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Quality-improved local refinement of tetrahedral mesh based on element-wise refinement switching

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Abstract

This paper presents an effective sliver-free and quality-improved local refinement algorithm of a tetrahedral mesh for an adaptive solution strategy. The method proposed is composed of controlled local refinement and a conventional quality improvement process. The new feature of the proposed method is the introduction of element-wise refinement switching between longest side bisection and octasection, to boost the quality improvement process of face swapping and node relaxation. Numerical results show that this refinement switching plays a critical role in improving the quality of poorly shaped elements while preserving the quality of well-shaped elements. The results also show that the proposed method is more effective than the previously known methods, considering both the average and minimum quality.

Keywords: Switching enabled local refinement; Quality improvement; Tetrahedral mesh; Adaptive solution strategy; TCAD

1. Introduction

The solution of partial differential equations requires the partitioning of the domain into small subdomains, which are called elements. With decreasing device dimensions, the modeled structures of Technology Computer Aided Design (TCAD) have become highly non-planar, and three-dimensional (3D) simulations are required to predict real physical phenomena. The vast quantities of data required for 3D simulation produces the most dominant bottleneck in TCAD analysis [1]. To circumvent this computational burden, a sophisticated adaptive solution strategy is required. In general, the adaptive solution strategy is composed of one prerequisite step and two main steps. The prerequisite step is the initial mesh generation, while the main steps are finding the solution for the given mesh and re-refining the mesh according to some condition, such as error estimation [2]. The two main adaptive solution steps are repeated until the error obtained is below a given tolerance. The complex geometries of today's TCAD simulations, composed of curved surfaces and thin layers, are prone to containing poorly shaped elements

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in the initial mesh; therefore a local refinement algorithm yielding good quality meshes independent of the initial mesh is desired, especially for the quality-sensitive Finite Element Method [3,4].

The generation of an initial mesh without poorly shaped elements in two dimensions is well known, as is the improvement of the quality of the given mesh topology [5–10]. Mesh-quality improvement techniques are generally classified into two categories: smoothing (also called node relaxation) and local transformation. Smoothing is the movement of nodes without changes of mesh topology, i.e., without changes of edge connectivity, and local transformation is the change of mesh topology without moving nodes. Representatives of the best-known methods in each category are Laplacian node relaxation and edge swapping [5,9]. Unfortunately, these improvement techniques are not as effective in three dimensions [11]. In addition, the initial construction of a boundary conforming tetrahedral mesh without poorly shaped elements is not always possible [1,5,22,23]. To date, the octree is the only 3D initial mesh generation algorithm with a strong theoretical quality guaranty, but this is not a boundary conforming method [22]. There have been many studies to enable the generation of a good quality tetrahedral mesh. Most of these were designed to find a better node relaxation method, but it has been pointed out that node relaxation fails to give high-quality meshes when individually used, and does not guarantee global optimization [23–25]. As an alternative methodology, Joe [12] has proposed an improved-quality triangulation method that uses a combination of local transformations. Although this method succeeded in eliminating slivers, which are poorly shaped elements with almost zero volume, it cannot guarantee the elimination of all slivers, and it is poor at improving overall mesh quality. Another approach, by Golias, involved the tetrahedral refinement method based on Delaunay triangulation followed by node relaxation [13]. This method was partially successful, but showed degradation of the minimum quality.

In this paper, we propose a quality-improved local refinement method for an adaptive solution strategy based on the element-wise refinement switching. We present details of the proposed quality-improved refinement method in Section 2 and numerical experiments in Section 3. In Section 4, we present the conclusions of our research with the use of our local refinement method with a commercial initial mesh generator.

2. Proposed quality-improved local refinement

2.1. Overall process

It has been observed that Rivara's 3D longest side partition shows little overall quality improvement ability with poorly shaped elements, whereas the red/green 3D method preserved the quality regardless of the parent's shape [14–16]. In other studies, Golias' method partially succeeded in improving mesh quality, and has an appropriate property for the adaptive solution strategy because of its nature of repeated local refinement followed by the quality improvement process [13]. Rivara's 3D longest side partition has no provable upper bound for the number of elements produced, while Golias' method has the problem of degradation of the minimum quality. The defects of Golias' method stem from the unstable local refinement and Delaunay transformation, which are possible sources of slivers. To produce a better local refinement algorithm, which contains quality improvement while preserving the quality of a well-shaped parent, we combined Rivara's 3D longest side partition with quality-guaranteed octasection. We then adapted Golias' quality improvement process without the Delaunay transformation.

The basic concept of our quality-improved local refinement is shown in Fig. 1. Switching enabled local refinement (SELR) is conducted, and then mesh improvement composed of face swapping and constrained Laplacian node relaxation is performed until there is insignificant improvement. If the fineness or error

