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Parallel anisotropic mesh adaptation with boundary layers for automated viscous fow simulations

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Abstract This paper presents a set of parallel procedures for anisotropic mesh adaptation accounting for mixed element types used in boundary layer meshes, i.e., the current procedures operate in parallel on distributed boundary layer meshes. The procedures accept anisotropic mesh metric feld as an input for the desired mesh size feld and apply local mesh modifcations to adapt the mesh to match/satisfy the specifed mesh size feld. The procedures fully account for the parametric geometry of curved domains and maintain the semi-structured nature of the boundary layer elements. The effectiveness of the procedures is demonstrated on three viscous fow examples that include the ONERA M6 wing, a heat transfer manifold, and a scramjet engine.

Keywords Parallel mesh adaptation · Boundary layer mesh · Semi-structured mesh · Parallel adaptive viscous flow simulations

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1 Introduction

The application of fnite elements for reliable numerical simulations requires that the simulations are executed in an automated manner with explicit control of the approximations made. Since there are no a priori methods to control the approximation errors for complex problems, a posteriori methods along with adaptive discretization procedures must be applied [[2,](#page-26-0) [6,](#page-26-1) [24,](#page-27-0) [62\]](#page-28-0). Adaptive meshing is therefore an important component for reliable simulation of complex problems, such as for fow problems that exhibit highly anisotropic solutions which can only be located and resolved through a posteriori anisotropic adaptivity (e.g., see $[9-11, 21, 49, 51, 54]$ $[9-11, 21, 49, 51, 54]$ $[9-11, 21, 49, 51, 54]$ $[9-11, 21, 49, 51, 54]$ $[9-11, 21, 49, 51, 54]$ $[9-11, 21, 49, 51, 54]$ $[9-11, 21, 49, 51, 54]$ $[9-11, 21, 49, 51, 54]$ $[9-11, 21, 49, 51, 54]$. Furthermore, in a number of problem cases it is desirable to use highly anisotropic elements (e.g., with aspect ratio above 1000) in specifc locations and for these elements to have a semi-structured nature which must be maintained during mesh adaptation [[34,](#page-27-5) [53\]](#page-28-3). Of particular interest in this study are viscous flows with boundary layers that form near solid surfaces, e.g., in a wall-bounded fow.

The two major classes of mesh adaptation techniques are adaptive re-meshing methods and methods that use local mesh modifcation. Re-meshing methods [[19,](#page-27-6) [21](#page-27-3), [23](#page-27-7), [26,](#page-27-8) [51](#page-28-1)] construct the desired mesh by regenerating the entire mesh through the application of automatic mesh generation algorithms governed by specifed element size and shape information while accounting for curved domains. This comes at the cost of re-meshing the entire domain along with global transfer of the solution felds to the new mesh. On the other hand, methods based on local mesh modifcation retriangulate local subdomains (or cavities) until the specified mesh size field is satisfied (e.g., see [\[7](#page-27-9), [37](#page-27-10), [49](#page-27-4)]). Effectiveness of local methods depends on the richness of the underlying local mesh modifcation operations that are employed. Some local mesh modifcation methods strictly use subdivision operations which can be limited in the amount of coarsening and anisotropy that can be achieved. For example, in [[5,](#page-26-2) [31,](#page-27-11) [40](#page-27-12)] the coarsening or merging of child elements to recover parent elements is done by reversing the previous subdivision operations at desired locations (i.e., by applying a derefnement step). Thus, in such methods coarsening cannot be applied to create elements larger than those in the initial mesh. This aspect also limits the amount of anisotropy that can be achieved in elements. Similarly, some local mesh modifcation schemes only adapt to the faceted geometry (e.g., based on the initial mesh) and do not improve the geometric approximation of the curved domains as the mesh is refned. In contrast, other research work has shown that a richer set of local mesh modifcation operations [\[7,](#page-27-9) [20,](#page-27-13) [29,](#page-27-14) [37,](#page-27-10) [49\]](#page-27-4) can be utilized to support general (local) coarsening, reconnection and anisotropy in the mesh as well as to account for curved domains [[38\]](#page-27-15). These local operations also support a localized transfer of solution felds [\[5](#page-26-2), [44](#page-27-16)] at the cavity level as the mesh is incrementally modifed to attain the desired mesh.

In viscous flows with boundary layers, hybrid or semistructured mesh generation methods have been used extensively [\[8](#page-27-17), [15](#page-27-18), [22,](#page-27-19) [25,](#page-27-20) [27](#page-27-21), [28](#page-27-22), [33,](#page-27-23) [41–](#page-27-24)[43](#page-27-25), [52\]](#page-28-4). For such problems, local mesh modifcation operations have been extended to account for mixed topology elements [[30,](#page-27-26) [34](#page-27-5), [53\]](#page-28-3), wherein the semi-structured nature of the mesh is taken into consideration. Specifcally the layers or stacks of wedges (triangular prisms) or hexes are modifed to attain the desired local mesh resolution while the overall layered structure is maintained. In [\[34](#page-27-5)], subdivision of mixed elements is employed along with mesh movement to improve the geometric approximation of the curved domains. In [\[30\]](#page-27-26), derefnement is also carried out for transient problems, whereas in [\[53](#page-28-3)] a richer set of local mesh modifcation operations are utilized for mixed element meshes. In these studies, layered mesh is modifed in conjunction with the rest of the interior mesh consisting of unstructured tetrahedral elements as well as pyramidal elements. The latter are used when necessary to transition between the semi-structured/layered and unstructured portions of the mesh. These studies have focused on serial boundary layer meshes, i.e., where the mesh is not partitioned or distributed over multiple parts.

Mesh adaptation techniques must operate in parallel on distributed meshes. This is because most problems of interest involve complicated geometries and complex physics, that even with adaptivity, the resulting meshes are very large. Adaptive simulations for such problems, where only the analysis or solve step is parallelized (see, for example, [\[65](#page-28-5)]), face a limitation in terms of the problem size and/or time-to-solution due to the serial mesh adaptation step. The serial mesh adaptation step may take as much time, or even more, as compared to the analysis step and thus, becomes a bottleneck. Therefore, to efficiently execute parallel adaptive simulations, both the analysis and mesh adaptation steps must be parallelized and executed on distributed or partitioned meshes (e.g., see [\[13](#page-27-27), [59](#page-28-6), [66](#page-28-7)]).

Performing mesh adaptation in parallel requires that all mesh operations are carried out in such a way that the resulting distributed mesh properly fts together, i.e., at the inter-part boundaries. Subdivision or refnement operations can be understood at the level of a single element and therefore, can be performed in parallel on each processor including for lower-order mesh entities that reside on inter-part boundaries. This must be followed by a communication step between processors to update the inter-part links based on new mesh entities introduced at the inter-part boundaries (e.g., see $[16, 47]$ $[16, 47]$ $[16, 47]$ $[16, 47]$). In $[47, 50]$ $[47, 50]$ $[47, 50]$, parallel refinement and derefnement steps are used for unsteady problems, where child elements of a given parent element always reside on the same processor. This makes the merging of child elements straightforward in which a communication step is required to delete the necessary vertices at inter-part boundaries due to derefnement. As in the serial case, this parallel approach is limited in terms of the amount of coarsening and anisotropy that can be achieved. In contrast to a parallel scheme that is based on refnement and derefnement steps, parallel re-meshing is used in $[26]$ $[26]$. In such an approach, mesh elements marked for adaptation (based on a selection criterion) are removed from the distributed mesh leading to cavities or holes in the mesh that are re-meshed. This intermediate mesh is repartitioned with the constraint that every hole to be re-meshed resides solely on a single part or processor in the re-distributed mesh. This scheme is more fexible in terms of shape and orientation of the resulting elements, however, the overall process can be time consuming. For example, a global repartitioning of the mesh, or a re-meshing of a relatively large hole due to concentrated adaptation in a contiguous portion of the domain, leads to signifcant work and memory imbalances between processors. On the other hand, in an adaptation approach that is based on local mesh modifcations only small portions of the mesh are affected at any given time. Therefore, mesh operations for which the associated cavity resides solely on one part can be carried out in a similar fashion to the serial case while for a cavity which spans multiple parts a migration of associated mesh elements is needed. A naive sequence of steps, which intermingles on-part mesh modifcation and mesh migration steps at a low level, will be ineffective due to signifcant wait times between these steps. However, with a proper control of the on-part mesh modifcation and mesh migration steps, parallel mesh adaptation based on local mesh modifications has been shown to be efficient $[3, 16]$ $[3, 16]$ $[3, 16]$ $[3, 16]$. So far such parallel mesh adaptation methods have focused on fully

unstructured/tetrahedral meshes and do not take boundary layer meshes into consideration.

