

1 Adaptive deformation of 3D unstructured meshes
2 with curved body fitted boundaries with
3 application to unsteady compressible flows

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10 **Abstract**

11 We present an adaptive moving mesh method for unstructured meshes which is a three-
12 dimensional extension of the previous works of Ceniceros et al. [9], Tang et al. [38]
13 and Chen et al. [10]. The iterative solution of a variable diffusion Laplacian model on
14 the reference domain is used to adapt the mesh to moving sharp solution fronts while
15 imposing slip conditions for the displacements on curved boundary surfaces. To this
16 aim, we present an approach to project the nodes on a given curved geometry, as well as
17 an a-posteriori limiter for the nodal displacements developed to guarantee the validity
18 of the adapted mesh also over non-convex curved boundaries with singularities.

We validate the method on analytical test cases, and we show its application to
two and three-dimensional unsteady compressible flows by coupling it to a second order
conservative Arbitrary Lagrangian-Eulerian flow solver.

19 *Keywords:* Constant-connectivity mesh adaptation, Unstructured meshes, Unsteady
20 compressible flows, Conservative formulations

21 **1. Introduction**

22 Mesh adaptation is a powerful tool to improve the representation of complex fields for
23 a given computational expense. In computational fluid dynamics in particular, adapta-
24 tion has become nowadays a customary tool [35]. Adapting the mesh also has a relative
25 computational overhead, which motivates the quest for efficient and robust methods.

26 Techniques improving the discrete representation of the fields of interest by inserting
27 and removing mesh entities (so called h-adaptation) have proven to be quite mature [35].
28 However, solution transfer between meshes with different topologies may be non-trivial
29 and may have a non-negligible computational cost, especially if conservation constraints
30 need to be satisfied [19, 2, 24, 31, 36].

31 By contrast, mesh nodes relocation with constant element connectivity (so called
32 r-adaptation), offers the possibility of a minimally intrusive coupling with existing com-
33 putational mechanics solvers, as no modification of the data structures is required. As

34 h-adaptation methods, they also provide considerable improvement in the quality of
 35 the solutions obtained, especially in unsteady simulations of traveling waves, like shock
 36 waves and water waves, where uniform refinement would be way too costly. More-
 37 over, with r-adaptation methods devising conservative projections is much simpler. In
 38 fact, the preservation of the one-to-one mapping from the old to the new mesh entities
 39 allows the easy construction of a conservative remapping [32], or the use of Arbitrary-
 40 Lagrangian-Eulerian (ALE) formulations compliant with the Geometric Conservation
 41 Law (GCL) [46, 41].

42 Unfortunately, the preservation of the initial mesh topology undeniably imposes se-
 43 vere restrictions on nodal displacements in order to avoid mesh folding with tangled (i.e.
 44 inverted) elements, especially when the boundary exhibits singular points. Moreover,
 45 the accuracy attainable for complex solutions is limited by the initial density of mesh
 46 nodes, and less finely-tunable than in metric-based h-adaptation [1].

47 Anyway, the advantages brought by the effortless coupling with external flow solvers
 48 and the conservative solution remapping can counterbalance the mesh quality limitation
 49 as long as the r-adaptation technique is computationally efficient. Simply put, the error
 50 reduction brought by adapting the mesh must offset the computational overhead. A
 51 measure of this efficiency can be evaluated by comparing with the cost of a simulation
 52 run on a uniformly refined mesh, providing the same resolution of the flow field. Hybrid
 53 adaptive approaches combining well timed re-meshing and adaptive deformation at every
 54 time step, which are perhaps the ones computationally most appealing, still require the
 55 r-adaptation step to perform well.

56 Extensive reviews of r-adaptation can be found in [30, 8]. We focus here on methods
 57 based on the numerical solution of an elliptic partial differential equation for the posi-
 58 tion of the mesh nodes, often referred to as the mesh PDE. This equation is typically
 59 formulated to find a mapping $\xi : \Omega_{\mathbf{x}} \rightarrow \Omega_{\xi}$ from the physical domain to a reference (com-
 60 putational) one. This mapping needs to be injective and surjective in order to guarantee
 61 that the produced mesh neither folds nor breaks the domain. Historically the Winslow
 62 or homogeneous Thompson-Thames-Mastin generator [43, 44] $\Delta_{\mathbf{x}}\xi = \mathbf{0}$ has been the
 63 basis for structured boundary-fitted grid generation (see for example the review in [42])
 64 and it has been extended to also adapt the mesh in the domain either by adding source
 65 terms to the equation, or through a variable-diffusion approach [51]. A more general
 66 formulation of the last method has been given in [15] by means of harmonic maps and
 67 extended in [6].