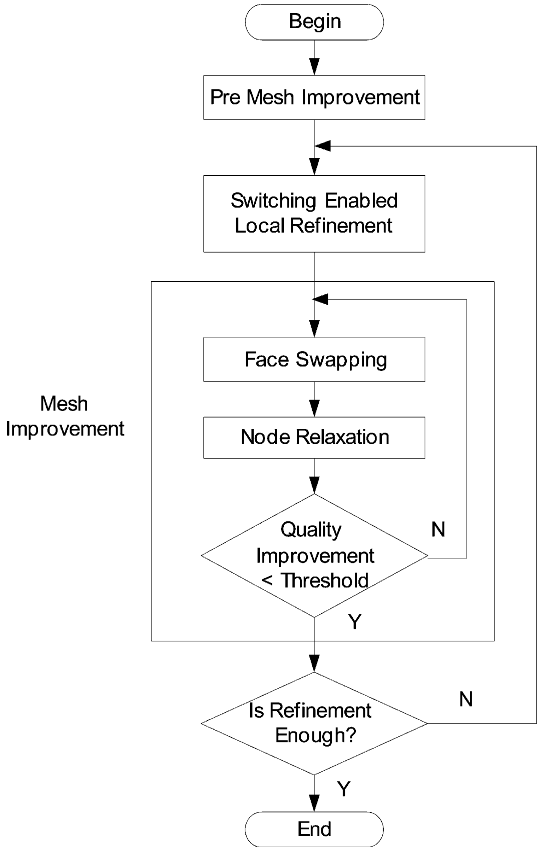

Fig. 1. Overview of quality-improved local refinement (cf. [13]).

estimation calculated with the refined mesh is not satisfactory, adaptive refinement steps are taken until the requirement is satisfied. To eliminate avoidable computational burden, prerequisite mesh improvement is conducted for the given initial mesh before the first refinement. In Fig. 1, face swapping was introduced first, then the node relaxation, because it was observed that the resultant mesh of octasection of SELR becomes close to that of red/green 3D if face swapping follows immediately.

2.2. Outline of the SELR

The SELR comprises refinement of marked elements, and conformation of the mesh to remove inconsistency in the refinement at the common face between two adjacent tetrahedral elements. Elements are marked, based on the error estimator, mesh quality or other given criteria. Each tetrahedron has one of SUB_0, SUB_1 and SUB_2 depth information, and the original tetrahedral elements are initialized with depth of SUB_0. The types of depth information of uniformly refined elements are shown in Fig. 2. By applying only refinements on the elements with this depth information, a conformative quality guaranteed mesh could be obtained.

The SELR algorithm

/* Let τ be the 3D tetrahedral grid.

Let T be the set of marked tetrahedral elements to be refined.

Let V be the set of non-conforming tetrahedral elements.

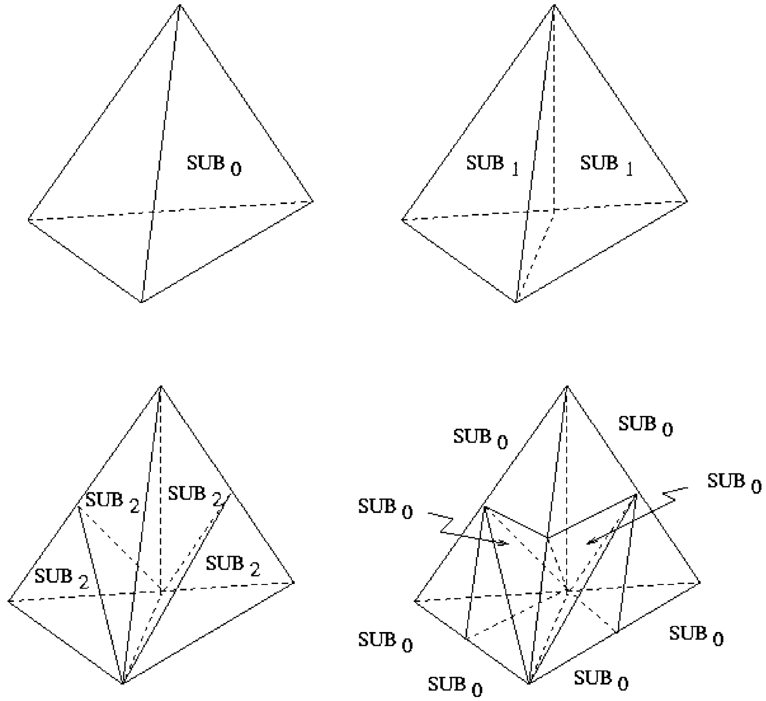

Fig. 2. Depth information of the SELR under uniform refinement.

Let t denote tetrahedral element.
Let $t_{i=1,2}$ be the possible child of t, and $t_{i,j=1,2}$ be the possible child of t_i for given i.
Let LE_0 be the longest edge of t.
Let LE_1 be the unique edge of t_i, which is also the longest edge of a common face of t_i with the original tetrahedron t.
Let LE_2 be the unique edge of $t_{i,j}$ corresponding to an edge of the original tetrahedron t.
Let bisection_flag be the indicator of bisection or octasection. Set true for bisection.
RefineSub$_0$(t) function bisects t across LE_0 and sets children's depth as SUB_1.
RefineSub$_1$(t) function bisects given $t := t_i$ across LE_1 and sets children's depth as SUB_2.
RefineSub$_2$(t) function bisects given $t := t_{i,j}$ across LE_2 and sets children's depth as SUB_0. */
/* 1. Refinement of Marked Elements : */
$\tau =$ initial mesh
while ($T \neq$ empty set) {
  $t \in T$;
  set bisection_flag for t;
  switch (depth of t) {
   case SUB_0: RefineSub$_0$(t); if(bisection_flag) return;
    for(each i) RefineSub$_1$(t_i);
    for(each i, j) RefineSub$_2$($t_{i,j}$);
   case SUB_1: RefineSub$_1$(t); If (bisection_flag) return;
    for (each i) RefineSub2(t_i);
   case SUB_2: RefineSub2(t); }
  $\tau = (\tau$-refined elements) $\cup$ newly created elements;

```
}
/* 2. Conformation: */
While(V ≠ empty set ) {
    t ∈ V;
    RefineSub_(depth index of t)(t);
    V = (V − t) ∪ newly created non-conforming elements;
    τ = (τ − refined elements) ∪ newly created conforming elements
}
```