A parallel mesh adaptation scheme for distributed boundary layer meshes has been presented in [\[32](#page-27-30)], where refnement and derefnement steps are employed for mixed elements. Similar to refnement and derefnement of fully unstructured distributed meshes discussed above, the technique in [[32\]](#page-27-30) requires the child elements of a given parent element to always reside on the same processor such that mesh derefnement step is completed with minimal communication. As mentioned before, such a scheme limits the amount of coarsening and anisotropy that can be achieved for hybrid meshes. Whereas an approach that is based on a richer set of local mesh modifcation operations for distributed boundary layer meshes can overcome these limitations, but to the best of our knowledge so far there has been no study on such an approach. The current work presents such an approach based on parallelization of a richer set of local mesh modifcation operations for distributed boundary layer meshes, i.e., this paper presents parallel procedures for boundary layer mesh adaptation and builds on our prior work on serial boundary layer meshes [[53\]](#page-28-3).

The organization of the paper is as follows. Section [2](#page-2-0) briefy provides the terminology used for boundary layer meshes. Section [3](#page-3-0) discusses the local mesh modifcation operators that are used for the layered portion of the mesh and its interface with the rest of the unstructured interior mesh. Section [4](#page-10-0) describes the procedures that are currently used to parallelize different local mesh modifcation operations for hybrid or boundary layer meshes. Section [5](#page-15-0) demonstrates the effectiveness of the current procedures based on three viscous fow problems.

1.1 Nomenclature

2 Boundary layer mesh terminology

A common method to construct boundary layer meshes with layered elements on walls is the advancing layers method [\[8](#page-27-17), [15,](#page-27-18) [22](#page-27-19), [25,](#page-27-20) [27](#page-27-21), [28,](#page-27-22) [33](#page-27-23), [41–](#page-27-24)[43,](#page-27-25) [52](#page-28-4)]. It infates the unstructured surface mesh on no-slip surfaces, where the boundary layer fow forms. This infation into the volume is performed along the local surface normals in the form of stack or layers of elements in a graded fashion up

Fig. 1 Cut of the boundary layer mesh for a pipe geometry

Fig. 2 Boundary layer mesh terminology

to a specifed distance. Rest of the domain is flled with unstructured tetrahedral elements while pyramids are used when necessary. An example of a boundary layer mesh for a pipe geometry is shown in Fig. [1](#page-2-1). In addition to the layers of prismatic elements and interior tetrahedral elements, this example includes a few pyramids. Note that pyramids are used to transition into the unstructured tetrahedral mesh when quadrilateral faces of the layered mesh are exposed, for example, when the number of prisms in neighboring stacks change due to a difference in the number of layers in those stacks.

The layered portion of the boundary layer mesh has a structure that can be decomposed into a tensor product of a layer surface (2D) mesh and a thickness (1D) mesh [[53](#page-28-3)]. The mesh composed of triangles located at the top or bottom end of any layer is referred to as a layer surface, while the lines normal to the wall composed of mesh edges are called growth curves, see Fig. [2.](#page-2-2) The mesh edges that belong to layer surfaces are referred to as layer edges and ones that reside on growth curves are called growth edges as depicted in the fgure. Each layer of elements is formed with the help of two layer surfaces, one above and one below, while the in-between growth edges join these layer surfaces. The height of each layer is referred to as layer thickness whereas the collective height of all the layers is the total thickness of a layered stack of elements. The number of total vertices (or edges) on growth curves determine its level. The vertices on walls from which growth curves originate are referred to as the originating vertices. The top most layer in a layered stack shares an interface with the unstructured interior mesh. The interior tetrahedral or pyramidal elements, sharing lower-order mesh entities with layered portion of the mesh, are referred to as the interface elements.

3 Mesh modifcations in the layered portion of the mesh

The goal of mesh modifcation operations for boundary layer meshes is to maintain the overall layered structure in the mesh. To do this, the mesh modifcation operations are decomposed such that operations that affect the layer triangulation of the layers are applied consistently throughout the stack. It is also necessary to apply modifcation to the corresponding unstructured mesh at the top of the stack. This section describes the control of mesh modifcations for the layered and unstructured portions of the mesh.

3.1 Mesh metric tensor

A mesh metric feld is used to specify the anisotropic mesh size distribution over the problem domain (e.g., see [[37,](#page-27-10) [49,](#page-27-4) [51](#page-28-1)]). In an adaptive process, the error estimator or indicator information is used to specify the desired mesh size or metric feld. This specifcation at any given point *P* is done by a symmetric positive definite tensor $T(P)$, referred to as the mesh metric tensor. A mesh metric tensor contains the desired directional mesh resolution at a point and geometrically follows an ellipsoidal surface. Specifcally, a mesh metric tensor transforms an ellipsoid into a unit sphere. The transformation: $e^T T e = 1$ (where *e* denotes the edge vector), defnes a mapping of the edge in the physical space into a unit edge in the metric or transformed space. Any tetrahedron that perfectly satisfes the mesh metric feld should be a unit equilateral tetrahedron in the metric space as depicted in Fig. [3](#page-3-1). However, in an unstructured mesh it is often not possible to exactly satisfy the specifed mesh metric feld. Therefore, mesh modifcation algorithms constrain edge lengths in the metric space to be within an interval around unity: $[L_{min}, L_{max}]$ (e.g., $[1/\sqrt{2}, \sqrt{2}]$), while elements are desired to achieve a mean ratio in the metric space to be close to 1 (with 1 being the ideal value). Mean ratio for a

Fig. 3 Transformation of a tetrahedral element based on a mesh metric tensor

Fig. 4 Decomposition of a mesh metric tensor in layered part of the mesh

tetrahedron was defned in [\[39](#page-27-31)]. In the metric space, mean ratio is defined as [\[37](#page-27-10)]: $\eta = 12(3V_T)^{2/3}/(\sum_{i=1}^6 l_{T,i}^2)$, where V_T is the volume of the tetrahedron and $l_{T,i}$ is the length of the *i*th edge of the tetrahedron in the metric space. As discussed later, we employ the cube of the mean ratio as the measure for element shape quality (e.g., see [\[37](#page-27-10)]).

In the layered part of the mesh, the mesh metric tensor can be decomposed into an ellipse as the planar (2D) part along a layer surface, which dictates the local in-plane mesh resolution, and a normal (1D) component that controls the local layer thickness [[53\]](#page-28-3). Note that layer thickness can also be based on flow physics, for example, in turbulent boundary layer fows [[14\]](#page-27-32). Figure [4](#page-3-2) illustrates the decomposition of a mesh metric tensor in layered part of the mesh.

3.2 Local mesh modifcation cavity

With the input of mesh metric feld, the local mesh modifcations are carried out to adapt the mesh to match the specifed size feld. As discussed before, a richer set of local mesh modifcation operations [[7,](#page-27-9) [37,](#page-27-10) [49](#page-27-4)] is needed for fully unstructured anisotropic meshes. Each modifcation operation involves a local cavity or subdomain which is retriangulated. The cavity for a given operation is defned as the union of sets of mesh entities that are changed by the application of the modifcation operation with the restriction that the triangulation of the cavity's boundary remains unchanged. This means that the boundary of the cavity can be shared with unchanged mesh entities outside of the cavity or in unaffected portion of the mesh (under this operation).

In 3D, the cavity is defned as the set of mesh regions along with its closure (i.e., lower-order mesh entities), which will be modifed by the modifcation associated with entity M_k^d and is denoted as:

$$
\{C(M_k^d)\} = \{M_i^3 \cup \{\partial M_i^3\} | M_i^3
$$

is affected by mesh modification
operation applied to M_k^d . (1)

The cavity's boundary is defned as:

$$
\left\{\partial C(M_k^d)\right\} = \left\{M_j^2 \bigcup \left\{\partial M_j^2\right\} \in C(M_k^d) | \newline M_j^2 \notin \left\{\partial M_i^3\right\} \bigcap \left\{\partial M_j^3\right\} \newline \forall M_i^3, M_j^3 \in \left\{C(M_k^d)\right\} \right\}.
$$
\n(2)

Equation [2](#page-4-0) states that the cavity's boundary contains the set of lower-order entities $\left\{ M_j^d \right\}$ ($d = 0, 1, 2$) that are located on the outer boundary of the closed set of regions comprising cavity $\{C(M_k^d)\}$. This way the cavity's boundary is shared with adjacent mesh regions that are outside and thus, not part of the cavity.

The application of a local mesh modifcation operation then is a retriangulation of the cavity, $\{C(M_k^d)\},$ which changes the mesh topology and results into a set of mesh entities contained in the set {*S*} with the following conditions:

$$
\{S\} \neq \Big\{ C(M_k^d) \Big\},\tag{3}
$$

$$
\{\partial S\} = \left\{\partial C(M_k^d)\right\}.
$$
 (4)

There can be situations when an entity M_k^d which requests modifcation is (only) repositioned within the cavity with no change in local mesh topology (for example, in case of a vertex motion as considered in Sect. [3.3](#page-4-1)). In this scenario, Eq. [3](#page-4-2) will have the equality.