68 These equations describe the mapping $\xi = \xi(\mathbf{x})$ and need to be inverted for the
 69 physical coordinates $\mathbf{x} = \mathbf{x}(\xi)$, leading to a nonlinear system of PDEs which is iteratively
 70 solved. In order to ease the cost of the iterative solution of the inverted equations, an
 71 alternative mesh generator was proposed in [9] based on a variable-diffusion Laplace
 72 equations directly formulated in the physical domain for the mapping $\mathbf{x} : \Omega_{\xi} \rightarrow \Omega_{\mathbf{x}}$.
 73 This generator is not based on a theoretical derivation, but on the observation that the
 74 variable-diffusion Laplacian in the reference domain is sufficient to adapt the mesh in
 75 the desired regions while the equations, which are still nonlinear, can easily be solved
 76 through a relaxation procedure. The efficiency of the method was shown in application
 77 to two-dimensional Boussinesq convection on structured grids, and the method was later

78 applied in [38] to hyperbolic conservation laws and extended in [10] to multicomponent
79 flows on two-dimensional unstructured grids. More recently, the same method was
80 applied to the two-dimensional shallow water equations both in Cartesian and spherical
81 coordinates [3, 4, 5].

82 Robustness to mesh folding in r-adaptation is a delicate matter, similarly critical in
83 the context of mesh deformation related to moving boundaries, curved mesh generation
84 and smoothing (see for example [29, 16, 45, 20, 47]). Obtaining non-singular meshes
85 requires two main conditions to be met. The first is that the continuous map, appro-
86 priately modified to account for all boundary conditions, should verify the appropriate
87 conditions as e.g. the non-negativity of the determinant of the deformation Jacobian.
88 Until quite recently, sufficient conditions were known only in the framework of harmonic
89 maps [15, 34]. Recent work by [26], has allowed to prove similar properties for other
90 types of mesh PDEs, as e.g. some of those proposed by Huang [25] or Huang and Rus-
91 sel [27], by resorting to energy arguments borrowed from the theory of gradient flows.
92 The second important aspect is that the discretization used to approximate the mesh
93 PDE should have the appropriate “property preserving” character, so that the fully
94 discrete moving mesh method is also guaranteed to provide non-singular meshes. This
95 is in itself a subject of investigation. It is in general well known that discrete moving
96 mesh methods can lead to mesh tangling even with properly chosen mesh PDEs [15],
97 and the impact of the truncation error is stressed for example in [30]. In the setting of
98 gradient flow maps, geometrical discretizations have been shown in [26] to answer the
99 discrete positive Jacobian requirement. However, even in the last reference, the issue of
100 accounting for complex curved boundaries is overlooked, even though mesh movement
101 along a given surface does not appear to be necessarily a natural boundary condition of
102 the PDEs considered.

103
104 In this work we proceed differently. We want to be able to handle domains with
105 boundaries as general as possible in three space dimensions. and propose a relaxation
106 technique embedding a geometrical limiter allowing to achieve this objective. We focus
107 on the simple reference-domain variable-diffusion Laplacian approach originally pro-
108 posed in [9], however the ideas proposed in this paper can be extended to other mesh
109 PDEs. To the best of the authors’ knowledge, very few applications of r-adaptation to
110 three-dimensional meshes are available to date, see for example [33] as well as some
111 simple applications in [26]. The original approach in [9] does not offer theoretical guar-
112 antees against folding, although it has been successfully used in many applications with
113 non-convex boundaries. R-adaptation in three dimensions exhibits even stronger limi-
114 tations than in two dimensions, as sufficiency results for unfolded continuum maps are
115 typically based on requirement of smoothness and convexity of the boundary. These are
116 easily violated especially in application to external flows, where the boundary is not con-
117 vex and several singularities (like corners and ridges) are present. We have experienced
118 that tangling is a major concern in the three-dimensional extension of these techniques.
119 Smoothing or untangling methods for unstructured meshes already developed in the
120 literature require nontrivial procedures [23, 45].

121 Our contribution is thus related to a mesh displacement method allowing to guar-

122 antee that nodes move and always remain on a given parametrizaion of curved domain
 123 boundaries, and for an *a-posteriori* limiter for the nodal displacement which, when em-
 124 bedded in the mesh relaxation iterations, allows to prevent the occurrence of tangled
 125 elements, thus enforcing the validity of the discrete mapping while avoiding smoothing
 126 procedures. The resulting moving mesh library **Fmg** has been developed on top of the
 127 open source platform **Mmg** [11, 12] to exploit, among other things, its built-in cubic Bézier
 128 patch representation of complex manifolds.

