LA-UR-10-02144

Approved for public release; distribution is unlimited.

Title: Accurate Volume Calculations for Unstructured Mesh Elements When Used to Model Primitive Objects (U)

Author(s): Roger L. Martz
David L. Crane

Intended for: American Nuclear Society
RPSD 2010 Meeting
Las Vegas, NV, April 18-23, 2010
and
Nuclear Technology

Accurate Volume Calculations for Unstructured Mesh Elements When Used to Model Primitive Objects

Roger L. Martz and David L. Crane

Los Alamos National Laboratory
PO Box 1663, Los Alamos, NM 87545
martz@lanl.gov; dcrane@lanl.gov

INTRODUCTION

A new geometry capability has been implemented in MCNP [1] that permits the existence of an unstructured mesh representation of a geometry with its legacy Constructive Solid Geometry (CSG) capability to form an hybrid geometry. This new feature enables the user to build complex 3-D models with Computer Aided Engineering (CAE) tools, such as Abaqus [2], and perform a Monte Carlo neutronics analysis on the same geometry mesh that is used for thermo-mechanical analyses.

A requirement in implementing this new geometry capability is accurate volume calculations for all mesh elements. This is complicated due to the fact that first and second order elements, where the elements may be 4-, 5-, or 6-sided, may have bilinear or quadratic faces. This paper discusses the adoption of a methodology for use in calculating these volumes and evaluates its use when modeling some common primitive objects.

METHODOLOGY

Numerous finite element text books and papers have shown the advantage of transforming or mapping from a curvilinear coordinate system (global space) to a Cartesian coordinate system (master space) where it is easier to perform certain calculations. We pursue this approach in order to calculate accurate volumes for unstructured mesh elements.

Let u^d be the coordinates in the global space with $d = 1, 2, or\ 3$, representing *x, y,* or *z*. Correspondingly, let θ^d be the coordinates in the master space with $d = 1, 2, or\ 3$, representing *g*, *h*, and *r*.

The mapping function from one space to the other depends upon the element type. The six different functions with which we have dealt can be factored so that there exists one term, f_m, for each node, M total nodes.

$$f_m(g,h,r) \in [1, g, h, r, gh, hr, gr, ghr, g^2, h^2, r^2, \cdots]$$

Mapping of a node *w* in master space to its corresponding node *w* in global space (i.e., we do not intend to permit excessively twisted or inverted elements during the mapping process) requires evaluation of the f_m terms at the *w* node in the master space. Hence, $f_{wm}(g,h,r)\,|_w$ denotes the evaluation at node *w* with the corresponding values of *g*, *h*, and *r* so that the terms evaluate to either -1, 0, or 1. Then in general, the mapping for each dimension between the two spaces for each node *w* can be written as

$$\left[u_w^d\right] = \left[f_{wm}\right] \cdot \left[a_w^d\right] \qquad (1)$$

a_w^d are coefficients for each dimension and can be found from

$$\left[a_w^d\right] = \left[f_{wm}\right]^{-1} \cdot \left[u_w^d\right] \qquad (2)$$

To calculate an element's volume, we use the expression for the differential volume [3]

$$dV_{global} = \left|J\right| dg\,dh\,dr = dV_{master} \qquad (3)$$

Where J is the Jacobian and

$$\left|J\right| = \sum_{i=1}^{M}\sum_{j=1}^{M}\sum_{k=1}^{M} \left|A_{ijk}\right| \frac{\partial f_i}{\partial g}\frac{\partial f_j}{\partial h}\frac{\partial f_k}{\partial r} \qquad (4)$$

With

$$\left|A_{ijk}\right| = \begin{vmatrix} a_i^x & a_j^x & a_k^x \\ a_i^y & a_j^y & a_k^y \\ a_i^z & a_j^z & a_k^z \end{vmatrix} \qquad (5)$$

The indexes, i, j, k, extend over the three dimensions.

The volume is found by integrating Equation (3) in the master space where the limits of integration are generally -1 to 1 or 0 to 1, depending on the element shape and dimension.

The triple summation of Equation (4) implies a large number of terms for the volume evaluation. In reality, a great many of these terms are zero. Table I summarizes the maximum number of partial terms and the number of non-zero partial terms by mesh element type.

