

# Efficient Computation of Volume in Flow Predictions

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## Introduction

IN this Note we propose an efficient method of calculating cell volumes for time-dependent three-dimensional flow predictions. The computation of volume, as defined by eight arbitrary corner points (see Fig. 1), is required in numerical methods based on integral or "finite volume" approaches. If the time-dependent method is used solely to obtain a steady-state solution, it is not necessary that the computation of the volume or its change with time be accurate, since the governing equations essentially require the surface integrals to vanish; hence, only the volume needs to be closed. However, in order to eliminate purely geometric errors for time-accurate marching, the volume integral has to be accurate. Given eight arbitrary corner points, the simplest way to define a shape whose volume can be precisely calculated is to partition each face into two planar triangles. Then the volume depends on the orientation of the partitioning, since the diagonals of four nonplanar points do not intersect. In order for neighboring cells to be contiguous, neighboring cell faces must have the same surface partitioning.

Rizzi and Erickson<sup>1</sup> partitioned a general hexahedron, defined by eight arbitrary corner points, into five tetrahedra (see Fig. 2). The volume of a tetrahedron is given by one-sixth of the triple product of the three vectors emanating from one of the vertices and ordered according to the right-hand directions. For example,

$$6V_{1438} = r_{41} \cdot (r_{31} \times r_{81}), \quad r_{ij} = r_i - r_j$$

This can be expressed as a  $4 \times 4$  determinant<sup>1</sup> whose entries involve the Cartesian components of the position vectors of the vertices. In order to avoid gaps or overlaps at cell junctures, one needs to employ a checkerboard-type strategy of partitioning in all three directions. This leads to inconvenient programming.

In the approach of Coakley,<sup>2</sup> the cell volume is simply given by the triple product of vectors in the three coordinate directions  $x^i$ , where each vector is the average of the four corresponding edge vectors of the hexahedron. However, the actual cell boundaries are not defined in this procedure.

## New Method

Here, a very simple decomposition of a hexahedron is proposed that does not require checkerboard-like strategies for partitioning the cells in order to avoid gaps or overlaps. Noted first is that the integral of the outward-oriented surface normal over a closed surface vanishes. This is a consequence of the divergence theorem as applied to a constant vector. It follows that any open surface whose boundary is a given closed curve has a unique surface vector independent of the

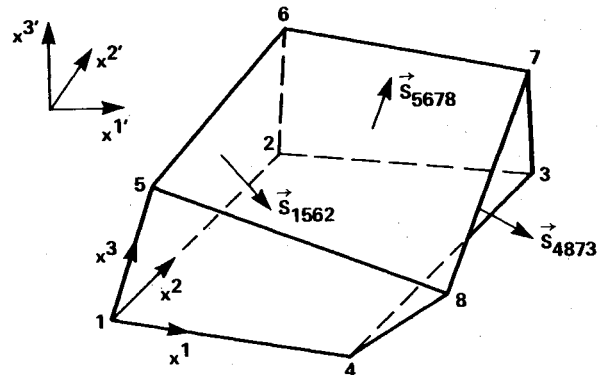


Fig. 1 General computational cell in physical space.

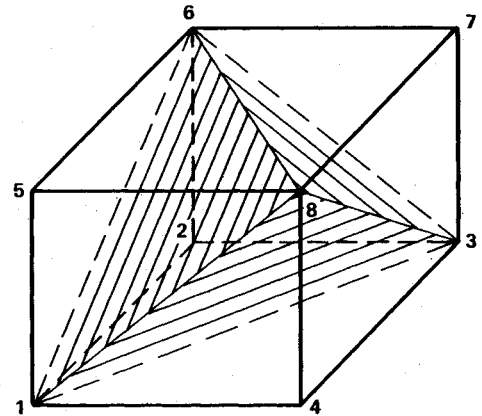


Fig. 2 Suggested partitioning of a general hexahedron into five tetrahedra.

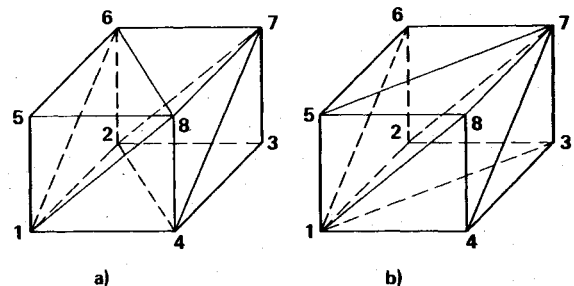


Fig. 3 Two independent ways of partitioning cell surfaces with the same orientation on opposite faces.

shape of the surface. In this context the surface vector  $S_{5678}$  for the surface with the corners 5678 in Fig. 1 is independent of the choice of the partitioning surface diagonal needed to uniquely define the volume. Thus, the alternate expressions can be written as

$$S_{5678} = 0.5(r_{75} \times r_{68}) \quad (1a)$$

$$= 0.5[(r_{85} \times r_{65}) + (r_{67} \times r_{87})] \quad (1b)$$

$$= 0.5[(r_{56} \times r_{76}) + (r_{78} \times r_{58})] \quad (1c)$$

$$= 0.25[(r_{85} + r_{76}) \times (r_{78} + r_{65})] \quad (1d)$$

The use of Eq. (1d) is suggested by Coakley,<sup>2</sup> whereas Rizzi and Erickson,<sup>1</sup> as well as the present authors, favor the simpler Eq. (1a).