As a tie-breaking rule, we chose the edge with lower vertex index if the lengths of edges are the same. After mesh conformation, the depth information of τ is reset to SUB_0 to make the first bisection of an original element in each refinement step be the longest side partition. In the refinement of each marked element, if the total number of elements is too large or the mean ratio is poorer than the threshold, the bisection_flag is set to true for the given marked element. The mean ratio is defined by

$$\text{Mean ratio } \eta = \frac{12\sqrt[3]{9v^2}}{\sum_{0 \leqslant i<j \leqslant 3} l_{ij}^2}, \tag{1}$$

where l is the length of edge and v is the volume of the tetrahedral element [21]. The quality threshold was determined based on numerical experiments. We did many tests with varying marking ratios, and the resultant quality of Fig. 1 had an approximate upper bound of mean ratio 0.5. This value was set as the quality threshold for the decision of refinement switching. In the mesh conformation, non-conforming elements are refined repeatedly according to the depth information until there is no non-conforming element. Fig. 3 shows the mesh conformation process of SELR. In this figure dashed planes represent newly created faces during the bisection of the to-be-refined edge with depth information of LE_0, LE_1 or LE_2. Bisection of each edge produces two child elements with corresponding depth information as shown in Fig. 3. For example, bisection of LE_0 produces two child elements with depth SUB_1.

2.3. Property of SELR

The SELR algorithm contains the characteristics of both Bansch's bisection and 3D-SBR (skeleton based refinement) [17,18]. If we initialize the depth information as SUB_0 in each refinement step, its characteristics are similar to 3D-SBR; otherwise it is similar to Bansch's method. In the former case, SELR is distinguishable from 3D-SBR, because it is capable of refinement switching and there is no need for the tetrahedron searching that is required in 3D-SBR [18].

In general, the refinement algorithm must provide two characteristics: boundedness and stability of the mesh. Boundedness means that the number of elements produced by refinement should not be able to increase to infinity and stability means that the quality of recursively refined elements should have a lower bound on the quality. In our SELR algorithm, the proof of boundedness is trivial. Let M_n and M_n' represent the mesh of the nth uniform octasection and nth local refinement, respectively. Although M_n' is not fully nested in M_n, the number of children of M_n' is smaller than that of M_n in each refinement step, because in the mesh conformation process of SELR, non-conforming element cannot be further refined than the octasection of original element. Therefore if M_n is bounded then M_n' is also bounded. The stability of the SELR was examined numerically for several examples, including the test problem proposed by Maubach [19]. We examined the Mean Ratio, Radius Ratio, Edge Ratio and Aspect Ratio [20,21], and all showed no degradation below a certain level during local refinement regardless of bisection, octasection or mixture of these. We show the results from the Maubach test with mixture of bisection and octasection in Fig. 4. Here