3.3 Boundary layer stack modifcation

To preserve the layered nature of the boundary layer stacks, the mesh adaptation process for layer surfaces utilizes layer edge split, collapse and swap operations [\[53\]](#page-28-3), while adjustment of layer thicknesses and movement of newly created originating vertices to the curved domain boundary are accomplished through vertex movement (that may involve direct repositioning or local mesh modifcation operations as discussed later).

The layer edge split operation splits edges in the boundary layer stack and applies the appropriate subdivisions to the unstructured interior mesh at the interface. When edge split is requested for a single layer edge, all edges in the stack are subdivided. This scheme is conservative in nature in that it may provide a fner mesh than desired for some layer surfaces. Namely, if M_i^1 , where $i \in [1..N]$, is the layer edge to be split in a stack of *N* layer edges, then the cavity associated with it consists of a set of unique regions ${C$ ${M_i}$ } $}$ = ${U_{i=1}^N$ ${M_i}$ ${M^3}$ } $}$. Figure [5](#page-4-3) illustrates the layer edge split operation. The subdivision of pyramids and tetrahedra at the interface follows the stack split.

The layer edge collapse operation is performed on stacks that contain all short edges in the metric space. It is carried out under this condition to avoid any oscillation between collapse and split operations [\[53](#page-28-3)]. The edge collapse operations can only be applied when the affected unstructured mesh entities at the top of the stack also remain valid after the collapse operation. Let $\{(M_i^1, M_i^0)\}\$ (with $i \in [1..N]\$ be *N* pairs of layer edges (to be collapsed) and their corresponding vertices (to be deleted) in a stack. Then the cavity associated with the layer edge collapse operator is $\{ C\{M_i^0\} \} = \left\{ \bigcup_{i=1}^N \{ M_i^0\{M^3\} \} \right\}$ in which regions $\left\{\bigcup_{i=1}^{N} \left\{M_i^1\left\{M^3\right\}\right\}\right\}$ are deleted. Figure [6](#page-5-0) shows the local mesh cavity before and after the layer edge collapse operation.

The layer edge swap operation changes the connectivity of neighboring boundary layer stacks. In comparison to an edge swap operation for tetrahedra, which are reconfgured based on the equatorial plane, there is only one other possible confguration for layer faces in case of a layer edge swap operation [\[53](#page-28-3)]. If $\{M_i^1\}$ (with $i \in [1..N]$) are the layer edges to be swapped, then the layer edge swap operation retriangulates the cavity $\{C\{M_i^1\}\} = \left\{\bigcup_{i=1}^N \{M_i^1\{M^3\}\}\right\}$ and new layer edges are introduced inside the cavity while

old layer edges $\{M_i^1\}$ are deleted. The unstructured interior regions at the interface are also retriangulated and in general are not guaranteed to be in a valid confguration after the swap operation. Thus, appropriate checks are required to ensure that the layer edge swap operation results in a valid mesh after its completion. Figure [7](#page-5-1) gives an example of the layer edge swap operation.

When edge split operations are applied to layer edges on curved wall surfaces, the newly introduced originating vertices must be moved to the curved boundary to maintain the proper geometric approximation. All the vertices on a growth curve should gradually be moved to follow the originating vertex, i.e., based on a movement vector [\[53\]](#page-28-3). The movement vector is determined for each stack of vertices based on the target location of the originating vertex on the curved domain boundary. This is given as: $\mathbf{m} = \mathbf{v}_0^t - \mathbf{v}_0$, where \mathbf{v}_0^t is the target location of the new originating vertex on the curved boundary (superscript *t* is used to denote target) and \mathbf{v}_0 is the location of the new originating vertex on the original layer edge. The movement vector **m** is then applied to all the vertices on that growth curve. The procedure frst evaluates the target location of every vertex on all new growth curves, with each vertex's target location calculated as: $\mathbf{v}_i^t = \mathbf{v}_i + \mathbf{m}$, where v_i is the current or original location of the *i*th vertex

on a growth curve and \mathbf{v}_i^t is its target location. The procedure then moves the vertices to their computed target locations. An example is depicted in Fig. [8.](#page-6-0) Similar to the repositioning of a newly created vertex in the unstructured mesh to the curved boundary, direct repositioning of a new originating vertex is not always possible without additional local mesh modifcation. Specifcally for the top most vertices, as it may introduce inverted elements. In this case local mesh modifcation operations are applied to the unstructured interior mesh for it to allow in a successful repositioning of the top most vertex. This step is followed by repositioning the rest of vertices on the growth curve.

3.4 Subdivision of transition pyramids

For pyramids we consider more subdivision templates than those presented in our previous work on serial boundary layer meshes [\[53](#page-28-3)]. This is done to achieve more fexibility in parallel mesh adaptation of boundary layer meshes. Pyramids are subdivided during the refnement of the unstructured part of the mesh.

There are three ways the quadrilateral face of a pyramid, which caps an exposed side of a stack, can be subdivided, see Fig. [9.](#page-6-1) While a refnement in the lateral direction splits

Fig. 9 Subdivision of a quadrilateral face based on different edge splits

Fig. 10 Subdivision templates

for a triangular face

the quadrilateral face using layer edges only (see the left image in Fig. [9\)](#page-6-1), the request to change the number of layers or the resolution along the normal or thickness direction can be achieved with bisection of the quadrilateral face along the growth edges (see the middle image in Fig. [9](#page-6-1)). Additionally, subdivision can be performed in both directions with the split of both layer and growth edges (see the right image in Fig. [9\)](#page-6-1).

In this study templates subdividing growth edges are not exploited. The reason for this is not due to any limitation in the ability to split the elements, but rather because thickness adjustment based on vertex repositioning was found to be sufficient for the problem cases considered in this work.

The rest of triangular faces of a pyramid is subdivided by counting the number of layer edges that are marked or tagged to be split, see Fig. [10.](#page-6-2) The triangular face templates are the same for the subdivision of layer faces and unstructured interior faces, and thus, do not introduce any additional ambiguity associated with the refnement of triangular faces.

The templates for a pyramid depend on the number of marked edges and the selection of the diagonal edge on a triangular face when two of its edges are marked [\[37](#page-27-10)]. This leads to a total of twenty-fve subdivision templates for a pyramid. The most frequently used templates for subdividing pyramids are shown in Fig. [11.](#page-7-0)

3.5 Unstructured decomposition of boundary layers

Figure [12](#page-7-1) shows a close-up of an adapted mesh on a pipe geometry without unstructured decomposition of prisms (on the left) and with prisms divided into tetrahedra and pyramids (on the right). One can observe that on the left part of the fgure there are boundary layer regions with low aspect ratio. It includes some layered regions that have growth edges that are longer than the layer edges which is counterintuitive in a boundary layer mesh and are not desirable. To satisfy the desired mesh resolution in such cases the corresponding regions in top portion of the stacks are converted into unstructured part of the mesh

Fig. 11 Subdivision templates for a pyramid

Fig. 12 Mesh adaptation without and with unstructured decomposition of regions with relatively low aspect ratio in the *top* portion of the stacks

Fig. 13 Different number of layers in neighboring boundary layer stacks. The number of vertices on growth curves is indicated by the count shown at originating vertices. Bold solid and dashed lines at the bottom represent edges on the wall

and subsequently more fexible unstructured mesh modifcation operations can be applied to achieve the appropriate level of mesh resolution and anisotropy. This is an additional feature to our previous work on serial boundary layer meshes [\[53](#page-28-3)].

The process of unstructured decomposition of prisms or reducing the numbers of layers in selected stacks, also referred to as trimming, leads to introduction of additional quadrilateral faces that must be capped with pyramids so that the mesh can be transitioned into tetrahedral elements in the unstructured interior mesh. This step can be reversed when a thicker boundary layer or more layers are desired. It can be done by splitting growth edges that will reintroduce more layers (locally). However, as mentioned before, split of growth edges is not considered currently since it was not necessary for the problems cases considered in this work.

The current algorithm for stack decomposition relies on adjacent stacks of regions that share a face to differ in the number of layers (or prisms) by only one, in which case the top prism on the higher stack must be connected to a pyramid. This is done to transition between different number of layers in face-neighbor stacks of regions. This condition can be enforced by controlling the number of vertices in neighboring growth curves in a preprocessing step before executing the trimming step.

Figure [13](#page-8-0) shows boundary layer stacks with different number of layers where any two face-neighbor stacks have no more than one layer difference. Note that with this condition the corresponding number of vertices between growth curves of a given stack can vary by as much as two. In the trimming step, the number of layers for a given growth curve is dictated by the lowest level regions being decomposed. The lowest level boundary layer vertices are given a priority to bisect the quadrilateral faces adjacent to it. If vertices next to each other are of the same level, the priority is granted to the one having the smallest local

vertex identifer (ID) which eliminates any possible ambiguity in selecting the diagonal edge of the quadrilateral face.

