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ABSTRACT

In Delaunay-based grid generation algorithms the in-sphere criterion plays a central role. An accurate and robust algorithm for employing the in-sphere criterion is proposed. In the derivation of the circumcentre and radius of the circumscribing sphere of a tetrahedral element needed for the in-sphere criterion round-off errors and propagation errors are introduced. The new algorithm is designed such that these errors are minimised. Furthermore, it is shown that the in-sphere criterion can be made invariant for scaling transformations.

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An accurate and robust algorithm for the in-sphere criterion for automated Delaunay-based Tetrahedral Grid Generation

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Summary

In Delaunay-based grid generation algorithms the in-sphere criterion plays a central role. An accurate and robust algorithm for employing the in-sphere criterion is proposed. In the derivation of the circumcentre and radius of the circumscribing sphere of a tetrahedral element needed for the in-sphere criterion round-off errors and propagation errors are introduced. The new algorithm is designed such that these errors are minimised. Furthermore, it is shown that the in-sphere criterion can be made invariant for scaling transformations.

1 Introduction

Currently, much effort is devoted towards the development of automatic tetrahedral grid generation algorithms. Tetrahedral grid generation algorithms can be categorised into three approaches: the advancing front approach (Refs. 1, 2, 3, 4), the Delaunay node insertion approach (Refs. 5, 6, 7, 8, 9) and the quadtree/octree approach (Refs. 10, 11).

The present paper focusses on the in-sphere criterion which is used in the Delaunay-based node insertion approach. The objective of the paper is to develop a more accurate and robust algorithm for the in-sphere criterion. The in-sphere criterion decides whether a node is inside or outside the circumscribing sphere associated to a given tetrahedral element.

Advantageous property of using the in-sphere criterion in the Delaunay-based node insertion approach is that the resulting tetrahedral grid is non-overlapping and that all tetrahedral elements have a positive volume. Disadvantage, however, is that current implementations of the in-sphere criterion lack accuracy and robustness.
Ill-conditioned tetrahedral elements appear in each stage of the Delaunay-based node insertion algorithm, particularly in the initial stages of the grid generation algorithm when the nodes of an input surface triangulation are inserted into an existing tetrahedral grid. The derivation of the circumcentre and radius for an ill-conditioned matrix can be inaccurate.
Furthermore, a degeneracy occurs in case a node is exactly located on the circumscribing sphere of a tetrahedral element. In case this node is connected to the grid the uniqueness of the tetrahedral grid is lost. This situation is handled by rejecting a node which is located on the sphere within some specified tolerance. The degeneracy cannot be circumvented and provides an inherent difficulty of the in-sphere criterion. To ensure that all surface nodes of an input surface triangulation (representing the flow domain) are inserted into the tetrahedral grid a rejected surface node is moved over a small distance. As a result the input surface triangulation has been changed on termination of the tetrahedral grid generation algorithm which is clearly undesirable. By designing a more accurate and robust algorithm for handling the in-sphere criterion the movement of surface nodes can be alleviated.

In Refs. 13, 14, 15 it is proposed to use integer arithmetic to exactly compute the circumcentre and the radius. To this purpose the physical coordinates of the nodes in the tetrahedral grid need to be scaled, so that they can be modelled by an integer representation.

In the present paper it is shown that the in-sphere criterion can be handled with the same ac-

curacy as an integer arithmetic approach. The crux of the new algorithm is that the nodes of a tetrahedral element (for which one derives the circumscribing sphere) and the coordinates of these nodes can be permuted in such a way that round-off errors and propagated errors (amplified due to matrix decomposition) are minimised. As a result of the approach the volume of the tetrahedral element under consideration is computed with the best attainable accuracy (under the assumptio=n that the physical coordinates of the nodes are specified in floating point format).

2 Circumscribing sphere of a tetrahedral element

The in-sphere criterion decides wether a node $\underline{x}$ is located inside, on or outside the sphere which passes through the four nodes of a tetrahedral element. The construction of the circumscribing sphere is explained here.