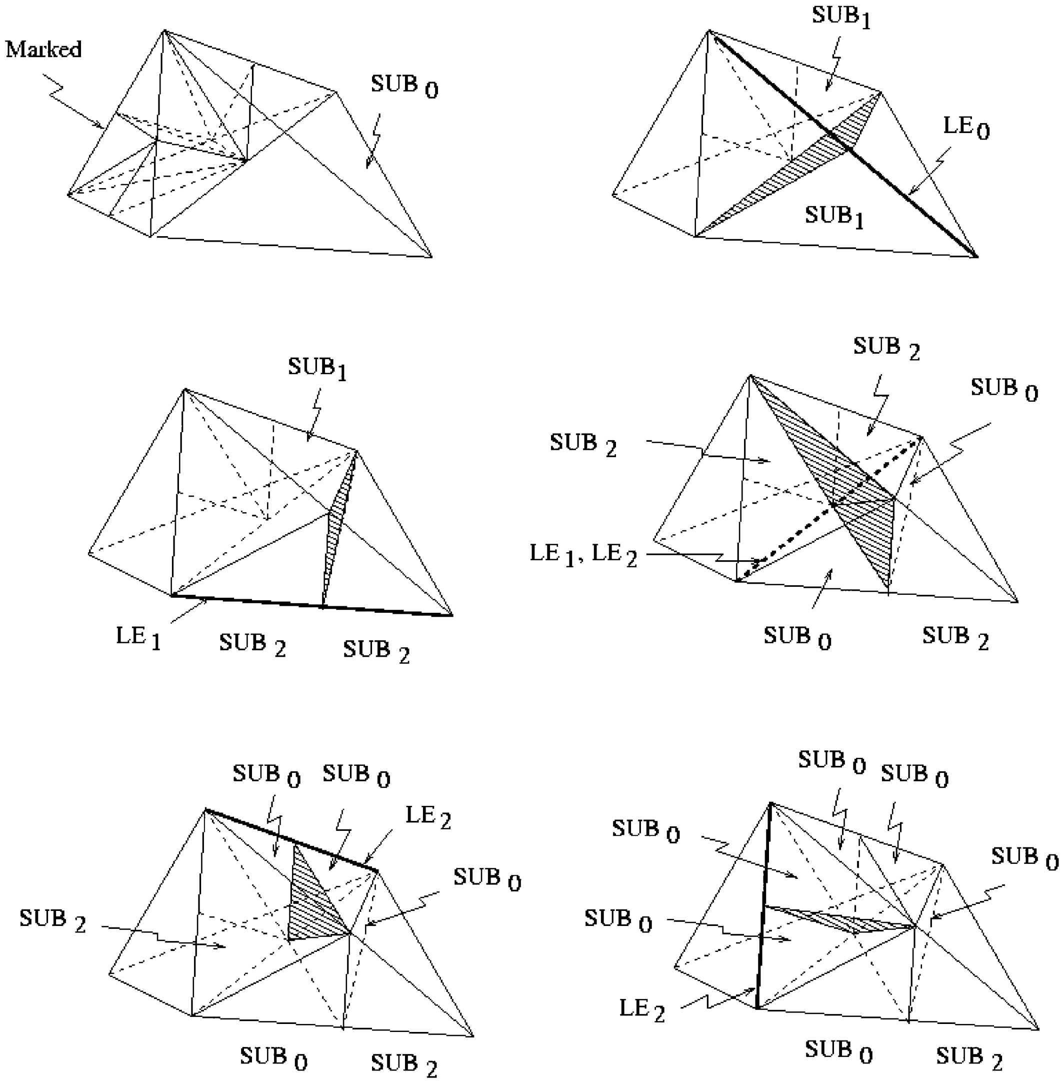

Fig. 3. Schematic representation of mesh conformation (cf. [18]). Dashed plane represents a newly created face during the bisection of to-be-refined edges represented by LE_0, LE_1 or LE_2.

octasection was applied three times and then six bisections were applied, and this result shows a lower bound of SELR.

3. Numerical experiments

In this section, we present numerical experiments for the role of SELR on quality improvement ability, comparison of quality improvement ability with previously known methods, and use the method with more realistic problems.

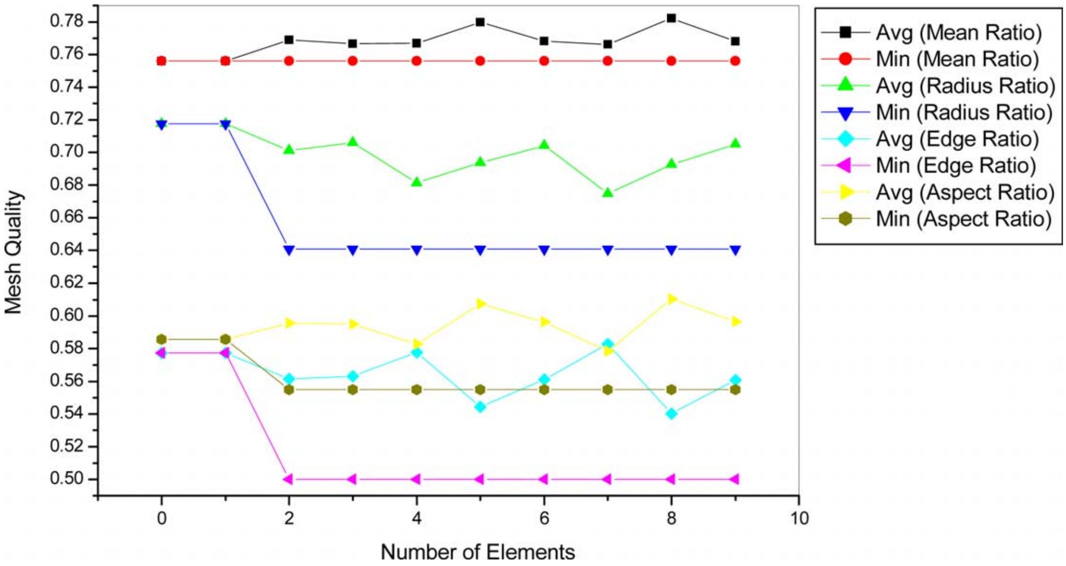

Fig. 4. Stability result of Maubach test using SELR. In the refinement, octasection is conducted three times and then bisection conducted six times. No mesh improvement was applied.

3.1. Role of refinement switching

To investigate the role of refinement switching on the quality improvement with SELR, we tested Rivara's Problems, which are conventionally used as stability tests of refinement algorithms [14]. The test results of well and poorly shaped meshes of Problems 1 and 3 are shown in Fig. 5. All elements are uniformly refined at each refinement step. In Problem 1 (mean ratio = 0.885) with a well-shaped element, bisection produced a lower average and minimum mean ratio than using SELR or octasection. This is because the quality of the parent tetrahedron is more effectively maintained by applying octasection once