Table I. Number of partial terms by element type

Faces	Nodes	Max # of Partial Terms	Non-zero Partial Terms
4	4	64	1
5	6	216	6
6	8	512	8
4	10	1000	64
5	15	3375	222
6	20	8000	222

It should be recognized that this methodology holds for area calculations as well once the appropriate simplifications have been made in Equations (1) to (5).

RESULTS

Even when creating complex 3-D geometry models with CAE tools, simple primitive objects such as spheres, cylinders, and parallelepipeds are often used in some fashion. Other times, objects may be created from synthetic surfaces in lieu of analytic surfaces. Regardless, it is from this collection of objects that the unstructured mesh is created. Given a fixed set of element types, the accuracy of the mesh to represent the model depends upon its granularity. For example, it is impossible for any standard, single 1st order mesh element type to accurately model a sphere as it might be feasible to use a single 1st order mesh element to model certain parallelepipeds. A single 2nd order hexahedron would fare better, due to its ability to possess more curvature with it quadratic faces, but it too would fall short. However, if the elements are small enough, more can be used to approximate the sphere really well. The question then is how many and of what size need they be? The answer lies in determining how well the sum of the mesh element volumes represents the volume of the sphere.

We examine this issue with several primitive objects that possess curvature: a sphere and a right circular cylinder.

First, we chose to mesh a sphere with radius 3 using 1st and 2nd order hexahedrons with various meshing seeds. The seed parameter presented in the table is an Abaqus/CAE parameter used to set the element size. Abaqus attempts to make elements with edges of this length; no attempt was made to force edges to this length. The number of total elements in the model is dictated by the seed number. The volume results using the current method along with the actual volume are presented in Table II.

Next, we chose to mesh a right circular cylinder with radius 5 and height 5 using 1st and 2nd order tetrahedrons with various meshing seeds to obtain representations with various number of mesh elements. The volume results using the current method along with the actual volume are presented in Table III.

Table II. Volume comparisons for a sphere (r = 3 cm) with different numbers of hex elements

Seed (cm)	Number of Elements	Mesh Volume (cm^3)	% Difference*
1st Order Hexahedrons			
1.5	56	95.0270	19.0
1.0	224	110.2924	2.54
0.5	1320	111.6583	1.29
0.4	3456	112.2451	0.76
0.3	7168	112.6199	0.42
2nd Order Hexahedrons			
2.0	32	111.4489	1.50
1.5	56	112.4322	0.59
1.0	224	113.0342	0.056
0.5	1320	113.0941	0.003
0.4	3456	113.0960	0.001
0.3	7168	113.0968	0.0004
Actual		113.0973	n/a

* from actual volume

Table III. Volume comparisons for a right circular cylinder (r = 5 cm, h = 5 cm) with different numbers of tet elements

Seed (cm)	Number of Elements	Mesh Volume (cm^3)	% Difference*
1st Order Tetrahedrons			
4.0	123	719.709	9.0
3.0	345	754.154	4.0
2.0	621	762.589	3.0
1.5	2170	778.478	0.9
1.0	5295	780.139	0.7
0.5	33369	784.023	0.2
2nd Order Tetrahedrons			
5.0	38	784.635	0.1
4.0	123	784.955	0.056
3.0	345	785.296	0.013
2.0	621	785.343	0.007
1.5	2170	785.393	0.0006
1.0	5295	785.395	0.0004
0.5	33369	785.398	0.0
Actual		785.398	n/a

* from actual volume

CONCULSIONS

We have successfully shown that by transforming from a curvilinear coordinate system to a Cartesian system through a well-behaved mapping, accurate volume calculations can be achieved for mesh elements that possess bilinear and quadratic faces.

When modeling primitive objects that possess curvature, fewer numbers of 2nd order mesh elements, by several orders of magnitude, are needed to accurately reproduce the intended volume. This will have a direct impact on particle tracking times and accuracy of results.

REFERENCES

1. X-5 MONTE CARLO TEAM, "MCNP – A General Monte Carlo N-Particle Transport Code, Version 5, Volume I: Overview and Theory," LA-UR-03-1987, Los Alamos National Laboratory (April 2003).
2. Dassault Systemes Simulia, Inc., "ABAQUS USER MANUALS, Version 6.9," Providence, RI (2009).
3. O. C. Zienkiewics, *The Finite element Method in Engineering Science*, p. 511, McGraw-Hill, London (1971).