### Acknowledgment

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#### References

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<sup>2</sup>Bartz, D. R., "Heat Transfer from Rapidly Accelerating Flows," in *Advances in Heat Transfer*, edited by J. P. Hartnett and T. F. Irvine Jr., Vol. 2, Academic Press, New York, 1965.

<sup>3</sup>Cebecci, T. and Smith, A. M. O., Analysis of Turbulent Boundary Layers, Academic Press, New York, 1974.

<sup>4</sup>Eckert, E. R. G., Analysis of Heat and Mass Transfer, McGraw Hill, New York, 1972.

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# **Technical Comments**

# Comment on "Singularity-Free Extraction of a Quaternion from a Direction-Cosine Matrix"

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LUMPP<sup>1</sup> describes a direction-cosine matrix to quaternion conversion algorithm which, although valid for all rotations, is unnecessarily sensitive to numerical imprecision. This imprecision can come from the algorithm which produces the direction-cosines or simply from the limited length of the registers that realize the direction-cosines. The sensitivity can be seen by noting that the magnitudes of the quaternion components are computed from the diagonal elements of the direction-cosine matrix. For a rotation of an angle  $\phi$  about the first axis, the diagonal elements are, in order, 1,  $\cos \phi$ ,  $\cos \phi$ . For small  $\phi$  the off-diagonal elements,  $\sin \phi$  and  $-\sin \phi$ , are more suitable numerically for determining  $\phi$ .

In general, since the magnitudes of the quaternion components are computed as square-roots, the squares of the components are most closely related to the direction-cosine matrix elements. The sensitivity of the magnitude  $\theta$  of a rotation caused by an error in the square of a quaternion component  $q_i$ , to the error, can be expressed

$$\frac{\partial \theta}{\partial q_i^2} = \frac{\sqrt{1 - q_i^2}}{|q_i|} \tag{1}$$

Thus precision is reduced whenever any quaternion component is small. This occurs for small rotations, for rotations about an axis nearly perpendicular to a reference axis, and for rotations of nearly 180 deg about any axis. Floating-point arithmetic is of little benefit because the expression for the square of each quaternion component contains a large constant term which limits the scaling reduction.

The following algorithm retains precision for all rotations by computing only the component of largest magnitude as a square-root and by using only this component as a divisor in computing the other components. Since there is always at least one component of magnitude greater than or equal to ½, numerical imprecision will have a limited effect on precision and will not cause a negative square-root argument or division by zero. The expressions follow immediately from the expression for a direction-cosine matrix in terms of quaternion components (given in Klumpp¹). Klumpp's notation is followed but, in some cases, the (equivalent) negative quaternion is computed.

Choose the largest (algebraically) of  $\operatorname{tr}(M)$ ,  $M_{i,i}$  (i=1-3). If  $\operatorname{tr}(M)$  is largest, compute the quaternion using the following expressions:

$$q_0 = \sqrt{I + \operatorname{tr}(M)}/2 \tag{2}$$

$$q_i = (M_{k,i} - M_{i,k})/4q_0$$
 (i=1-3)

where j and k are chosen so that i, j, k is a cyclic permutation of 1, 2, 3. If tr(M) is not largest, use the following expressions:

$$q_i = \sqrt{M_{i,i}/2 + (I - \text{tr}(M))/4}$$
 (4)

$$q_0 = (M_{k,i} - M_{i,k}) / 4q_i$$
 (5)

$$q_{i} = (M_{l,i} + M_{i,l})/4q_{i}$$
  $(l = j, k)$  (6)

where i, j, k is the cyclic permutation of 1, 2, 3 such that  $M_{i,i}$  is the largest above.

The precision of this algorithm was verified with a Fortran program. Quaternions were converted to direction-cosine matrices and then converted back using both algorithms. Precision, with respect to the magnitude of the error, was reduced with Klumpp's algorithm whenever any quaternion component was small, while full precision was always retained with the above algorithm. Precision, with respect to the direction of the rotation (of interest when computing the eigenvector of the direction-cosine matrix), was reduced with Klumpp's algorithm whenever a quaternion vector component was small, while full precision was retained with the above algorithm even (because of the floating point arithmetric) for small rotations.

## References

<sup>1</sup>Klumpp, A. R., "Singularity-Free Extraction of a Quaternion from a Direction-Cosine Matrix," *Journal of Spacecraft and Rockets*, Vol. 13, Dec. 1976, pp. 754-755.

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