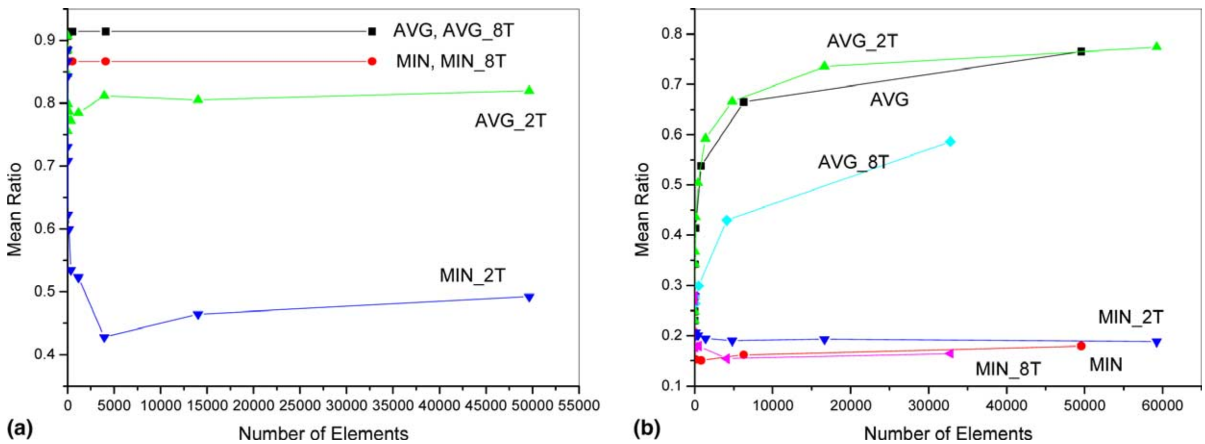

Fig. 5. The role of refinement switching in SELR. The curves annotated with AVG and MIN represent average and minimum mean ratios, respectively, for our approach, while AVG and MIN with 2T or 8T denote those of bisection-only and octasection-only cases of SELR, respectively. (a) Problem 1. (b) Problem 3.

rather than three bisections, even though a quality improvement process is followed. In Problem 3 (mean ratio = 0.278), with a poorly shaped element, bisection and SELR showed nearly the same superior effect for quality improvement process, compared to octasection. From these results, it is evident that switching enabled refinement is the better choice in the early stage of refinement where the number of elements is not of concern.

3.2. Comparison with other methods

We compared our results from testing Rivara's Problems with quality local refinement based on subdivision (QLRS) without local transformation and quality local refinement based on bisection (QLRB) with Joe's mixed local transformation [15,16]. In the case of QLRS, mixed local transformation was not shown in the original paper, because local transformation rarely improves quality with QLRS in the uniform refinement of a single element, as we also found using our implementation with face swapping. The results of the comparison are shown in Fig. 6. Here all elements are uniformly refined at each refinement step. Because the reported final mesh of QLRB contains only 64 elements [15], the quantity of data used in the QLRB graph is less than that of QLRS or of our method. In Problems 1, 2 and 4, where the parent of the