Consider a tetrahedral element which is defined by four nodes with physical coordinates $\underline{x}_p$, $\underline{x}_q$, $\underline{x}_r$, and $\underline{x}_s$; the nodes are ordered so that the volume of the tetrahedral element is positive. The circumcentre and the radius of the circumscribing sphere for a tetrahedral element are derived by requiring that the distance between each node of the tetrahedral element and the circumcentre are equal to the radius. This leads to 4 (quadratic) equations with 4 unknowns (the 3 coordinates of the circumcentre and the radius) which can be written as

$$\mathbf{s} = \begin{bmatrix} (\underline{x}_p - \underline{x}_c, \underline{x}_p - \underline{x}_c) \\ (\underline{x}_q - \underline{x}_c, \underline{x}_q - \underline{x}_c) \\ (\underline{x}_r - \underline{x}_c, \underline{x}_r - \underline{x}_c) \\ (\underline{x}_s - \underline{x}_c, \underline{x}_s - \underline{x}_c) \end{bmatrix} = \begin{bmatrix} L^2 \\ L^2 \\ L^2 \\ L^2 \end{bmatrix} \tag{1}$$

where the circumcentre of the sphere is $\underline{x}_c$, the radius is L and $(,)$ denotes the innerproduct.

The radius L can be eliminated by for instance selecting the first equation and substracting this equation from the second, third and fourth equation. This operation can be expressed by means of the permutation matrix

$$\mathbf{\Pi} = \begin{bmatrix} -1 & 1 & 0 & 0 \\ -1 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \tag{2}$$

By pre-multiplying system (1) with the permutation matrix (2) shown a system of three equations in the three unknowns (physical coordinates of the circumcentre $\underline{x}_c$) remains

$$\begin{cases} (\underline{x}_q, \underline{x}_q) - 2(\underline{x}_q, \underline{x}_c) - (\underline{x}_p, \underline{x}_p) + 2(\underline{x}_p, \underline{x}_c) = 0, \\ (\underline{x}_r, \underline{x}_r) - 2(\underline{x}_r, \underline{x}_c) - (\underline{x}_p, \underline{x}_p) + 2(\underline{x}_p, \underline{x}_c) = 0, \\ (\underline{x}_s, \underline{x}_s) - 2(\underline{x}_s, \underline{x}_c) - (\underline{x}_p, \underline{x}_p) + 2(\underline{x}_p, \underline{x}_c) = 0. \end{cases} \tag{3}$$

The permutation matrix (2) represents a tree which spans the four nodes of the tetrahedral element. This can be seen by forming edges between the two nodes of a tetrahedral element which have non-zero entries in the permutation matrix. It is well-known that a graph having n nodes has n^{n-2}

trees, hence for a tetrahedral element 16 different permutation matrices exist.
The three equations (3) form a linear system which can be written as

$$\begin{bmatrix} x_q - x_p & y_q - y_p & z_q - z_p \\ x_r - x_p & y_r - y_p & z_r - z_p \\ x_s - x_p & y_s - y_p & z_s - z_p \end{bmatrix} \underline{x}_c = \frac{1}{2} \begin{bmatrix} (\underline{x}_q, \underline{x}_q) - (\underline{x}_p, \underline{x}_p) \\ (\underline{x}_r, \underline{x}_r) - (\underline{x}_p, \underline{x}_p) \\ (\underline{x}_s, \underline{x}_s) - (\underline{x}_p, \underline{x}_p) \end{bmatrix}. \tag{4}$$

The determinant of the 3×3 matrix A (on the left hand-side) equals two times the volume of the tetrahedral element: $det(A) = 2\ V$. The inverse of matrix A exists only if the volume of the tetrahedral element is non-zero. The physical coordinates of the circumcentre are then obtained by solving equation (4). The radius of the circumscribing sphere is calculated from the inner product

$$L^2 = (\underline{x}_c - \underline{x}_p, \underline{x}_c - \underline{x}_p). \tag{5}$$

The circumcentre obtained by solving system (4) is rotation, translation and scaling invariant. Let the operator $\mathbf{R}^x_\theta$ be a rotation of θ radians around the x-axis (for the y- and z-axis a similar operator is defined), the operator $\mathbf{T}_{\underline{a}}$ is the translation $\mathbf{T}_{\underline{a}}\underline{x} = \underline{x} - \underline{a}$ and the operator $\mathbf{S}_\delta$ is a scaling with $\mathbf{S}_\delta \underline{x} = \delta\ \underline{x}$. Transform the physical coordinates of the tetrahedral element as

$$\underline{x}^\star = \mathbf{R}^x_{\theta_x}\ \mathbf{R}^y_{\theta_y}\ \mathbf{R}^z_{\theta_z}\ \mathbf{S}_\delta\ \mathbf{T}_{\underline{a}}\ \underline{x}. \tag{6}$$

