau = (\mathbf{S}^\xi \cdot \mathbf{r}_\tau)_\xi + (\mathbf{S}^\eta \cdot \mathbf{r}_\tau)_\eta + (\mathbf{S}^\zeta \cdot \mathbf{r}_\tau)_\zeta \quad (36)$$

Equation (36) is called the differential statement of the geometric conservation law (GCL).⁷

Free-Stream Capturing Metrics in Space and Time

Following Ref. 1, let the edges of the hexahedron in Fig. 1 be redefined as a double-sized cell in the FD grid ($\mathbf{r}_1 = \mathbf{r}_{i-1,j-1,k-1}$, $\mathbf{r}_2 = \mathbf{r}_{i-1,j+1,k-1}$, $\mathbf{r}_3 = \mathbf{r}_{i-1,j+1,k+1}$, ..., $\mathbf{r}_8 = \mathbf{r}_{i+1,j-1,k+1}$). Also let the time level advance from t_1 to t_2 . Then, all the discussions for the FV formulation in the previous section can be applied to the FD formulation for the central differencing.

The surface vector evaluations, Eqs. (11) and (12), can be regarded as the evaluations of the free-stream capturing metrics in the stationary grid for the FD method. For example, Eq. (11) has been applied for the central-differencing part in Ref. 4. Equation (12) can be rewritten as

$$\begin{aligned} \mathbf{S}_{i-1,j,k}^\xi &= (\mathbf{r}_{56} - \mathbf{r}_{12}) \times (\mathbf{r}_{15} - \mathbf{r}_{26}) \\ &= \frac{(\mathbf{r}_5 - \mathbf{r}_1) + (\mathbf{r}_6 - \mathbf{r}_2)}{2} \times \frac{(\mathbf{r}_1 - \mathbf{r}_2) + (\mathbf{r}_5 - \mathbf{r}_6)}{2} \\ &= -\frac{1}{4}(\delta_\zeta \mathbf{r}_{i-1,j-1,k} + \delta_\zeta \mathbf{r}_{i-1,j+1,k}) \times (\delta_\eta \mathbf{r}_{i-1,j,k-1} + \delta_\eta \mathbf{r}_{i-1,j,k+1}) \end{aligned} \quad (37)$$

where δ denotes the difference operator. After scaling by one-fourth to adjust the area from double-sized to regular cell, the first component of the above expression can be written as

$$\frac{\xi_x}{J} = (\mu_\zeta \delta_\eta y)(\mu_\eta \delta_\zeta z) - (\mu_\zeta \delta_\eta z)(\mu_\eta \delta_\zeta y) \quad (38)$$

where μ denotes the arithmetic averaging operator. Thus, Eq. (12) is equivalent to the consistently differenced metrics in Ref. 3 that are based on the averaging procedure so as to satisfy the differential chain rules numerically.

The main discrepancy between the FV and FD formulations appears in the definition of cell volume. The cell volume defined by Eq. (13) is different from the one defined by the discretized form of Eq. (32) because the FD method does not use the cell concept. Nevertheless, Eq. (13) can be applied to the FD method with a scaling factor of one-eighth instead of Eq. (32). Then, the FV space metrics on the double-sized cell become identical to the FD ones.

The FD time-metric evaluation is also considered from the FV point of view. It is easily found that the time-metric evaluation, Eq. (34), will not maintain the free stream even with the use of the free-stream capturing metrics, Eqs. (11) or (12), in case of a rotating frame because of Eq. (23). Also, it can be shown that such inconsistent time metrics do not satisfy GCL. The discretized form of GCL can be written as

$$\Delta V = \Delta \tau [\delta_\xi (\mathbf{S}^\xi \cdot \mathbf{r}_\tau) + \delta_\eta (\mathbf{S}^\eta \cdot \mathbf{r}_\tau) + \delta_\zeta (\mathbf{S}^\zeta \cdot \mathbf{r}_\tau)] \quad (39)$$

Let the grid move in the rigid rotation, that is, $V_\tau = 0$ and $\mathbf{r}_\tau = \Omega \times \mathbf{r}$. Then the left-hand side of Eq. (39) is zero. But the right-hand side results in $\delta_\xi (\mathbf{r} \times \mathbf{S}^\xi) + \delta_\eta (\mathbf{r} \times \mathbf{S}^\eta) + \delta_\zeta (\mathbf{r} \times \mathbf{S}^\zeta) \neq 0$ (Eq. (23) appears again). This indicates that the use of the GCL condition, Eq. (39), for computing ΔV can be erroneous. In other words, the GCL condition, Eq. (39), is necessary to preserve the free stream, but not sufficient to construct consistent metrics in space and time.