The application of this restriction during trimming of the stacks yields a favorable situation in which all prisms subdivided into tetrahedra can be triangulated without the introduction of an interior vertex [[60\]](#page-28-9). Avoiding an interior vertex eliminates certain algorithmic complexities and typically results in a better control of the element shape quality [[35\]](#page-27-33).

Algorithm 1 Pseudo code for the unstructured decomposition of boundary layers.

- 1: for each boundary layer stack BL_i do
- for each region in the stack $M_i^3 \in BL_i$ from bot- $2:$ tom to top do
- $3.$ assign: AR_j = aspect ratio of M_j^3
- if AR_j < AR_{min} (where AR_{min} is the pre- $\overline{4}$: scribed limit for aspect ratio) then
- $5.$ tag BL_i for unstructured decomposition
- determine and assign the new number of lay-6. ers to BL_i
- assign the new number of layers to corre- $7.$ sponding originating vertices (i.e., maximum of surrounding stacks)
- 8: break
- 9: end if
- $10:$ end for
- $11:$ end for
- 12: for each *level* starting from 0 do
- if number of layers assigned to any two face-13 neighbor stacks differ by more than 1 then
- reduce the number of layers assigned to the 14. higher stack BL_i to achieve a difference of 1
- tag BL_j for unstructured decomposition 15:
- assign the new number of layers to BL_i 16:
- $17:$ end if
- $18:$ end for
- 19: bisect quad faces of each stack BL_i tagged for unstructured decomposition
- 20: subdivide regions adjacent to bisected quad faces
- 21: tetrahedralize any two pyramids sharing a quad face

A prism can be subdivided into a pyramid and a tetrahedron when two of its quadrilateral faces are split and the two diagonal edges share a common vertex, or into three tetrahedra when all quadrilateral faces are subdivided and there is at least a common vertex between any two diagonal edges. This is depicted in Fig. [14.](#page-9-0) This logic eliminates the possibility for a prism being subdivided to have only one quadrilateral face that is split, or that there is no common vertex between diagonal edges.

Fig. 14 Subdivision of a prism based on bisection of quadrilateral faces with diagonal edges sharing a common vertex

The algorithm for unstructured decomposition of the appropriate portions of a boundary layer mesh consists of three parts. The frst part is responsible for determining the layers in each stack that need to be decomposed based on the allowed minimum value of the aspect ratio. The second part adjusts the number of layers for any two face-neighbor stacks of regions such that they have difference of no more than one after the unstructured decomposition is accomplished. The third step assigns each quadrilateral face with an appropriate diagonal edge using the rules described above. Algorithm 1 presents the overall process of the unstructured decomposition of boundary layers.

3.6 Overall boundary layer mesh adaptation algorithm

Before we present our approach for parallel boundary layer mesh adaptation, the overall adaptation procedure is described. It is executed in three stages: mesh coarsening, iterative mesh refnement and shape improvement [\[53](#page-28-3)]. The frst two stages are controlled by analysis of mesh edge length in the metric or transformed space, whereas the third stage is dictated by both mesh edge length and element shape or quality control. The layered part of the mesh is given a priority in applying mesh modifcation operations of a specifc type followed by the same operation for the unstructured entities. This is done because size requests for entities in boundary layer stacks are more involved (e.g., layer edge split is applied throughout the stack) and thus, resolved frst.

The overall procedure is given in Algorithm 2. It starts with the coarsening stage. The coarsening stage applies local mesh modifcation operations to eliminate the majority of edges shorter than that requested by the local mesh size feld. A mesh edge is considered to be short if its length in the transformed space is smaller than the specifed value *Lmin* [\[37](#page-27-10)]. An advantage to coarsening frst is that it will make the traversals required during mesh adaptation faster and limit the peak memory used during the adaptation process. Thickness adjustment is applied on the coarsened mesh so that it is only applied to entities that will remain in the mesh.

Algorithm 2 Pseudo code for boundary layer mesh adaptation.

- 1: get mesh metric field from the application
- 2: apply metric decomposition in layered part of the mesh
- 3: coarsen short layer edges in the metric space
- 4: coarsen short interior edges in the metric space
- 5: adjust thickness for each growth curve
- while mesh resolution is not satisfied do $6 -$
- $7¹$ tag layer edges that are long in the metric space
- split tagged layer edges, their adjacent faces and 8. regions except for the interior ones
- tag interior edges that are long in the metric $9:$ space
- split tagged interior edges, their adjacent faces $10:$ and regions
- move new originating vertices at curved bound- $11:$ aries onto solid surface
- move new unstructured vertices at curved bound- $12.$ aries onto solid surface
- $13²$ coarsen short layer edges introduced in this refinement iteration
- apply unstructured decomposition to top portion $14:$ of stacks with relatively low aspect ratio
- 15: coarsen short interior edges introduced in this refinement iteration
- 16: end while
- 17: eliminate poorly shaped layer faces by layer edge swap or collapse operators
- 18: eliminate poorly shaped interior regions by swap or compound operators

The second stage refnes mesh regions using refnement templates that split the mesh edges longer than *Lmax* in the transformed space. *Lmin* and *Lmax* are typically selected to be $1/\sqrt{2}$ and $\sqrt{2}$, respectively [\[37](#page-27-10)]. The procedure ensures that the refnement is applied to stacks of prisms along with interior elements located at the interface. This stage also places newly created boundary vertices onto the domain boundary (e.g., as defned by the CAD model). It also coarsens any new short mesh edges introduced by refnement templates. At the end of an iteration in this stage, any elements in the stack that have relatively low aspect are tetrahedralized and made part of the unstructured interior mesh. Thus, removing them from the stack by applying unstructured decomposition of boundary layers. The refnement iterations terminate when no long layer or interior edges are left.

The third stage applies shape improvement operations to improve the quality of poorly shaped entities in the transformed space. We use mean ratio [[39\]](#page-27-31) as the measure for element shape quality, specifcally the cube of the mean ratio in the transformed space [\[37](#page-27-10), [53](#page-28-3)]. This is done for both layer faces (in layered part of the mesh) and tetrahedra (in unstructured interior part of the mesh).

Poorly shaped entities (i.e., those below a certain value of quality measure) are modifed using sets of swap and compound operators [\[37,](#page-27-10) [53](#page-28-3)] to obtain the best possible element quality while preserving the desired edge length in the transformed space [\[4,](#page-26-4) [17](#page-27-34), [39](#page-27-31)]. Again, the shape correction operations are first carried out in the layered part of the mesh and then followed by mesh optimization in the unstructured interior part [[53\]](#page-28-3).

4 Parallel implementation

The execution of parallel mesh adaptation is based on the fact that the mesh is distributed $[3, 57]$ $[3, 57]$ $[3, 57]$ $[3, 57]$ into a number of parts, where each part consists of a set of mesh entities and is treated as a partitioned mesh with the addition of interpart boundaries within the mesh. A partitioned mesh is managed by the parallel mesh database that tracks the mesh entities residing on inter-part boundaries.

The application of a local mesh modifcation in parallel involves a cavity of mesh entities that are all on one part or are on multiple parts. In the case where the entities associated with a cavity are on a single part, the mesh modifcation can be carried out on that part and thus making the parallel execution straightforward. However, in cases where the entities in the cavity are distributed on multiple parts, some form of inter-part or inter-processor coordination is needed.

4.1 Distributed mesh infrastructure

The effective implementation of parallel mesh modifcation requires a parallel mesh infrastructure and associated parallel mesh control tools. The parallel mesh representation [\[57](#page-28-10)] employed maintains the information on mesh entities on inter-part boundaries such that all parts sharing an entity maintain an on-part copy as well as remote copies corresponding to other parts. It supports the ability to update mesh entities on inter-part boundaries if they are modifed (e.g., due to an edge split). It also supports the movement or migration of mesh entities from one part to another, which is referred to as a mesh migration step and in which the inter-part boundaries are automatically updated.

Mesh migration is needed to localize a cavity associated with a mesh modifcation operator. For certain mesh modifcation operations, such as collapse and swap, the direct consideration of cavities spanning multiple parts leads to a complex and expensive procedure since it requires a number of communication steps to properly carry out the mesh modifcation operation and update the local mesh in each part. Thus, before applying the mesh modifcation operation, such cavities are localized on one part or processor such that the cavity retriangulation can be carried out as in the serial case. In cavity localization, all regions and stacks of regions involved in the mesh modifcation operation are migrated onto a single part [\[3](#page-26-3), [57](#page-28-10)].

Note that during mesh adaptation, mesh migration is also needed to control the memory usage since the adaptive mesh modifcation process will alter the numbers of entities on a part (e.g., due to concentrated refnement in a part) and thus the mesh must be dynamically repartitioned. The Zoltan library [\[56](#page-28-11)] is used to perform the dynamic repartitioning.