129 The paper is organized as follows. We recall the continuous mesh partial differential
 130 equations in section §2, while a thorough discussion of their numerical solution is given
 131 in section §3, including a-posteriori limiting and projections to obtain a valid mesh
 132 satisfying all the boundary conditions, and the application to unsteady simulations.
 133 We discuss the validation of the method proposed considering the adaptation w.r.t.
 134 analytical functions in two and three space dimensions in section §4, and application
 135 to two and three dimensional unsteady compressible flows are discussed in section §5
 136 Finally, conclusions are presented in section 6.

137 2. Variable-diffusion Laplacian r-adaptation in the reference domain

138 We focus here on Laplacian-based r-adaptation, which is the mesh PDE currently
 139 implemented in the **Fmg** library. However, the ideas proposed in this paper can be
 140 immediately extended to other mesh PDEs. We recall here the continuous mesh problem,
 141 and in particular we discuss the boundary conditions, as well as the definition of the
 142 monitor functions used for adaptation.

143 Following [10], we look for a mapping $\mathbf{x} : \Omega_{\xi} \rightarrow \Omega_{\mathbf{x}}$ from the reference domain Ω_{ξ}
 144 (the original mesh) to the computational domain $\Omega_{\mathbf{x}}$ (the adapted mesh). Within the
 145 reference domain, the computational coordinates satisfy the variable-diffusion Laplace
 146 equation

$$\nabla_{\xi} \cdot (\omega(\mathbf{x}) \nabla_{\xi} \mathbf{x}) = \mathbf{0} \quad \text{in } \Omega_{\xi} \quad (1)$$

147 The above problem is in general a system of coupled non-linear PDEs, which needs to be
 148 complemented by appropriate boundary conditions. Nonlinearity is introduced by the
 149 monitor function $\omega(\mathbf{x})$ which depends on an external field evaluated in the computational
 150 domain. In this work, we have used a classical scalar definition for this quantity, which
 151 allows to decouple the equations for the three spatial coordinates.

152 In particular, given a quantity of interest $f(\mathbf{x})$, the scalar monitor function used in
 153 the examples discussed later is evaluated as

$$\omega(\mathbf{x}) = \sqrt{1 + \alpha \|\nabla_{\xi} f(\mathbf{x})\|_{\gamma_{\alpha}}^2 + \beta \|\mathbf{H}_{\xi}(f)(\mathbf{x})\|_{\gamma_{\beta}}^2 + \tau \|f\|_{\gamma_{\tau}}^2} \quad (2)$$

154 where ∇_{ξ} and \mathbf{H}_{ξ} denote the gradient and Hessian computed on the reference domain
 155 Ω_{ξ} . Norm $\|f\|_{\gamma}$ is defined as

$$\|f\|_{\gamma} = \min \left(1, \frac{\|f\|}{\gamma \max(\|f\|)} \right). \quad (3)$$

156 This normalization, already used in [10], allows to introduce some saturation near the
 157 norm maximum according to the value of γ . The idea behind this normalization is to
 158 spread a little bit the peak values of the function f around the peak locations, in order
 159 to filter out small inhomogeneities in the numerical approximation of the sharp fronts of
 160 f . The above definition gives the user some control on the behaviour of the spatial map-
 161 ping via the parameter pairs (α, γ_α) , (β, γ_β) , (τ, γ_τ) . As in the original works [9, 10],
 162 these parameter pairs are not related to an error estimate, thus they are determined
 163 empirically and they are intrinsically dependent on the application. However, in our
 164 experience a short test on a few time steps is sufficient to assess the behaviour of these
 165 parameters on the whole simulation time range.

167 2.1. Boundary conditions

168 Despite the decoupling of equation (1) into separate scalar equations, even for a
 169 scalar monitor function a strong coupling of the coordinate equations may arise through
 170 the boundary conditions, especially in domains including general shapes. In particular,
 171 we will split the boundary on two parts as $\partial\Omega_\xi = \Gamma_\xi^D \cup \Gamma_\xi^S$. A full set of Dirichlet
 172 conditions are imposed on Γ_ξ^D