In order to use the same computational formula for each computational cell, the partitioning diagonals must have the same orientation for opposite faces of the cell. This can be

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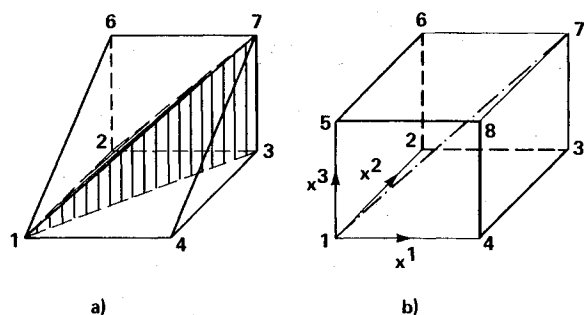


Fig. 4 Suggested decomposition of the cell volume.

done in only two independent ways, as shown in Fig. 3. The decomposition of Fig. 3a is characterized by the fact that six of the eight corners are vertices of two surface diagonals, yielding the maximum number of 12 diagonal ends. The decomposition of Fig. 3b has two corners, each of which is the vertex of three diagonals, and six corners which are vertices of one diagonal. It turns out that the second decomposition yields a more convenient and simpler formula for the computation of the corresponding cell volume. For the computation of the volume consider, for example, the decomposition of the cell into two, as indicated in Fig. 4a. Each portion consists of three tetrahedra such that the total volume is given as

$$6 \text{ Vol} = r_{71} \cdot [(r_{31} \times r_{21}) + (r_{21} \times r_{61}) + (r_{41} \times r_{31}) + (r_{81} \times r_{41}) + (r_{51} \times r_{81}) + (r_{61} \times r_{51})] \quad (2a)$$

$$= r_{71} \cdot [(r_{31} \times r_{24}) + (r_{61} \times r_{52}) + (r_{81} \times r_{45})] \quad (2b)$$

$$= 2r_{71} \cdot (S_{1485} + S_{1234} + S_{1562}) \quad (2c)$$

The expected six triple vector products reduce to three, having one single factor. They do not even require any volume calculations, since the surface vectors are available. Equation (2c) reflects the formula for calculating the volume of a pyramid: the complete cell consists of three topological pyramids with the three faces intersecting in  $r_1$  as base surfaces and with  $r_7$  determining the height with respect to each base. The volume for each pyramid is one-third of the corresponding height times the base surface, resulting in Eq. (2c) (see Fig. 4b). It is noted that for this kind of decomposition, four different volumes can be determined, depending on the choice of main diagonal of the general hexahedron.

### Conclusions

In this Note we have shown how to compute efficiently the nonunique cell volume, based on a partitioning of cell surfaces with the same orientation on opposite faces. Because of its simplicity the new method is particularly suited to handle a time-dependent mesh. The computational effort involved is nominally reduced by at least 40%, compared with Ref. 1. In finite volume approaches where surface vectors are stored, the computational effort reduces further to the dot product of the chosen main cell diagonal with the sum of three surface vectors.

### Acknowledgment

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### References

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<sup>2</sup>Coakley, T. J., "Numerical Method for Gas Dynamics Combining Characteristic and Conservation Concepts," AIAA Paper 81-1257, June 1981.

## Unsteady Transonic Small Disturbance Approximation with Strong Shock Waves

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### Introduction

THE most common methods of predicting steady flow aerodynamic characteristics at transonic speeds use either the transonic small disturbance (TSD) equation<sup>1</sup> or the full potential equation (FPE).<sup>2</sup> The more general Euler equations<sup>3</sup> are expensive to solve, although for flows with strong shock waves such solutions are essential. The FPE is derived on the assumption that the flow is isentropic and irrotational but it generally has a (numerically) exact treatment of the wing boundary conditions. The TSD equation is a further approximation to the full potential equation for small perturbations about freestream conditions. Thin wing boundary conditions are used in the solution procedure. There is some flexibility in deriving the TSD equation. This flexibility generally is utilized by a choice of a transonic scaling parameter. The basic assumptions of isentropy and irrotationality in both these theories are only valid when there are no shock waves in the flow, although a reasonable approximation to flows with shock waves is possible if the local Mach number just ahead of the shock is less than 1.3. If the flow has strong shock waves, however, then there is considerable disagreement between both TSD and FPE solutions and Euler equations solutions. Generally, the predicted shock location for the potential theories is much further aft than that for the Euler equations solutions. This is because the isentropic assumption is invalid in these flows. The causes of the error in the shock location in the steady TSD solutions for two-dimensional flow have been examined in Ref. 4 where a correction procedure has been derived that alters the basic equation within the formal accuracy bounds of the small disturbance approximation. A nonisentropic formulation for the full potential equation is given in Ref. 5. In the present paper, this procedure is extended to unsteady transonic flows, implemented in a modification to the low-frequency unsteady transonic small disturbance code LTRAN2,<sup>6</sup> and the results compared to solutions of the Euler equations.

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