For a boundary layer mesh, the mesh modifcations in the layered part of the mesh are applied to the entire stack, and therefore, maintaining the knowledge of the stack is critical. In parallel, managing this information would be diffcult if the mesh regions in a stack were distributed over multiple parts. Thus, the implementation of parallel boundary layer mesh adaptation requires all the mesh regions in a boundary layer stack to be placed in a mesh set [\[64](#page-28-12)] and each such mesh set is required to reside on a single part along with the ability to migrate such a set to another part.

Additionally, mesh modifcation and migration involve many irregular or unstructured messages of relatively small sizes. Thus, the parallel efficiency and scalability depend on effectively controlling the underlying message-passing processes. The Inter-Processor Communication Manager (IPComMan) is used [[48\]](#page-27-35) for efficient parallel communications between processors. It is a general-purpose communication package built on top of MPI [\[1](#page-26-5)] which signifcantly improves the inter-processor communications by exploiting mesh neighborhood of a given part and by packing small messages into larger messages.

Algorithm 3 Pseudo code for refinement of the parallel boundary layer mesh.

- 1: for all edges M_i^1 (and faces M_i^2) which are tagged for refinement ${\bf do}$
- $\overline{2}$: split M_i^1 (and M_i^2)
- $3:$ if the entity being split resides on inter-part boundary then
- attach the list of newly created entities $4:$ *NewEntList* to corresponding M_i^1 (and M_i^2)
- add M_i^1 (and M_i^2) to the list on update of inter- $5:$ part links UpdateLinksList
- end if $6:$
- 7: end for
- 8: for all M_i^1 (and M_i^2) in UpdateLinksList do
- 9: send the attached NewEntList to remote copies of M_i^1 (and M_i^2)
- receive and set up links between $NewEntList$ of $10:$ M_i^1 (and M_i^2) on local part with ones from remote parts
- $11:$ end for
- 12: subdivide layered and unstructured regions

4.2 Refnement and boundary vertex repositioning

Subdivision of mesh edges and their adjacent mesh faces on inter-part boundaries happens the same way as it is done in serial [\[3](#page-26-3), [16](#page-27-28)]. The duplicate faces on inter-part boundaries maintain the bounding edges and vertices in the same order on each part to ensure the triangulations are consistent across face neighbors. Note that triangular faces can be split using any combination of edges tagged for refnement whereas quadrilateral faces (which are part of the boundary layer stacks) are subdivided using opposite edges, see Figs. [9](#page-6-1) and [10.](#page-6-2) When a quadrilateral face is bisected for unstructured decomposition of boundary layers (see Fig. [14\)](#page-9-0), then the procedure ensures that the diagonal edge of the face is created in the same way on both parts sharing the face. This way no invalidity is introduced during mesh triangulation and matching of the newly created entities on inter-part boundaries.

The inter-part links between newly created mesh entities are updated across the parts in a communication step such that the distributed mesh is correctly connected. In the execution of the refnement step, the corresponding old-tonew entity mapping is formed such that the links for newly created entities can be effectively set during the communication step. The communication step is carried out after all tagged edges and faces have been split. The mesh regions are subdivided using the same templates as in serial without any communication (i.e., only lower-order entities on inter-part boundaries require a communication step). The pseudo code of the parallel refnement algorithm is given in Algorithm 3.

The algorithm for updating the inter-part links involves the same logic for both layered and unstructured parts of the mesh. The only difference for the layered part is that the update for any stack involves the entire subdivided portion of that stack.

Figure [15](#page-12-0) demonstrates an example of the parallel refnement procedure. The initial distributed mesh is depicted in Fig. [15](#page-12-0)a, where thick lines indicate edges and

adjacent faces which are going to be split and communicated during the refnement step. One of those edges is represented as M_0^1 on P_0 and M_1^1 on P_1 (Fig. [15](#page-12-0)a). Consider top view of the stack (Fig. [15b](#page-12-0), c) showing refnement of edges M_0^1 and M_1^1 on each part. Figure [15](#page-12-0)b shows the introduction of the vertex M_0^0 splitting the edge M_0^1 , and Fig. [15c](#page-12-0) shows M_1^0 splitting the edge M_1^1 . On each part, the newly created vertex and two edges are the child entities and attached to the parent edge on inter-part boundary, namely: $M_0^1 \rightarrow \{M_0^0, M_2^1, M_3^1\}$ on P_0 and $M_1^1 \rightarrow \{M_1^0, M_4^1, M_5^1\}$ on *P*1. To set up the correct inter-part links between the new entities, a communication step is carried out for remote copies between $\{M_0^0, M_2^1, M_3^1\}$ on *P*₀ and $\{M_1^0, M_4^1, M_5^1\}$ on *P*₁. On *P*₀, M_0^1 has a link to M_1^1 and using this link it sends to P_1 the list of child entities, whereas on P_1 , M_1^1 has a link to M_0^1 and using this link it sends the list of child entities to P_0 . This way P_1 receives the message for M_1^1 containing the list of remote copies of its children on P_0 and vice-versa. Then on P_1 , the old-to-new mapping is used to update the links such that M_0^0 corresponds to M_1^0 , M_2^1 corresponds to M_4^1 , and M_3^1 corresponds to M_5^1 . Same is done on P_0 . This is depicted in Fig. [15c](#page-12-0). After all edges and faces are split on the inter-part boundaries and the links are updated, the regions are subdivided with no further communication. The resulting mesh is depicted in Fig. [15](#page-12-0)d.

In the process of refnement, each part maintains a list of new mesh vertices that reside on curved domain boundary and need to be projected [[3\]](#page-26-3). For the layered part of the mesh, the newly created originating vertices are projected onto to the curved surfaces with the help of the movement vector as described in Sect. [3.3](#page-4-1). In cases where a direct repositioning will introduce invalidities in the unstructured part of mesh (i.e., at the top of the stack), a more extensive set of local mesh modifcation operations, which includes collapses, swaps and/or splits, is used. This is done in parallel which involves mesh migration (as discussed above). Algorithm 4 describes vertex repositioning procedure for the parallel boundary layer mesh.

Fig. 15 Example of layer edge split in parallel

Algorithm 4 Pseudo code for vertex repositioning for the parallel boundary layer mesh.

- 1: for all new originating vertices M_i^0 on model boundary with target locations $\mathbf{x}_{M_{i_{orgn}}^{0}}^{t}$ do
- calculate target locations for each vertex on cor- $\overline{2}$: responding growth curve GC_j (i.e., $M_i^0 \in GC_j$)
- add the top most vertex $M_{i_{top}}^0 \in {^{c}C_{j}}$ with 3: its corresponding target location $\mathbf{x}_{M_e^0}^t$ $VtxListToMove$
- 4: end for
- 5: while $VtxListToMove$ is not empty in all parts do
- for all $M_i^0 \in VtxListToMove$ do 6:
- $7:$ move M_i^0 to its target location
- 8: **if** movement introduces flat or inverted regions then
- **if** M_i^0 is on inter-part boundary **then** 9:
- add M_i^0 to $VtxAdjRgnMigrate$ $10:$
- else $11:$
- if possible then apply local mesh modifi- $12:$ cation to ensure the movement of M_i^0 to its target location
- 13: end if
- $14:$ else
- remove M_i^0 from $VtxListToMove$ 15:
- end if 16:
- end for $17:$
- send each vertex $M_i^0 \in VtxAdjRgnMigrate$ to 18: its remote copies
- move vertices which receive messages from re- $19:$ mote copies (based on $VtxAdjRqnMigrate$) to their original location
- 20: perform mesh migration based **on** $VtxAdjRgnMigrate$
- update VtxListToMove on each part after mi- $21:$ gration
- 22: end while
- 23: for all growth curves GC_i in which repositioning of the top most vertex was performed do
- move each vertex in the stack to its target $24:$
- 25: end for

4.3 Coarsening and swapping

Layer edge collapse operation is always performed on a localized or on-part cavity [\[3](#page-26-3), [16\]](#page-27-28). For applying a layer edge collapse operation on a growth curve, the boundary layer stacks adjacent to the growth curve are checked. In this step, all the layer edges that are adjacent to the vertices on the growth curve, starting at the originating vertex $M_{j_{orgn}}^0$ and ending at the top most vertex $M_{j_{top}}^0$, are considered. If

no surrounding stack of short layer edges can be collapsed locally, then the boundary layer coarsening procedure migrates all the layered and interface regions adjacent to growth-curve vertices (from $M_{j_{orgn}}^0$ to $M_{j_{top}}^0$) onto a single part. The procedure then checks for the validity of the layer edge collapse operation for the given growth curve and proceeds with it.

Figure [16](#page-14-0) shows the example of an layer edge collapse operation requiring migration. It can be seen from the fgure that growth-curve vertices $[M_{j_{orgn}}^0, \ldots, M_{j_{top}}^0]$ reside on the inter-part boundary and the collapse operation cannot be carried out. Thus, all the adjacent layered and interface regions are migrated to one part P_2 to perform the layer edge collapse operation.