The physical coordinates of the circumcentre are then

$$\underline{x}^\star_c = \mathbf{R}^x_{\theta_x}\ \mathbf{R}^y_{\theta_y}\ \mathbf{R}^z_{\theta_z}\ \mathbf{S}_\delta\ \mathbf{T}_{\underline{a}}\ \underline{x}_c. \tag{7}$$

which satisfy system (4) for the transformed coordinates. The circumcentre is invariant with respect to any sequence of the above listed operations. By adopting these tranformations the di-hedral angles of the initial tetrahedral element are preserved.

3 Model tetrahedral element

A tetrahedral element defined by 4 nodes has 12 degrees of freedom. Without loss of generality the construction of the circumscribing sphere can be analysed for a tetrahedral element which has only 5 degrees of freedom. This is accomplished by transforming the tetrahedral element according to (6).

Let the nodes of the tetrahedral element be ordered in such a way that the distance between nodes p and q is the largest in the element, viz:

$$||\underline{x}_p - \underline{x}_q|| \geq ||\underline{x}_i - \underline{x}_j|| \quad \text{with } (i,j) \neq (p,q) \text{ and } i,j \in \{p,q,r,s\}.$$

The tetrahedral element is transformed according to (6) by taking $\delta = 1/||\underline{x}_p - \underline{x}_q||$ and $\underline{a} = \underline{x}_p$. The rotation angles θ_y and θ_z are defined so that node q coincides with $[1,0,0]^T$ and the rotation angle θ_x is defined so that node r or s is located in the $z = 0$ plane.

The initial tetrahedral element is then transformed into a model tetrahedral element which has only 5 degrees of freedom:

$$\begin{aligned}
\underline{x}_p &= [0,0,0]^T, \\
\underline{x}_q &= [1,0,0]^T, \\
\underline{x}_r &= [R_2\cos(\alpha), R_2\sin(\alpha), 0]^T, \\
\underline{x}_s &= [R_3\cos(\beta)\cos(\gamma), R_3\sin(\beta)\cos(\gamma), R_3\sin(\gamma)]^T.
\end{aligned} \tag{8}$$

with $R_2, R_3 \in [0,1]$ and $\alpha \in [0,\pi]$, $\beta \in [-\pi,\pi]$ and $\gamma \in [0,\pi]$. In Figure 1 the model tetrahedral element is shown. Substitution of the transformed coordinates in the 3×3 system (4) yields the

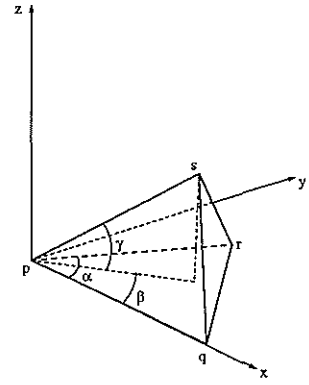

Fig. 1 The model tetrahedral element

system

$$\begin{bmatrix} 1 & 0 & 0 \\ R_2\cos(\alpha) & R_2\sin(\alpha) & 0 \\ R_3\cos(\beta)\cos(\gamma) & R_3\sin(\beta)\cos(\gamma) & R_3\sin(\gamma) \end{bmatrix} \underline{x}_c = \frac{1}{2}\begin{bmatrix} 1 \\ R_2^2 \\ R_3^2 \end{bmatrix}. \tag{9}$$