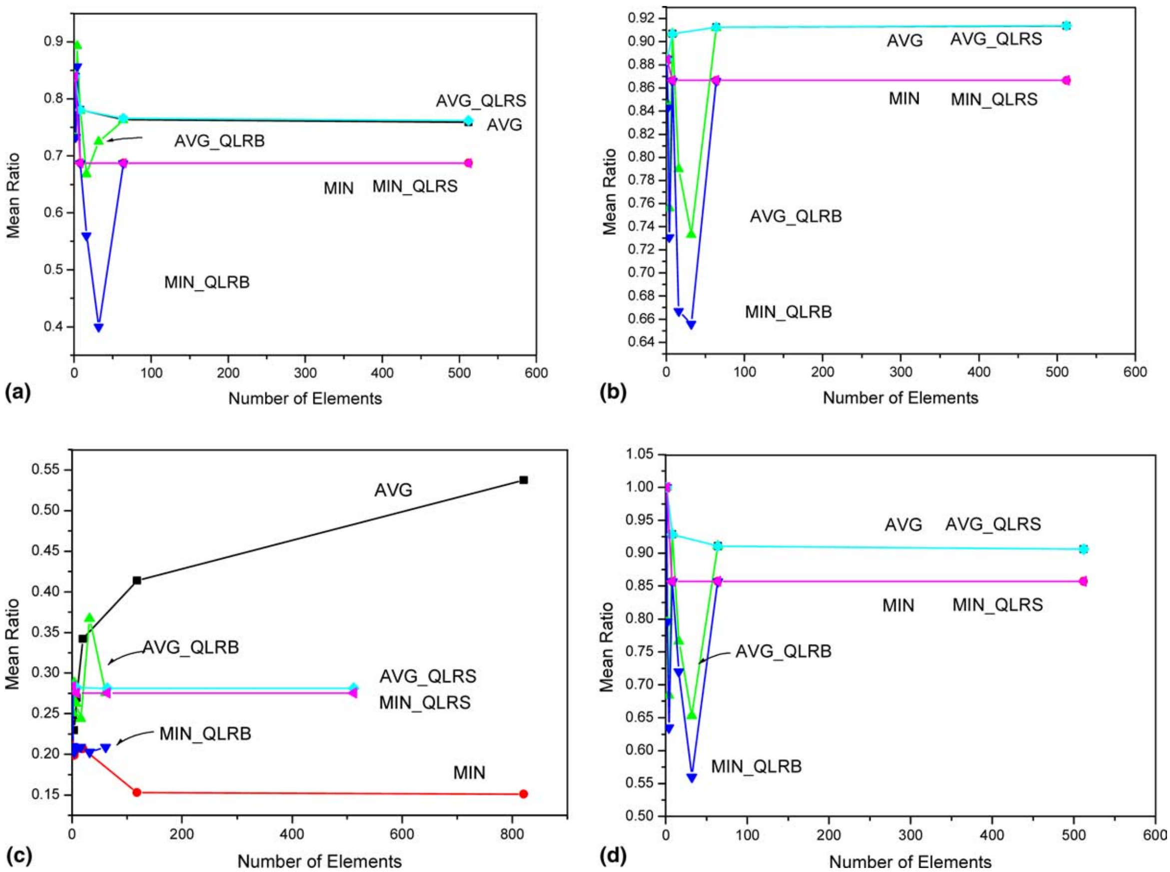

Fig. 6. Comparison of improvement between the proposed methods and previously reported methods. AVG and MIN represent the average and minimum mean ratios, respectively, of our approach, while AVG and MIN with a suffix represents those of the method corresponding to the suffix. (a) Problem 1. (b) Problem 2. (c) Problem 3. (d) Problem 4.

element has rather good shape, our method and Joe's two methods have similar results. However, in Problem 3 with a poorly shaped element, Joe's method failed to improve mesh quality because Joe's mixed local transformation is aimed at removing slivers, rather than at improving the quality of poorly shaped elements. Only our method showed improvement in the average value while guaranteeing a lower bound for the minimum value; see Table 1 for the truncated average and minimum quality data of our results. In Problem 3, the geometry has a wedge shape; therefore the quality of bisected element near a wedge cannot be improved by the following mesh improvement process. This resulted in a slight reduction of minimum quality; however, a lower bound was guaranteed, with slight quality recovery as refinement proceeded, as shown in Table 1.

3.3. Use with realistic problems

Fig. 7 shows how well our approach improves distorted element by refining poorly shaped elements. Because our approach has an approximate quality upper bound of mean ratio 0.5, we set this value as marking threshold. Figs. 7(a) and (b) show the initial mesh composed of very poorly shaped elements and the final mesh from the proposed method, respectively. Fig. 7(c) shows the quality improvement trend during local refinement. To visualize the quality improvement ability of our approach, we showed the quality trend with the red/green 3D method, which is the most widely accepted method in the adaptive solution strategy. In this quality trend, nine times, the proposed quality-improved local refinement improved the average and minimum value of the mean ratio from 0.2552 and 0.06935 to 0.73427 and 0.28614, respectively, whereas the red/green 3D method only preserves mesh quality by unintentional uniform refinement resulting from poor quality of the whole elements. While Golias' method shows minimum quality degradation even with well-shaped elements, the proposed method shows no such degradation; on the contrary, it improves minimum quality in an overall sense or at least guarantees a lower bound [13].

Fig. 8 shows how the proposed local refinement can be used in combination with a conventional advancing front initial mesh generator. As in the previous example, elements with a mean ratio below 0.5 were marked for refinement. Fig. 8(a) shows the initial mesh produced by the advancing front method, and (b) shows the final mesh obtained using our approach. In Fig. 8(a), the initial mesh produced by the advancing front method contained a few severely distorted elements, and containment of a small portion of bad elements is the typical problem of the advancing front method [1]. In Fig. 8(b), because local refinements were conducted on these poor elements, refinement is heavily localized. In the quality trends of Fig. 8(c), the average mean ratio of the red/green 3D method decreased because the relative portion of poor elements increases as the refinement on poor elements increases. In the case of the proposed method, the initial average mean ratio of 0.82904 decreased to 0.74166 but gradually increased to 0.7706,

Table 1
Mean ratio vs. the number of elements on Rivara's Problem 3; see Fig. 1

# of Elements	Problem 3	
	AVG	MIN
1	0.27806	0.27806
2	0.24822	0.20682
4	0.22971	0.19873
8	0.26962	0.20583
20	0.34219	0.20682
118	0.41381	0.15304
821	0.53742	0.15107
6277	0.66459	0.16193
49 594	0.76546	0.17965