Algorithm 5 Pseudo code for coarsening of the parallel boundary layer mesh.

- 1: Create and fill the list of originating vertices $VtxListToCips$ connected to atleast a stack of layer edges with all short edges in the metric space
- 2: while $VtxListToClps$ is not empty in all parts do 3:
- for all originating vertices $M_{j_{organ}}^0$ in the list of vertices VtxListToClps do
- find stack of shortest adjacent edges corre- $4:$ sponding to vertices M_i^0 on growth curve GC_i
- if adjacent layered and interface regions are on 5: one part then
- check for validity of the layer edge collapse 6: operation and apply it
- update VtxListToClps $7:$

else 8:

add vertices on inter-part boundary $Q₂$ $[M_{j_{orgn}}^0, \ldots, M_{j_{top}}^0] \in GC_j$ into the list $VtxToMigrate$

- $11:$ end for
- $12:$ perform mesh migration based on the list $VtxToMigrate$
- update $VtxListToCips$ based on migration 13:
- 14: end while

Algorithm 5 presents the procedure for coarsening of the parallel boundary layer mesh. It starts with a (dynamic) list on each part which consists of originating vertices that are connected to atleast a stack of layer edges with all short edges in the metric space and must be collapsed. This list is repeatedly traversed until it is empty.

In each traversal, the adjacent boundary layer stacks are checked for the layer edge collapse operation based on the shortest adjacent edges to a given growth curve. If all layered and interface regions are on one part, then the collapse operation is checked for validity and applied as in the serial case and the dynamic list of originating vertices to

end if $10:$

Fig. 17 A schematic of the adaptive loop with different simulation components

be collapsed is updated. Otherwise, the corresponding layer vertices on inter-part boundaries are added to the list of vertices to be migrated. After each traversal, the migration list is used to request migration of surrounding layered and interior regions. These requests then drive the mesh migration step and also updating of the on-part list of originating

Algorithm 6 Pseudo code for layer surface optimization of the parallel boundary layer mesh.

- 2: while $FaceListToOpt$ is not empty in all parts do
- $3:$ for all faces M_k^2 in $FaceListToOpt$ do
- check for the layer edge swap operation to ap- $4:$ ply on bounding edges
- if layered and interface regions associated with $5:$ the swap operation are on one part then
- apply the operation and update $6:$ $FaceListToOpt$
- $7:$ else
- obtain the top most layer face $M_{k_{\text{tan}}}^2$ (corre-8: sponding to M_k^2)
- add the top most vertices $M_{j_{top}}^0 \in \{\partial M_{k_{top}}^2\}$ 9: into the list $VtxToMigrate$
- end if $10:$
- end for $11:$
- perform mesh migration based on the list $12:$ $VtxToMigrate$
- update $FaceListToOpt$ based on migration 13:

14: end while

vertices to be collapsed.

Parallelization of the layer edge swap operation follows the same overall logic as the layer edge collapse operation. Layer edge swaps are applied at the end of the boundary layer mesh adaptation procedure, i.e., within the mesh optimization step for the layered part of the mesh [\[53](#page-28-3)]. The only difference in such an optimization step is that it is driven by a traversal process focused on improving the shape quality of the layer faces. Algorithm 6 describes the surface optimization procedure for the parallel boundary layer mesh.

5 Results and discussions

5.1 Adaptive loops and applications

An adaptive loop is constructed using a set of interoperable components that includes analysis code along with libraries for geometry-based problem specifcation, automatic mesh generation, error estimation and generalized mesh modifcation (e.g., see [\[12](#page-27-36), [58](#page-28-13)]). The adaptive loop links the analysis and adaptation components needed for the successful simulation of the problem on the domain of interest. The solution obtained by the analysis code is evaluated to provide information for mesh adaptation, which in-turn results in an adapted mesh that enriches the solution approximation. In this step, the error distribution is determined on the current mesh and is converted into a mesh metric or size feld that is used to drive the adaptation procedure. In the adaptation procedure as the mesh is locally modifed, the necessary solution felds are transferred onto the modifed mesh. The resulting adapted mesh and associated solution felds are sent back to the analysis code to perform the next step of analysis and adaptation within the adaptive loop. The overall structure of the adaptive loop is shown in Fig. [17](#page-14-1).

The current capabilities of the parallel anisotropic mesh adaptation with boundary layers are demonstrated on three flow applications. The first case involves the ONERA M6 wing $[61]$ $[61]$ for which the FUN3D flow solver $[46]$ $[46]$ was used. In the second case, the simulation of a heat transfer manifold was executed. The analysis for this case was performed using the PHASTA fow solver [[63\]](#page-28-15). The third test case involves a scramjet engine (of the NASA CIAM configuration $[45]$ $[45]$, where the analysis was performed using the FUN3D flow solver.

The parallel boundary layer mesh adaptation procedure for these cases has been executed on Hopper Cray XE6 [[18\]](#page-27-39) at the National Energy Research Scientifc Computing Center. It is confgured with 2 twelve-core AMD 2.1 GHz processors per node, with separate L3 caches and memory controllers, 32 GB or 64 GB DDR3 SDRAM per node. Hopper has a Gemini interconnect with a 3D torus topology. Note that all available processors or cores on a node were used in this work.

In this work, both strong and weak scalings are studied. The strong scaling (for a fxed size mesh in an aggregate sense) is computed based on the execution time on base processors and is defned as:

$$
S_i^s = (np_{base} \times t_{base})/(np_i \times t_i),
$$
\n(5)

where *npbase* is the base number of processors or cores, *tbase* is the execution time on base processors, np_i is the number of processors on which strong scaling is tested, and *ti* is the execution time on test processors. A scaling factor of 1 indicates a perfect linear scaling (i.e., 100 % parallel efficiency) and a value below or above 1 denotes a sub-linear scaling (or below 100 $%$ parallel efficiency) or super-linear scaling (or above 100% parallel efficiency), respectively.

On the other hand, the weak scaling (with a fxed load per part) is computed using a correction factor. This is done to account for (slightly) different loads in an aggregate and average sense between different meshes considered under weak scaling. It is computed as:

Fig. 18 ONERA M6 wing: initial (*top left*) and three adapted meshes (frst and third adapted meshes are shown in the *right column*)

$$
f = M_{\text{incr}-i} / M_{\text{incr}-\text{base}},\tag{6}
$$

$$
S_i^w = f \times t_{base}/t_i,
$$
\n(7)

where M_{incr} is the mesh increase factor defined by the ratio of the number of regions from input to adapted meshes for a test case and *Mincr*−*i* and *Mincr*−*base* are the mesh increase factors for the test and base cases, respectively. *f* is a factor which is the ratio of the mesh increase factors of the test and base cases.

5.2 ONERA M6 wing

The ONERA M6 wing is a classic validation case [[61\]](#page-28-14). Air enters the wind tunnel at transonic speed and is accelerated over the wing to a supersonic speed causing a shock to appear on the wing. The free-stream Mach number is 0.84 and the angle of attack is 3.06° . The free-stream pressure and temperature are 42.89 psi and 255.5 *K*, respectively. The Reynolds number is 11.72 million based on the mean aerodynamic chord. This flow marks a strong need for mesh adaptivity since the location and structure of the complex lambda shock is unknown a priori. The reference experimental data are from Schmitt and Charpin in [\[61](#page-28-14)]. We used FUN3D flow solver for this case.

Three cycles of mesh adaptation were applied for this case, where Hessian of pressure was used to compute the mesh metric feld. Initial mesh contained 0.28M regions with pre-defned boundary layers (where M denotes a million). The frst adapted mesh had 0.37M regions, the second adapted mesh had 1.24M regions while the third and fnest adapted mesh had 3.8M regions. Figure [18](#page-16-0) shows the surface mesh on the upper side of the wing for the initial and three adapt meshes. The imprint of the lambda shock on the adapted mesh can be clearly seen.

Figure [19](#page-17-0) presents the pressure coefficient for the initial and three adapted meshes. The surface pressure contours (along with surface meshes in Fig. [18](#page-16-0)) show that the mesh is refned in the shock region and the shape of the lambda shock is clearly captured. The mesh away from the shock is coarsened, due to a low variation in pressure in those regions. The surface pressure contours become sharper and more regular with adaptivity. One thing to notice is that the elements start to align with the shock in the frst adapted mesh.

To perform a more quantitative comparison, we look at the pressure coefficient profiles along the chord at certain spanwise locations on the wing. Figure [20](#page-18-0) shows pressure coefficient along the local chord at two spanwise locations. In this figure, experimental data are also included [\[61](#page-28-14)]. These plots show that as the mesh is adapted, the pressure coefficient becomes more accurate. To establish this aspect further we look at a zoomed view near the suction peak in Fig. [21.](#page-18-1) The zoomed view clearly shows that the agreement between experimental and numerical results are improved as the mesh is adapted further. The fnest or third adapted mesh shows the best agreement among all meshes. For example, at non-dimensional span location of $y/b = 0.9$, the peak pressure value is captured far better

Fig. 19 ONERA M6 wing: pressure on initial (*top left*) and three adapted meshes (frst and third adapted meshes are shown in the *right column*)

on the fnest adapted mesh as compared to other adapted meshes. Results on the initial mesh are the least accurate among all meshes.