$$\mathbf{x} = \boldsymbol{\xi} \quad \text{on } \Gamma_\xi^D \quad (4)$$

173 as this is the portion of the boundary that is not allowed to move. Since fixed boundary
 174 nodes are not convenient whenever adaptation is performed on flow waves approach-
 175 ing the boundary, we want to limit as much as possible usage of Dirichlet conditions,
 176 preferring slip boundary conditions wherever we can formulate them while preserving
 177 sharp geometrical features of the boundary. Along the *slip* boundary Γ_ξ^S the coordinate
 178 positions are constrained to move along a given parameterized domain. For manifold sur-
 179 faces, we assume to have a known parameterization, for example in the form $\gamma^S(\mathbf{x}) = 0$.
 180 This provides one **position** constraint relating the d spatial coordinates. Thus, $d-1$ addi-
 181 tional conditions are required, which are here taken as the null normal stress conditions
 182 parallel to the local tangent space spanned by $\{\hat{\boldsymbol{\tau}}_j^S\}_{j=1, d-1}$. This gives the boundary
 183 conditions:

$$\begin{aligned} \gamma^S(\mathbf{x}) &= 0 \\ \hat{\mathbf{n}}^S \cdot (\omega(\mathbf{x}) \nabla \mathbf{x}) \cdot \hat{\boldsymbol{\tau}}_j^S &= 0 \quad \forall j = 1, d-1 \end{aligned} \quad \text{on } \Gamma_\xi^S \quad (5)$$

184 In three dimensions, the slip boundary Γ_ξ^S can be further generalized as the union
 185 of multiple manifolds with one-dimensional boundaries joining them. This leads to
 186 intersection curves where two sets of equations 5 should formally be satisfied at the
 187 same time, constraining the displacement to happen along the curve tangent direction.
 188 Points where multiple intersection curves meet are corner points and no displacement
 189 is possible, thus Dirichlet conditions are imposed on (and only on) these points. The
 190 approach used here for the numerical enforcement of boundary conditions is discussed
 191 in the following section.

192 **3. Discrete equations, a-posteriori limiting, slip on curved boundaries**

193 We discuss here the implementation choices made in the `Fmg` library, namely the dis-
 194 cretization of the mesh PDEs, as well as their iterative solution. Both the a-posteriori
 195 limiting of the displacement and the implementation of the slip boundary conditions are
 196 strongly tied to the relaxation iterations, and for this reason all the steps are discussed
 197 in this section. More specifically, to relieve the complexity of satisfying the bound-
 198 ary conditions (5), we formulate the discrete approximation by means of an iterative
 199 multiple-corrections procedure embedding the following three elements:

- 200 1. A finite element approximation of the variational form of (1) with natural (Neu-
 201 mann) boundary conditions;
- 202 2. An a-posteriori limiter for the nodal displacement enforcing local mesh validity;
- 203 3. A boundary correction in the local normal direction to enforce the first of (5) by
 204 projecting on the manifold parametrization **at hand**.

205 The intertwining of the a-posteriori limiter of the displacement, of the update of the lo-
 206 cal boundary normals, and of the projection on the parameterized manifold is essential
 207 for the proposed approach to provide valid adapted meshes both in the volume and on
 208 the boundaries.

209
 210 Concerning the representation of these, the `Fmg` library we developed makes use of
 211 the point-normal curved triangles parameterization proposed in [49], which is based
 212 on cubic Bézier patches with quadratically varying normals. For this we leverage the
 213 implementation provided by the open source platform `Mmg` [11, 12]. However note that
 214 the form of the manifold parametrization is not a necessary ingredient of our method.
 215 Other high order approximations can be used.

216 *3.1. Finite element approximation: Dirichlet and natural boundary conditions*

217 The discrete equations are built starting from a linear finite element approximation
 218 of the problem embedding **natural (Neumann) boundary conditions**, which corresponds
 219 to the simple variational form

$$\int_{\Omega_\xi} \omega(\mathbf{x}) \nabla_\xi v \cdot \nabla_\xi \mathbf{x} \, d\Omega_\xi = \mathbf{0}, \quad \forall v \in H^1(\Omega_\xi). \quad (6)$$

220 Note that this statement satisfies the **null normal stress conditions** in (5) but neither the
 221 remaining one in the system (the belonging to the surface), nor any Dirichlet conditions
 222 eventually assigned. Dirichlet conditions are strongly imposed on the solution space,
 223 **while the enforcement of the belonging to a slip surface will be detailed in the follow-**
 224 **ing 3.4)** Note also that ω being a scalar quantity, the above equations provide uncoupled
 225 nonlinear variational statements for each component of \mathbf{x} .