It is easily found that the time integration of Eq. (39) from t_1 to t_2 results in Eq. (18) and thus both equations are equivalent. Therefore, the consistent time metrics

can be obtained, for example in the ξ direction, by replacing $\mathbf{S}^\xi \cdot \mathbf{r}_r$ in the right-hand side of Eq. (34) with the time average, $V_{S\xi}/\Delta t$, of Eq. (16) as,

$$\frac{\xi_t}{J} = -\frac{1}{\Delta t} \int_{t_1}^{t_2} \mathbf{S}^\xi \cdot \mathbf{r}_r dt = -\frac{V_{S\xi}}{\Delta t} \quad (40)$$

Note that ξ_t defined by Eq. (40) contains all information about the movement of a cell surface, such as translation, rotation and deformation. In contrast, Eq. (34) is a simple product of surface area and velocity of cell centroid and thus can represent only a translational motion.

The free-stream subtraction technique will be useful for the rigid motion of the grid, because a rigorous evaluation of Eq. (40) is expensive computationally. Note that the subtraction is required only for the time-metric terms with the use of the free-stream capturing metrics in space.⁵

Concluding Remarks

This paper summarizes the free-stream capturing techniques for the finite-volume (FV) and finite-difference (FD) formulations following a 1989 journal article by M. Vinokur. For an arbitrary motion of the grid, the FV analysis shows that volumes swept by all six surfaces of the cell have to be computed correctly. This means that the free-stream capturing time-metric terms should be calculated not only from a surface vector of a cell at a single time level, but also from a volume swept by the cell surface in space and time. The error introduced by conventional inconsistent time metrics is also shown. The FV analysis also gives a guideline to construct free-stream capturing metrics in space and time for the FD formulation by regarding an FV cell as an FD mesh. The discretized geometric conservation law is shown to be a necessary condition but not a sufficient one.

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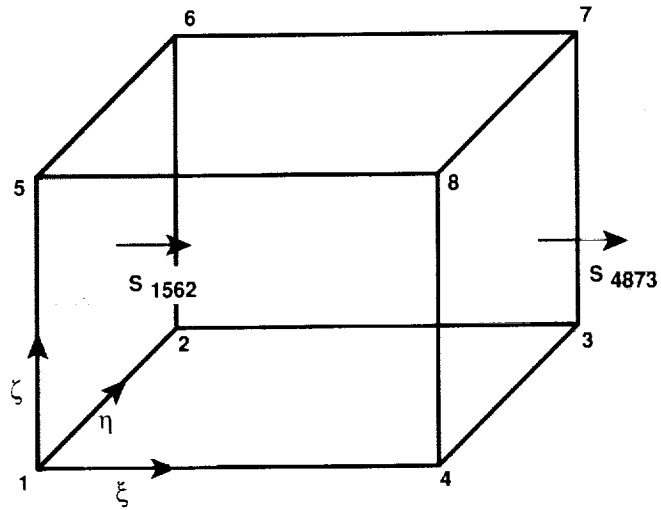


Fig. 1 Geometry of a hexahedral cell.

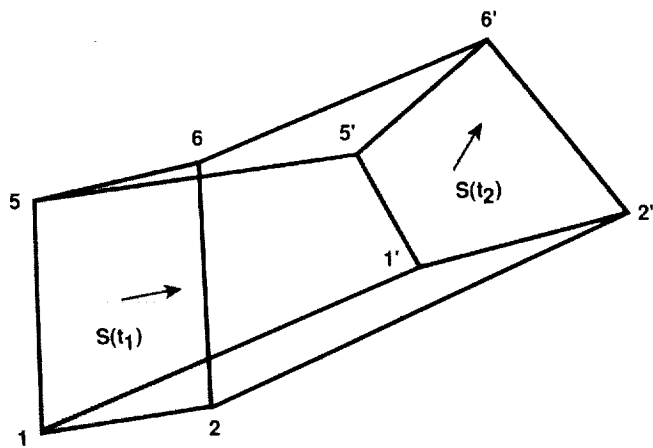


Fig. 2 Volume swept by a surface.



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