To evaluate the parallel performance of boundary mesh adaptivity, a strong scaling study was conducted. In this study we consider a refned mesh of the third adapted mesh resulting in 160M regions. Strong scaling study was executed on cores ranging from 512 (base) to 8192, which spans 4 doublings in core counts.

Table [1](#page-19-0) shows that the execution time for mesh adaptation procedure decreases with an increase in the number of processors. As the given mesh is distributed to more processors, there is little computation performed during mesh modifcations relative to the substantial increase in communications, and thus, the scaling decreases on high core counts.

5.3 Heat transfer manifold

The heat transfer manifold test case consists of a large diameter cylindrical pipe as the inlet, a relatively thin and fat manifold section, and twenty outlet pipes. Flow simulations for this case were performed using the incompressible Reynolds-averaged Navier-Stokes (RANS) simulations with the Spalart-Allmaras turbulence model. A turbulent velocity profle with a Reynolds number of 1 million was used at the inlet pipe. No-slip boundary conditions were assumed at walls and a homogeneous natural pressure was prescribed at the outlet. In this case, the Hessian-based error indicator used the static pressure combined with a scaled dynamic pressure. This was defined as: $p + \alpha \rho u^2/2$,

where the factor $\alpha = 0.2$ was chosen to attain an appropriate balance of static and dynamic pressure.

Two iterations or cycles of the adaptive loop (which consists of a flow solve and mesh adaptation within each cycle) were carried out, and at each cycle, fow solver was started from the solution of the previous cycle. The initial computation used a mesh of 3M elements with pre-defned boundary layers. The frst adapted mesh had 16M regions and the second adapted boundary layer mesh had 81M regions. The initial mesh along with the frst and second adapted meshes are shown in Fig. [22.](#page-19-1)

For this case we provide a qualitative assessment of the numerical results due to the lack of experimental or any reference data for comparison. The pressure distribution near the inlet pipe is provided in Fig. [23](#page-19-2), whereas near the outlet pipe is presented in Fig. [24](#page-20-0). The initial mesh is too coarse and these fgures demonstrate its inability to capture the dominant flow features. Critical flow locations, including stagnation and turns around fllets of the pipes, get signifcantly refned. For example, see the smoother solution obtained on adapted meshes. The walls of the manifold, especially the wall closest to the inlet pipe, get refned to a higher degree. The fllets of the outlet pipes also get more refnement. The central part of the fat manifold gets relatively lesser refnement because of a relatively small variation in the solution. Moreover, away from flow regions with stagnation and turns, highly anisotropic mesh elements are created to effectively capture the anisotropy present in the fow. This results in signifcant computational savings over isotropic meshes of equivalent resolution.

Fig. 20 Pressure coeffcient profles along the local chord on initial and three adapted meshes at two spanwise locations

Figure [25](#page-21-0) shows the magnitude of wall shear stress. With adaptivity, smoothness of the wall shear stress feld improves and its details are captured better. It has been shown in [[53\]](#page-28-3) that a wall shear stress field computed on an adapted boundary layer mesh is superior to that computed on a fully unstructured adapted mesh of a similar resolution.

In addition to these results, mesh statistics were also collected for this case. Specifcally, this was done for three quantities in the metric or transformed space: layer edge length, interior edge length and mean ratio for interior regions (for further details on such mesh statistics for fully unstructured, anisotropically adapted meshes see [\[37](#page-27-10), [49\]](#page-27-4)). Currently mesh statistics were collected for the fnal adaptation cycle, where it was done for both the input mesh and

Fig. 21 A zoomed view of the pressure coeffcient profles (near the suction peak) on initial and three adapted meshes at two spanwise locations

the resulting adapted mesh. Figure [26](#page-22-0) shows these statistics. It can be seen that the input mesh has a large number of interior and layer edges whose lengths in the metric space are outside the desired interval of $[1/\sqrt{2}, \sqrt{2}]$, however, for the adapted mesh interior edges fall within this interval indicating the satisfaction of the specifed mesh metric feld. Note that a large number of layer edges in the adapted mesh have a length (in the metric space) close to 0.5. This is due to the conservative nature of the split scheme used for layer edges (i.e., edge split of a single layer edge results in the split of all layer edges in that stack). Similarly, mean ratio plot shows that the shape quality measure of the elements in the adapted mesh is higher and respects the specifed mesh metric feld.

Table 1 Execution time and strong scaling of mesh adaptation for the ONERA M6 case

| Num. cores (np) | 512 (base) | 1024 | 2048 | 4096 | 8192 |
|--------------------------|------------|--------|------|----------------------|------|
| Time $(t \text{ in } s)$ | 1212.83 | 812.68 | | 507.36 322.82 241.94 | |
| Scaling factor (S^s) | | 0.75 | 0.60 | 0.47 | 0.31 |

As before, a strong scaling study was conducted to evaluate the parallel performance of boundary mesh adaptation procedure on this test case. In this case, mesh adaptation in the second cycle of the adaptive loop was executed on a range of processors from 256 (base) to 4096, which spans 4 doublings in processor counts. Table [2](#page-22-1) gives the scaling results for the input mesh with 16M regions and the fnal

Fig. 22 Heat transfer manifold: initial (*left*), frst adapted (*middle*) and second adapted (*right*) meshes

Fig. 23 Initial (*left*), frst adapted (*middle*) and second adapted (*right*) meshes (in *top row*) and pressure distribution (in *bottom row*) for the heat transfer manifold test case. The cut is applied at the end of the inlet pipe near the fat section

Fig. 24 Initial (*left*), frst adapted (*middle*) and second adapted (*right*) meshes (in *top row*) and pressure distribution (in *bottom row*) for the heat transfer manifold test case. The cut is applied at an outlet pipe

adapted mesh with 81M regions. In Table [2](#page-22-1) the execution time for mesh adaptation decreases with an increase in the number of cores. Again, on high core counts there is little computation performed during mesh modifcations relative to the substantial increase in communications, and thus, the scaling decreases on high core counts.

The flow solver has been shown to strongly scale $[55, 16]$ $[55, 16]$ $[55, 16]$ [66](#page-28-7)] on a large number of cores, i.e., for a fxed size problem in an aggregate sense. It is the analysis part of a simulation which defnes the number of processors on which the particular problem is being executed. The idea is to effciently execute the mesh adaptation procedure on the same number of cores since repartitioning and migrating the mesh to a smaller number of cores for adaptation, and then again to a larger number after adaptation, will introduce a substantial amount of additional work and data movement.

In this case, the mesh adaptation procedure took 0.7 % of the total simulation time on 256 cores and 3.2 % on 4096 cores. In either case, mesh adaptation cost do not dominate as compared to the cost of the analysis step. Thus, even with some loss of strong scaling in the mesh adaptation step, it is reasonable to execute it on the same number of processors together with the fow solver.

A weak scaling study was also performed for this case on three uniformly refned meshes starting with the frst mesh on 256 (base) cores. The second mesh was obtained by uniform refnement of the frst mesh and the third mesh by uniform refnement of the second. The mesh metric feld for the second and third meshes was constructed from that on the frst mesh by multiplying it uniformly by a factor of 1 / 2 and 1 / 4, respectively. Due to the existence of the layered elements in the mesh the second and third meshes had roughly six times more regions than the frst and second meshes, respectively. Thus, the numbers of processors used to adapt the second and third meshes was set to 1536 and 9216, respectively. This roughly spans a factor of 36 in the number of mesh regions and core counts. Considering the heuristics employed in the mesh adaptation procedure and the fact that the ratio of regions in the test and base meshes is not precisely six, the weak scaling factor is calculated using a correction factor as discussed above. The weak scaling results are presented in Table [3.](#page-23-0)

Fig. 25 Wall shear stress on the initial (*left*), frst adapted (*middle*) and second adapted (*right*) meshes

Table [3](#page-23-0) shows that the weak scaling does not degrade substantially with the increase in the number of cores while having relatively the same amount of workload in each test. The scaling is affected not only by the growing data exchange between cores at larger core counts, but also by the asynchronous application of mesh modifcation operations. Note that although the average workload is approximately the same per part, it might be very different for each specifc part depending on the amount of different types of mesh modifcation operations applied locally on any given part and its neighboring parts sharing inter-part boundaries.

5.4 Scramjet engine

The NASA CIAM scramjet case [\[45](#page-27-38)] was setup with a freestream Mach number of 6.2 and temperature of 203.5 *K*. The initial mesh had 2.86M regions. A cut of it is shown in Fig. [27](#page-23-1) along with a zoomed view near the tip of the nose cone. Hessian calculations were based on the Mach number to compute the mesh size feld.