226 The projection of (6) on the linear finite element space leads to the nonlinear alge-
 227 braic system

$$\mathbf{K}(\mathbf{x}) \mathbf{x}^\nu = \mathbf{0}, \quad \nu = 1, \dots, d \quad (7)$$

228 having introduced the array of unknown node positions $\mathbf{x}^\nu = [x_i^\nu]$ for each space com-
 229 ponent ν , with d the number of space dimensions, and where the stiffness matrix has
 230 the standard entries

$$K_{ij}(\mathbf{x}) = \int_{\Omega_\xi} \omega(\mathbf{x}) \nabla_\xi \phi_i \cdot \nabla_\xi \phi_j \, d\Omega_\xi \quad (8)$$

231 with $\{\phi_i\}_{i \geq 1}$ the linear base functions spanning the solution space. Please note that (7)
 232 is a set of decoupled systems, one for each spatial direction, as shown by the fact that
 233 K_{ij} are scalar entries. Note also due to the consistency of the finite element space with
 234 Dirichlet conditions, Dirichlet nodes are not included in the above sum.

235 In practice, by defining the displacement $\boldsymbol{\delta} = \mathbf{x} - \boldsymbol{\xi}$, the system is not written as in
 236 (7), but as

$$\mathbf{K}(\mathbf{x})\boldsymbol{\delta}^\nu = -\mathbf{K}(\mathbf{x})\boldsymbol{\xi}^\nu \quad (9)$$

237 which is better suited for the iterative corrections described in the following sections.

238 3.2. Scalar correction iterations

239 We introduce an iterative procedure which, while avoiding mesh tangling in 2D
 240 and 3D, and accounting for the directional coupling inherent to (5), retains the scalar
 241 structure of the decoupled variational form. Note however that the corrections proposed
 242 can be easily adapted to other iterative solution methods (as well as mesh PDEs).

243 The basic iteration used in our method starts from a standard diagonal Jacobi re-
 244 laxation to handle the nonlinearity of (9)

$$K_{ii}^{[k]} \boldsymbol{\delta}_i^{[k+1]} = - \sum_{\substack{j \in \mathcal{B}_i \\ j \neq i}} K_{ij}^{[k]} \boldsymbol{\delta}_j^{[k]} - \sum_{j \in \mathcal{B}_i} K_{ij}^{[k]} \boldsymbol{\xi}_j \quad (10)$$

245 where \mathcal{B}_i denotes the ball¹ of node i and vector $\boldsymbol{\delta}_i^{[k]} = [\delta_i^\nu]_{\nu=1, \dots, d}^{[k]}$ is now the vector made
 246 of the space components of the displacement of node i at iteration k (the same notation
 247 will be used for vectors \mathbf{x}_i and $\boldsymbol{\xi}_i$). Again, we stress that the above iteration is in fact
 248 a set of d relations for the components of the displacement. The matrix entries $K_{ij}^{[k]}$
 249 depend on monitor function ω at iteration k (cf. equation (8)), which in turn depends
 250 on the scalar field f evaluated at the actual positions $\mathbf{x}_i^{[k]}$, according to equation (2). In
 251 our current implementation, the re-evaluation is performed by linearly interpolating the
 252 scalar field f at the current nodal positions $\mathbf{x}_i^{[k]}$ through a standard search algorithm
 253 based on barycentric coordinates.

254 In our implementation we added and removed the term $K_{ii}^{[k]} \boldsymbol{\delta}_i^{[k]}$, to obtain the fol-
 255 lowing iterations

$$\boldsymbol{\delta}_i^{[k+1]} = \boldsymbol{\delta}_i^{[k]} - \frac{1}{K_{ii}^{[k]}} \sum_{j \in \mathcal{B}_i} K_{ij}^{[k]} \mathbf{x}_j^{[k]} \quad (11)$$

¹In the common lexicon of the mesh generation community, the *ball* \mathcal{B}_i of a mesh node i is defined here as the set of elements sharing vertex i [?]. To ease the notation, with a slight abuse of terminology we say that a node j *belongs* to the ball of node i if it is a vertex of an element belonging to the ball, and we denote this statement as $j \in \mathcal{B}_i$.

256 which are initialized with $\boldsymbol{\delta}_i^{[0]} = \mathbf{0}$.