The determinant of the matrix is

$$\det(A) = R_2 R_3 \sin(\alpha)\sin(\gamma). \tag{10}$$

The condition number of the 3×3 matrix is:

$$k(A) = \frac{1}{\min\{R_2\sin(\alpha), R_3\sin(\gamma)\}} \tag{11}$$

It can be seen that the matrix is ill-conditioned in case $k(A) >> 1$ which holds if the determinant $\det(A)$ equals zero or in other words the tetrahedral element has a volume near zero. Matrix A is ill-conditioned for the cases $R_2 \to 0$, $R_3 \to 0$, $\alpha \to 0$ or $\gamma \to 0$. The condition number of matrix A satisfies $k(A) \geq 1$. The condition number equals $k(A) = 1$ for a tetrahedral element with $R_2 = 1$, $R_3 = 1$, $\alpha = \frac{1}{2}\pi$, $\gamma = \frac{1}{2}\pi$ (β arbitrary)
The circumcentre of the sphere can explicitly be derived by inverting matrix A which yields the analytical solution

$$\underline{x}_c = \frac{1}{2}\left[1, \frac{R_2 - \cos(\alpha)}{\sin(\alpha)}, \frac{[\sin(\beta-\alpha) - R_2\sin(\beta)]\cos(\gamma) + R_3\sin(\alpha)}{\sin(\alpha)\sin(\gamma)}\right]^T \tag{12}$$

From this expression it can be observed that the location of the circumcentre is very sensitive to small disturbances in case the angles α or γ are close to zero. In fact the location of the circumcentre becomes unboundedly large for $\sin(\alpha) \to 0$ or $\sin(\gamma) \to 0$ (provided that $R_2, R_3 \neq 1$.

Starting point for the derivation of the circumcentre and radius of the circumscribing sphere are the physical coordinates of the four nodes $\underline{x}_p$, $\underline{x}_q$, $\underline{x}_r$ and $\underline{x}_s$ defined in floating point format. In the numerical solution of system (4) two kinds of errors can be made, these are:

1. Round-off errors which are introduced in the formation of matrix A
2. Propagation errors which can be made in the decompositioning of matrix A since the matrix is ill-conditioned.

In order to compute an accurate estimate of the circumcentre and radius (needed for the in-sphere criterion) these errors should be minimised.

4 Minimising the influence of the round-off error on the location of the circumcentre

In this section it is shown that the round-off errors arising in the formation of matrix A can be minimised by adopting an algorithm stemming from graph theory, namely the algorithm of Kruskal.

To illustrate the effect of round-off in the formation of matrix A consider the x-coordinates of the nodes and let

$$|x_p| > 10^d \max\{|x_q|, |x_r|, |x_s|\}. \tag{13}$$

with $|x_q|, |x_r|, |x_s| = O(1)$. Following the floating point notation of (Ref. 12) the x-components of matrix A equal

$$\begin{aligned} x_q - *x_p &= x_q - x_p + \varepsilon_{pq}, \\ x_r - *x_p &= x_r - x_p + \varepsilon_{pr}, \\ x_s - *x_p &= x_s - x_p + \varepsilon_{ps}, \end{aligned}$$

with $|\varepsilon_{pq}|, |\varepsilon_{pr}|, |\varepsilon_{ps}| = O(10^d\varepsilon)$. In an integer arithmetic approach the non-significant part of a coordinate would be approximated by zeros so that a round-off error of approximately the same size would be introduced.

By taking a different ordering in the construction of matrix A the influence of round-off can be reduced. Consider for instance the permutation matrix

$$\Pi = \begin{bmatrix} 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 1 \\ 1 & -1 & 0 & 0 \end{bmatrix} \tag{14}$$

The elements in the first column of matrix A are then equal to

$$\begin{aligned} x_r - *x_q &= x_r - x_q + \varepsilon_{rq}, \\ x_s - *x_q &= x_s - x_q + \varepsilon_{sq}, \\ x_p - *x_q &= x_p - x_q + \varepsilon_{pq}, \end{aligned}$$

with $|\varepsilon_{pq}| = O(10^d\varepsilon)$ and $|\varepsilon_{rq}|, |\varepsilon_{sq}| = O(\varepsilon)$. This illustrates that the round-off error can be minimised.

The problem of minimising the round-off error in the system (4) boils down to the minimisation of the global round-off error

$$\eta_1 = \min_{k=1,16} \sum_{i=1,3} \sum_{j=1,3} |a_{i,j,k}|, \quad \text{with} \quad A^k = \Pi^k \mathbf{s} \tag{15}$$

where $\mathbf{s}$ is the vector (1) and Π is the permutation matrix (2). Since the L_1-norm and L_2-norm are equivalent in an N-dimensional Euclidean space ($N = 9$ matrix elements exist) the minimisation can be restated as

$$\eta_2 = \min_{k=1,16} \sum_{i=1,3} \sum_{j=1,3} |a_{i,j,k}|^2. \tag{16}$$

This expression also minimised the round-off error occuring in the right-hand side vector of system (4) which can be proven by employing Schwarz' inequality.