Two adaptation cycles were carried out for this case. The frst adapted mesh had 7.2M regions and the second adapted mesh consisted of 16M regions. Figure [28](#page-23-2) presents

Fig. 26 Distribution of edge length (*left* plot for interior edges and *middle* plot for layer edges) and mean ratio (*right* plot) in the transformed space from the fnal adaptation cycle of the heat transfer manifold case

Table 2 Execution time and strong scaling of mesh adaptation for the heat transfer manifold case

| Num. cores (np) | 256 (base) 512 | | 1024 | 2048 | 4096 |
|--------------------------|----------------|--------|------|----------------------|------|
| Time $(t \text{ in } s)$ | 1194.34 | 785.44 | | 514.45 421.09 339.38 | |
| Scaling factor (S^s) | \mathbf{I} | 0.76 | 0.58 | 0.35 | 0.22 |

a cut of the frst and second adapted meshes, whereas Fig. [29](#page-23-3) shows a zoomed view near the nose cone. For this case also we provide a qualitative assessment of the numerical results. Figure [30](#page-24-0) presents the Mach number contour plots on the initial mesh and the frst and second adapted meshes. In addition, Fig. [31](#page-25-0) shows adapted meshes and contours of the computed Mach number near the cowl lip region of the inlet to the combustor region.

The solution resolution is greatly improved through the use of anisotropic mesh adaptation. The second adapted mesh captures the shocks far better than the initial mesh. In the far-feld region upstream of the primary shock, where flow is uniform and parallel, the mesh was appropriately coarsened. Expected mesh refnement was obtained at the nose cone, at the cowl lip, within the combustor region, at the sharp edges of the combustor liner as well as behind the engine. Mesh anisotropy follows the shock emanating from the nose cone, i.e., elements are longer in the tangential directions to the shock than in the normal direction.

Changes in the mesh evidently refect a sharper resolution of fow features in the relevant regions of the domain. The second adapted mesh captures the shocks better than the initial mesh, and a sharper resolution of the shocks can be seen in Fig. [30](#page-24-0). The resolution of the shocks in the far feld is limited since it is currently not of concern and far-feld resolution can easily be improved with more stringent adaptation criteria. Behind the engine also, the fow features are better resolved on the second adapted mesh. Finally, the fow solution in the combustor region is also better resolved which is important in proceeding forward to a combustion simulation.

In this case, an anisotropic mesh gradation procedure [[36\]](#page-27-40) is also used to reduce high variations in the mesh size around the tip of the nose cone. Figure [32](#page-25-1) illustrates the impact of anisotropic gradation near the tip of the nose cone. The requested sizes at the wall surface are over an order of magnitude smaller than those in the unstructured region directly at the top of the boundary layer stacks. As a result, the boundary layer stack at the tip is much more refned than in the adjacent unstructured interior mesh, leading to a so-called "spider web" behavior and poorly shaped elements locally. As shown in Fig. [32,](#page-25-1) gradation of the mesh size feld alleviates this issue.

Mesh statistics were collected for this case too. The same three quantities were collected in the fnal adaptation cycle. Figure [33](#page-26-6) shows these statistics. It can be seen

Table 3 Execution time and weak scaling of mesh adaptation for the heat transfer manifold case

| Num. cores (np) | 256 (base) | 1536 | 9216 |
|--|------------|-----------------------|-------------|
| Initial mesh—number of regions | | 16,319,606 94,487,988 | 604.853.414 |
| Adapted mesh—number of 80,890,803 527,501,893 3,702,376,095 regions | | | |
| Mesh increase factor (M_{incr}) | 4.96 | 5.58 | 6.12 |
| Time $(t \text{ in } s)$ | 1194.34 | 1381.55 | 1716.23 |
| Scaling factor (S^w) | 1 | 0.97 | 0.86 |

Fig. 27 Cut of the initial mesh for the scramjet case: whole body (*top*) and a zoomed view near the tip of the nose cone (*bottom*)

that the input mesh has a large number of interior and layer edges whose lengths in the metric space are outside the desired interval whereas interior edges in the adapted mesh fall in this interval. As before, many layer edges in the adapted mesh are fner (or shorter) than desired, which is due to the conservative nature of the split scheme used for layer edges. The percentage of fner layer edges in the metric space is higher in this case because the computed mesh size feld has more variation along the thickness of the layered mesh (e.g., in stacks near the tip region of the nose cone). As before, mean ratio plot shows that the shape quality measure of the elements in the adapted mesh is higher and respects the specifed mesh metric feld.

Fig. 28 Cut of the frst (*top*) and second (*bottom*) adapted meshes for the scramjet case

Fig. 29 Cut of the frst (*top*) and second (*bottom*) meshes for the scramjet case near the nose

Fig. 30 Mach contours on the initial (*top*), frst adapted (*middle*) and second adapted (*bottom*) meshes

Table [4](#page-26-7) provides execution time and scalability of the mesh adaptation procedure based on the second adapted mesh. The strong scaling studies were performed on cores ranging from 128 (base) to 4096, which spans 5 doublings in core counts.

Table [4](#page-26-7) shows that the execution time for mesh adaptation procedure is decreased on larger number of cores. Even though the mesh is relatively smaller for this case as compared to the heat transfer manifold case, the parallel scalability is better. Note that the mesh adaptation procedure took 1.2 % of the total simulation time on 128 cores and 3.6 % on 4096 cores, which is not signifcant when compared to the analysis time. As in the previous cases, even for a fxed size problem, mesh adaptation procedure is able to perform effectively on high core counts.

Table [5](#page-26-8) gives weak scaling results for the scramjet engine case, where the scaling factor is calculated the same way it was done for the heat transfer manifold case. It can be seen in Table [5,](#page-26-8) with a relatively equal amount of workload per part in each test, the drop in weak scaling is modest as the core count is increased. In contrast to the strong scaling results, the weak scaling is better for the heat transfer manifold case as compared to the scramjet case. Note that the mesh increase factors are less in the scramjet case by roughly $2\times$ as compared to the heat transfer manifold case. As noted earlier, the parallel performance of the mesh adaptation procedure is specifc to the types of mesh modifcation operations carried out on different parts and on the communication-to-computation ratio.

6 Closing remarks

In this paper, a parallel adaptive boundary layer meshing procedure is presented. The approach successfully works on distributed meshes and effectively supports layered structure in the mesh. It is based on local mesh modifcation operations which are carried out in parallel and dictated by the specifed mesh size feld. The current parallelization paradigm allows the adaptation procedure to be applied on large and complex problem cases (e.g., on meshes with billions of regions).

The adaptation procedure was executed in parallel for three viscous flow problem cases, namely: the ONERA M6 wing, a heat transfer manifold and a scramjet engine. It has been demonstrated that boundary layer mesh adaptation leads to an accurate prediction of fow quantities of interest (e.g., surface pressure and wall shear stress) and appropriately resolves critical fow features (e.g., lambda shock). In the ONERA M6 wing case, numerical results on the fnest adapted mesh showed good agreement with the experimental data. However, in the other two cases a qualitative assessment was made.

The parallel performance of the mesh adaptation procedure for these problems showed that the execution time decreases with an increase in the number of cores for a fxed size problem or under strong scaling (e.g., with 5 doublings in core counts). Weak scaling was also presented showing that the procedure is capable to scale for larger meshes on high core counts (e.g., spanning a factor of 36 in the number of mesh regions and core counts). With mesh adaptation taking a small fraction of the total simulation time within the adaptive loop, parallel boundary layer mesh adaptation can be effectively integrated into workfows to support large-scale automated flow simulations of complex problems on high core counts. In the future, we plan to include cases where change in number of layers is required

Fig. 31 Initial (*top*), frst adapted (*middle*) and second adapted (*bottom*) meshes (*left column*) and Mach number contours (*right column*) for the scramjet case near the cowl lip and at the inlet to the combustor region

Fig. 32 Anisotropic gradation near the nose cone for the scramjet case: without (*left*) and with (*right*) gradation

Fig. 33 Distribution of edge length (*left* plot for interior edges and *middle* plot for layer edges) and mean ratio (*right* plot) in the transformed space from the fnal adaptation cycle of the scramjet case

Table 4 Execution time and strong scaling of mesh adaptation for the scramjet case

| Num. cores (np) 128 (base) 256 | | 512 1024 | | 2048 | 4096 |
|----------------------------------|------|----------|-----------------------------------|------|------|
| Time $(t \text{ in } s)$ 957.80 | | | 532.29 339.39 202.17 136.83 90.85 | | |
| Scaling factor 1 (S^s) | 0.90 | | $0.71 \qquad 0.59$ | 0.44 | 0.33 |

Table 5 Execution time and weak scaling of mesh adaptation for the scramjet case

and far-feld solution features (e.g., far-feld shocks) play an important role.

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