257 The last step is the computation of the new nodal positions as follows

$$\mathbf{x}_i^{[k+1]} = \mathbf{x}_i^{[k]} + \widetilde{\Delta \mathbf{x}}_i^{[k+1]} \left(\boldsymbol{\delta}_i^{[k+1]}, \{\mathbf{x}_i^{[k+1]}\}_{j < i}, \{\mathbf{x}_i^{[k]}\}_{j \geq i} \right) \quad (12)$$

258 where $\widetilde{\Delta \mathbf{x}}_i^{[k+1]}$ are limited increments obtained by a-posteriori correcting $\boldsymbol{\delta}_i^{[k+1]}$ to ac-
 259 count for both mesh validity and boundary conditions (both Dirichlet and slip wall).
 260 In both cases, these corrections are local, albeit not only dependent on node i , and
 261 non-linear w.r.t. \mathbf{x} . The nonlinearity is readily handled in the iterations by using the
 262 last nodal positions available.

263 3.3. A-posteriori corrections for mesh validity enforcement

264 The Laplacian model in the reference domain does not guarantee that the Jacobian
 265 of the mapping is strictly positive everywhere, thus leading to the occurrence of tangled
 266 (invalid) mesh elements. In two space dimensions, our experience has shown that in
 267 most cases carefully tuning the monitor function $\omega(\mathbf{x})$ allows to solve this issue. This is
 268 not the case in three dimensions, where tangling occurs much more often.

269 To cope with this, we have devised an a-posteriori limiter to the nodal displacements
 270 which is activated whenever the displacement of a node causes the occurrence of an
 271 element whose volume is below a given threshold. This condition is of course implicit,
 272 in the sense that it couples the positions of all the mesh nodes. However, it can be
 273 easily embedded in an iterative setting. In particular, in our implementation we relax
 274 and update each nodal position $\mathbf{x}_i^{[k+1]}$, one after the other. As illustrated on figure 1
 275 (for simplicity in 2D), each displacement $\boldsymbol{\delta}_i^{[k+1]}$ is limited according to the validity of
 276 the configuration in the current ball $\mathcal{B}_i^{[k,k+1]}$ obtained using new values $\{\mathbf{x}^{[k+1]}\}_{j < i}$, for
 277 nodes updated before i , and old positions $\{\mathbf{x}_j^{[k]}\}_{j > i}$ for nodes not updated yet. This
 278 relax-update step has a *Gauss-Seidel* flavour, as the position of each node is updated
 279 based on the values of the previously-treated coordinates. In practice, the displacement
 280 of node i is iteratively limited by a factor $\mu_i^{s_{\max}}$ as follows

$$\begin{aligned} \mathbf{d}_i^0 &= \boldsymbol{\delta}_i^{[k+1]} + \boldsymbol{\xi}_i - \mathbf{x}_i^{[k]} \\ \mathbf{d}_i^{s+1} &= \begin{cases} \mu_i \mathbf{d}_i^s & \text{if } \min_{K \in \mathcal{B}_i^{[k,k+1]}} |\Omega_K| < \epsilon \\ \mathbf{d}_i^s & \text{otherwise} \end{cases} \quad \forall s \in [0, \dots, s_{\max} - 1] \\ \widetilde{\Delta \mathbf{x}}_i^{[k+1]} &= \mathbf{d}_i^{s_{\max}} \end{aligned} \quad (13)$$

281 The limiter is thus the result of local sub-iterations, which are stopped when a
 282 volume greater than ϵ is guaranteed for every element in the ball. This check allows
 283 to enforce the validity of every intermediate mesh configuration, effectively preventing
 284 the occurrence of invalid elements at a reasonable computational cost with respect to
 285 smoothing or untangling procedures for unstructured meshes [23, 45].

286 It must be remarked that for interior nodes in general one iteration of the above
 287 procedure is enough, while more iterations are required when applying the limiter within

288 the projection step enforcing the boundary conditions (cf. next section). For simplicity
 289 here the same value $\mu_i = 0.5$ has been adopted for all the nodes. **In this work, this value**
 290 **has proven to be effective in locally preventing tangling while allowing the position of**
 291 **blocked nodes to be naturally relaxed by the successive application of r-adaptation at**
 292 **the next time steps, as the monitor function moves with the flow.**

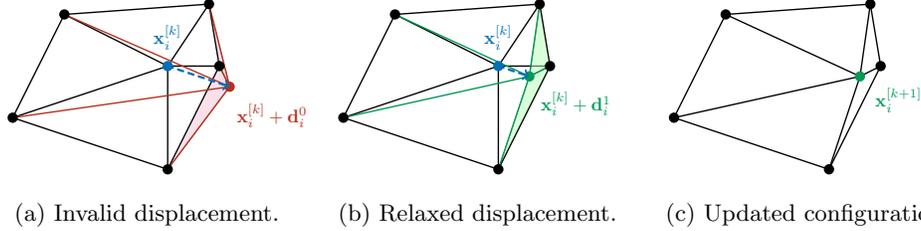


Figure 1: Two-dimensional illustration of the nodal displacement limiting. **1a**: Proposed displacement for node i right after the Jacobi iteration $k + 1$, that would produce inverted elements (in red). **1b**: Relaxed displacement producing valid elements (in green). **1c**: Updated configuration.