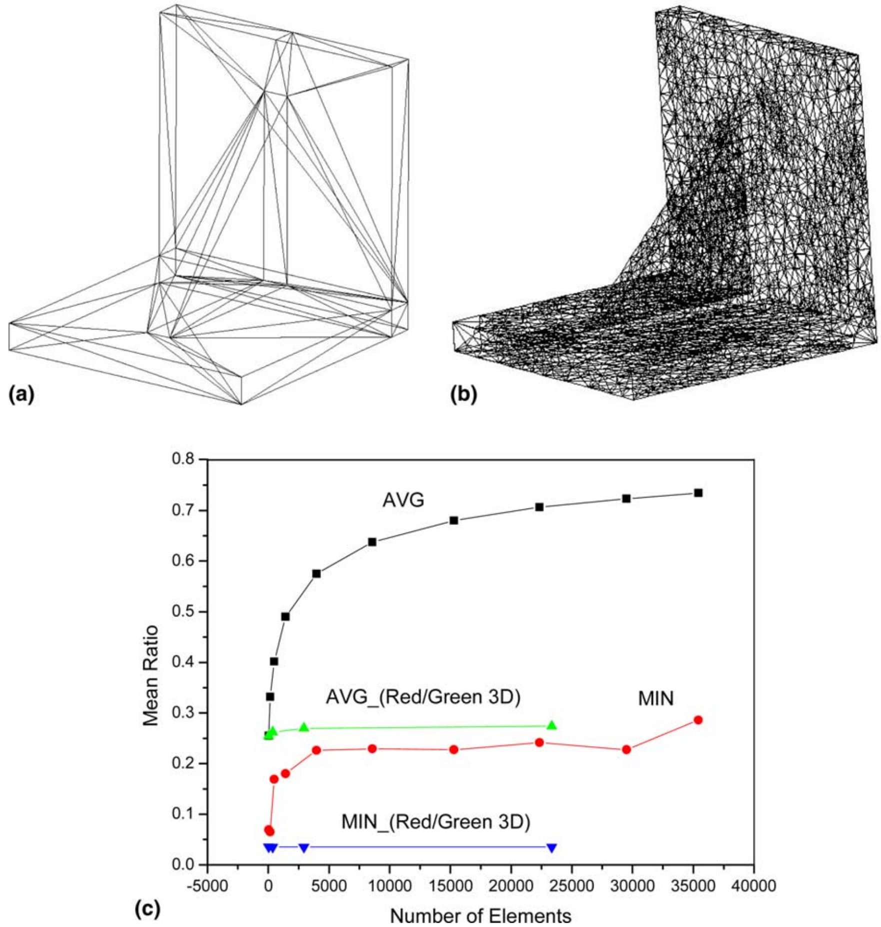

Fig. 7. Bracket problem. Elements with mean ratio below 0.5 were marked for refinement. AVG and MIN represent the average and minimum value of our approach, while those with suffix represent those of the red/green 3D method. (a) Initial mesh. (b) Final mesh with Fig. 1. (c) Quality improvement trend.

and the initial minimum mean ratio of 0.10618 increased to 0.50353 as refinement was repeatedly conducted on the poor elements. In the quality trend of Fig. 8(c), minimum quality decreased at some stage with the proposed approach. This is because, in some cases, bisection reduces quality a little, and this is not fully recovered by mesh improvement; but this temporary quality reduction disappears soon if there is no poor boundary constraint, such as a wedge. We observed that overall minimum quality, with the proposed method, tends to improve with small fluctuations as the number of refinements of poorly shaped elements increases.

Finally, as a real application, we show the mesh generation of a local oxidation of silicon (LOCOS) structure based on the gradient of doping concentration, which is a prerequisite step to solving the diffusion problem. The doping profile is assumed to have a maximum value of 1×18 cm^{-3} below 0.1 μm from the upper face of the LOCOS structure, and has a Gaussian shape. Fig. 9(a) shows the initial mesh composed of macro-elements using a layer-based method and Fig. 9(b) shows the mesh constructed after refinement on elements that have a doping concentration gradient in excess of 10% of element average using the proposed approach. During local refinement, the average and minimum values of mean ratio increased from 0.237 to

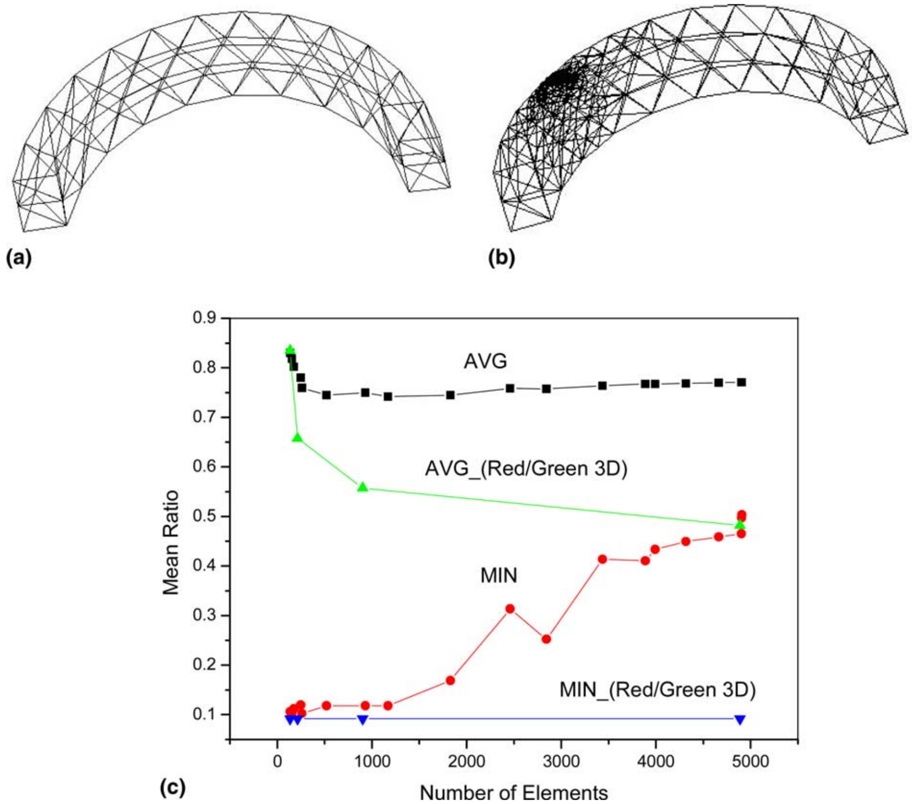

Fig. 8. The arch problem. Elements with mean ratio below 0.5 were marked for refinement. AVG and MIN represent the average and minimum value of our approach, while those with suffix represent those of the red/green 3D method. (a) Initial mesh using advancing front method. (b) Final mesh with Fig. 1. (c) Quality improvement trend.