The extremum in the minimisation (16) is obtained by deriving the minimal tree spanning the four nodes of the tetrahedral element. Assign to each edge of the tetrahedral element a weight which equals the square of the distance between the two nodes on the edge. The minimum tree is defined as the tree of minimal weight spanning the tetrahedral element. In order to compute this minimum tree efficiently the algorithm of Kruskal (Ref. 16) is adopted which has a computational cost of $M\,Log M$ where M is the total number of edges in the tree. For a tetrahedral element the computational cost amounts to $6\,Log 6$.

5 Minimising the influence of the propagated error

Since the condition number (11) is large for an ill-conditioned tetrahedral element care should be taken in the numerical inversion of matrix A. It is known that direct solution methods like Cramer's rule or Gaussian elimination are not stable so that round-off errors accumulate in these approaches (Ref. 12). Numerical stability is achieved by complete pivoting (Ref. 17), but this approach is computationally expensive since for each pivot all matrix elements of matrix A have to be accessed. Another more elegant approach similar to complete pivoting would be to choose suitable transformations (6) so that a 3×3 lower-triangular matrix (9) results which can be solved in a numerically stable manner. This method is computationally expensive since 5 matrix operations have to be performed.

For the latter practical reason LU-decomposition (Gaussian elimination) with partial pivoting of the rows of matrix A (Ref. 12) is considered here. LU-decomposition with partial pivoting can be written in the form (Ref. 17)

$$L_2 P_2 L_1 P_1 A = U \tag{17}$$

where L is a lower-triangular matrix, U is an upper-triangular matrix, P_1 and P_2 are permutation matrices (for row interchanges). The determinant of matrix A equals

$$\det(A) = s \det(U) \tag{18}$$

where s is the sign change induced by the number of permutations P_1 and P_2 needed.

6 Handling of the degenerate zero volume case

In order to avoid that during tetrahedral grid generation tetrahedral elements with a non-positive volume are formed it is required that

$$V > 0. \tag{19}$$

The volume is computed from (18) as $V = \frac{1}{2}\det(A)$. Since tetrahedral elements with a volume near zero are ill-conditioned according to (11) these elements receive a special treatment.
To improve the accuracy of the circumcentre and the radius one iterative improvement based on LU-decomposition with partial pivoting (Ref. 18) is adopted for an ill-conditioned tetrahedral element with a volume

$$0 < V < \varepsilon d_{\max}^3. \tag{20}$$

The upperbound has been made relative to the largest edge length $d_{\max}$.

7 In-sphere criterion

To arrive at a robust treatment of the in-sphere criterion the criterion should be invariant for scaling transformations. As a result of this invariance the in-sphere criterion has become independent of the reference length of a geometry under consideration.
A node $\underline{x}$ is located on the circumscribing sphere in case

$$|d_l(\underline{x})| < \varepsilon L^2. \tag{21}$$

where $d_l(\underline{x}) = (\underline{x}_c - \underline{x}, \underline{x}_c - \underline{x}) - L^2$ and $\varepsilon = 1 \times 10^{-11}$. Otherwise, if condition (21) is not satisfied node $\underline{x}$ is located inside the circumscribing sphere if

$$d_l(\underline{x}) < 0, \tag{22}$$

and outside the sphere in case

$$d_l(\underline{x}) > 0. \tag{23}$$

In such a way the in-sphere criterion is made invariant for scaling transformations.

8 Conclusions

In this paper an accurate and robust algorithm for the in-sphere criterion is proposed. The calculation of the circumcentre and the radius of the circumscribing sphere of a tetrahedral element is computed with the same accuracy as proposed by integer arithmetic based methods. The volume of a tetrahedral element is computed with the best attainable accuracy in floating point arithmetic.

Application of the proposed algorithm in a three-dimensional Delaunay based tetrahedral grid generation algorithm learns that the computational cost of the proposed algorithm is moderate.

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