293 3.4. *A-posteriori corrections on Dirichlet and slip boundaries*

294 The decoupling of the spatial coordinates obtained by initially accounting for natural
 295 boundary conditions only is particularly convenient in terms of computational cost and
 296 simplicity of implementation. It allows to store and assembly only a single smaller
 297 stiffness matrix to be used for every space coordinate, instead of a matrix of 3×3
 298 blocks. However, the resulting nodal displacements need to be corrected to account
 299 for conditions on Dirichlet and slip boundaries. This is achieved by the projection
 300 step discussed in this section, which is easily embedded in the scalar iterations. The
 301 description is given for slip wall boundaries, of which Dirichlet nodes are a particular
 302 case.

303 In the `Fmg` library boundary geometries are handled by means of curved point-normal
 304 triangles [50], i.e. piecewise cubic Bézier patches for the boundary position and quadratic
 305 for the boundary normal vector, relying on the implementation provided in `Mmg` [11, 12].
 306 In this setting an implicit surface representation of the slip boundary reading in the
 307 continuous case

$$\gamma^S(\mathbf{x}) = 0 \quad \text{on } \Gamma_\xi^S \quad (14)$$

308 is approximated by the explicit piecewise parametric representation

$$\begin{aligned} \chi_\tau[\mathbf{x}_j, \hat{\mathbf{n}}_j] : \Sigma \rightarrow \Gamma_\xi^S, \quad \Sigma = [0, 1] \times [0, 1], \quad \Gamma_\xi^S \subset \mathbb{R}^3 \\ \mathbf{x} = \chi_\tau[\mathbf{x}_j, \hat{\mathbf{n}}_j](\mathbf{w}), \quad \mathbf{w} \in \Sigma \end{aligned} \quad (15)$$

309 which is defined for each triangle τ in the triangulation of the slip boundary, from the
 310 positions and unit normals $\{\mathbf{x}_i, \hat{\mathbf{n}}_i\}_{i \in \tau}$ of the nodes of the triangle. Similarly, the Bézier
 311 patches also allow to evaluate surface normals as

$$\begin{aligned} \eta_\tau[\mathbf{x}_j, \hat{\mathbf{n}}_j] : \Sigma \rightarrow \Gamma_\xi^S, \quad \Sigma = [0, 1] \times [0, 1], \quad \Gamma_\xi^S \subset \mathbb{R}^3 \\ \hat{\mathbf{n}} = \eta_\tau[\mathbf{x}_j, \hat{\mathbf{n}}_j](\mathbf{w}), \quad \mathbf{w} \in \Sigma \end{aligned} \quad (16)$$

312 For some applications, as for example external aerodynamics, handling curved ge-
 313 ometries is a necessity. As a consequence, the geometric approximation becomes an
 314 integral part of the numerical method. In particular, in three dimensions even the sim-
 315 plest combination of boundary surfaces easily leads to intersection curves. Since sharp
 316 edges (ridges) in the initial geometry need to be preserved as well as corners (**intersec-**
 317 **tions of multiple ridges**), nodes cannot cross a ridge, but they are only allowed to move
 318 tangentially to it, and displacement of a corner node cannot happen. **As outlined in sec-**
 319 **tion 2.1**, **slip boundary conditions bring a position constraint expressing the belonging**
 320 **of the node to the surface, and a null normal stress condition on the local tangent plane.**
 321 **The latter being already fulfilled by the Neumann conditions naturally imposed on the**
 322 **weak formulation, only the former is of our interest here.** Although node belonging to an
 323 **intersection curve can be formally expressed as the belonging to the two surfaces sharing**
 324 **the curve, this is not practical from an implementation point of view.** Slip boundary
 325 conditions need thus to be specialized to the chosen geometry approximation and to
 326 distinguish among regular curved surfaces, ridges, and corners.

327 In the following, the boundary treatment is detailed for the supported geometri-
 328 cal features: manifold surfaces, ridges (i.e. intersections of two manifold surfaces) and
 329 corners (intersections of two or more ridges). Note that different geometrical repre-
 330 sentations involving other local or global manifold parametrizations can be easily embed-
 331 ded in the algorithm.