0.807 and 0.121 to 0.235, respectively. Because elements are marked based on the gradient of doping concentration, not on the quality threshold, the number of refinements on a poor element is relatively small and therefore the minimum mean ratio does not improve sufficiently compared with the previous examples. Nonetheless, from Fig. 9(c), the quality of our approach is superior to the red/green 3D method, which produces poorly shaped green tetrahedral elements, which are introduced to temporarily satisfy the requirement of conformity of the mesh.

In general, local refinement in adaptive solution strategy is not aimed at the poorly shaped elements; rather it has a tendency to depend on other criteria, such as error estimation or problem-specific conditions, such as in the previous LOCOS example. Therefore, the quality improvement of the proposed approach would typically be less than that of its maximum ability, and the amount of quality improvement would vary with the refinement number of the poorly shaped elements. In the point of time consuming proposed method is rather expensive. In the previous examples it took about 1 min, 75 min and 15 h, respectively, for the mesh having roughly 5000, 35 000 and 130 000 elements (with Pentium III 1 GHz and gcc 2.9.1.66). In our implementation mesh improvement was conducted until there is no additional improvement. Since the initial mesh of TCAD is composed of relatively few macro elements and the size of badly shaped elements is large, badly shaped elements could be removed at an earlier stage of adaptive refinement using the proposed approach, if element marking is properly controlled.

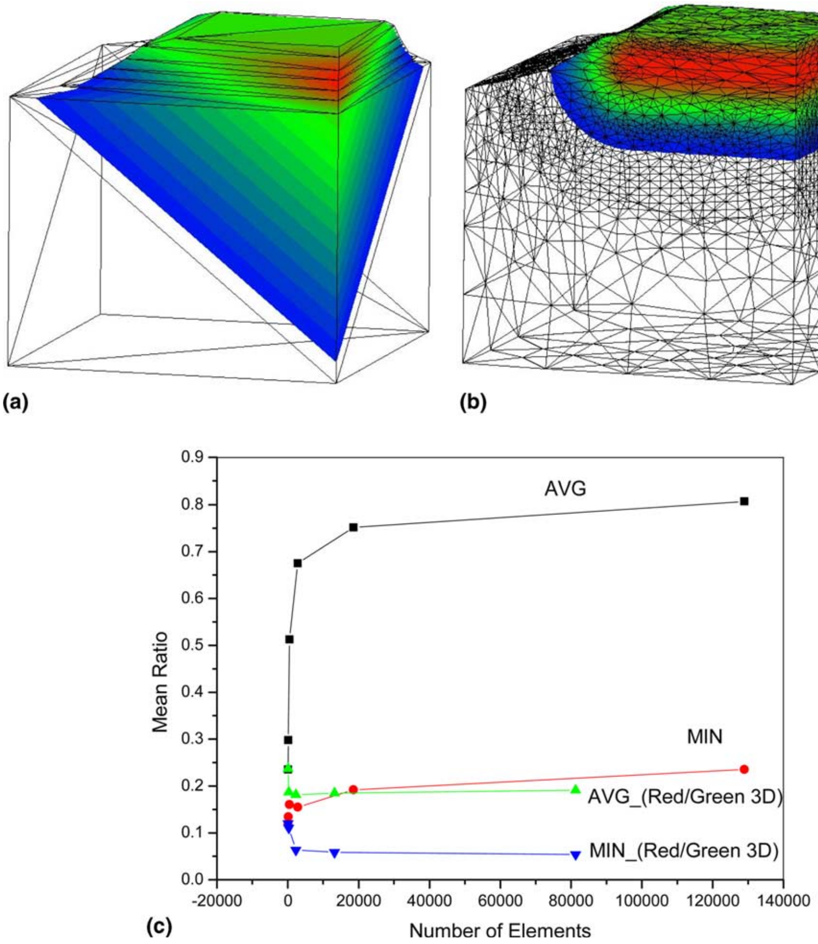

Fig. 9. Local refinement of LOCOS structure. Elements that have a doping concentration gradient in excess of 10% of element average were marked for refinement. AVG and MIN represent the average and minimum value of our approach, while those with a suffix represent those of the red/green 3D method. (a) Initial mesh by layered method. (b) Final mesh with Fig. 1. (c) Quality improvement trend.

4. Conclusion

The main contribution of this paper is the development of an effective quality-improved local refinement method for an adaptive solution strategy. The key idea of the proposed method is to improve the quality of poorly shaped elements while preserving the quality of well-shaped elements. We have accomplished this goal by using refinement switching between longest side bisection and octasection, followed by a conventional quality improvement process. We showed that refinement switching plays an important role in quality improvement. By applying the proposed method on the poorly shaped macro-elements produced manually, by the layered method, or by the advancing front method, well-shaped mesh could be easily obtained. It is observed that if the proposed local refinement is conducted on the poorly shaped elements, intentionally or unintentionally, the minimum quality improves in an overall sense. The method is boundary conforming and sliver-free, and could be combined with a conventional initial mesh generator, such as the advancing front method, to rectify the quality deficiency legacy of the initial mesh generator. From this it is expected that the proposed method can be used as a mesh generator for an adaptive solution strategy at an earlier stage of the adaptive solution strategy.

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