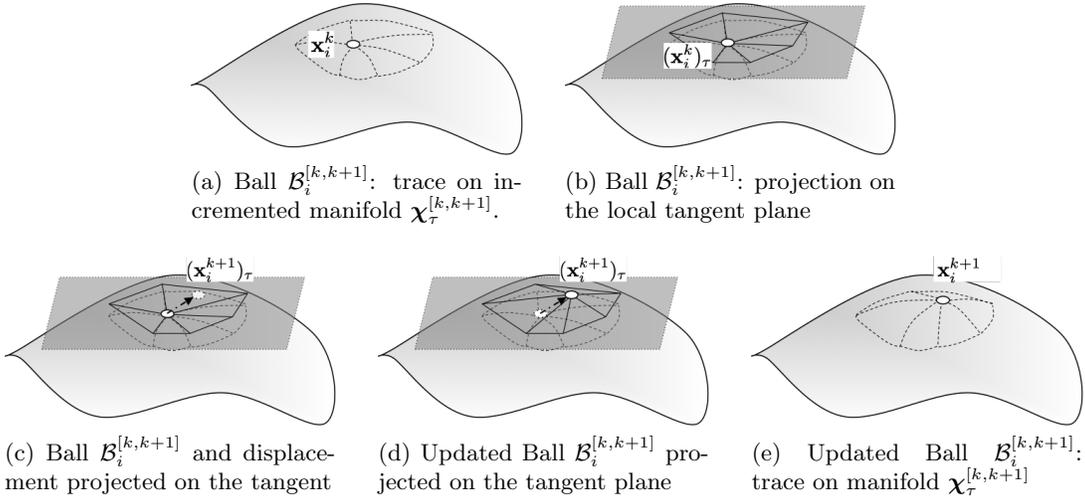


Figure 2: Illustration of the slip boundary projection procedure.

332 *Manifold surfaces.* The procedure adopted here to handle slip conditions along manifolds
 333 for a node i consists in iteratively projecting the point position on the surface, updating
 334 the Bézier patches, and limiting at the same time the displacement to ensure mesh
 335 validity. Tangling can typically occur on surface triangles if too large displacements are
 336 allowed, but also the adjacent volume elements can tangle when a point is projected on

337 a concave boundary. For this reason the mesh validity check is always performed on
 338 volume elements.

339 In the first step, we work based on the partially updated ball $\mathcal{B}_i^{[k,k+1]}$, which allows
 340 to build a local updated geometrical model. As before, this model is evaluated using the
 341 new updates for nodes already processed, and value from the previous iteration for the
 342 remaining ones. This provides the incrementally updated geometry model $\chi_\tau^{[k,k+1]} =$
 343 $\chi_\tau[\{\mathbf{x}_j^{[k+1]}, \hat{\mathbf{n}}_j^{[k+1]}\}_{j < i}, \{\mathbf{x}_j^{[k]}, \hat{\mathbf{n}}_j^{[k]}\}_{j \geq i}]$ (cf. (15)). In particular, as shown on figures 2-(a)
 344 and 2-(e), this allows to identify the trace of $\mathcal{B}_i^{[k,k+1]}$ on the updated manifold, and its
 345 projection on the local tangent plane.

346 The second step consists of four coupled ingredients:

- 347 1. projection of the displacement provided by the Jacobi iteration onto the local
 348 tangent plane, leading to an approximate tangent displacement $(\delta_i^{k+1})_\tau$; and pre-
 349 liminary nodal position $(\mathbf{x}_i^{k+1})_\tau$, as shown on figure 2-(c);
- 350 2. identification of the element containing the new node position, based on barycentric
 351 coordinates interpolation, as shown on figures 2-(c) and 2-(d);
- 352 3. Bézier interpolation $\chi_\tau^{[k,k+1]}(\mathbf{w})$ on the geometrical model, as shown on figure 2-(e);
- 353 4. limiting of the displacement based on the minimum element volume, as discussed
 354 in section 3.3.

355 The iterations providing the final displacement, and hence position, are similar to (13):

$$\begin{aligned}
 \mathbf{d}_i^0 &= \chi_\tau^{[k,k+1]} \left(\mathbf{w}(\mathbf{x}_i^{[k+1]})_\tau \right) - \mathbf{x}_i^{[k]} \\
 \mathbf{d}_i^{s+1} &= \begin{cases} \chi_\tau^{[k,k+1]} \left(\mathbf{w}(\mathbf{x}_i^{[k]} + \mu_i \mathbf{d}_i^s) \right) - \mathbf{x}_i^{[k]} & \text{if } \min_{K \in \mathcal{B}_i^{[k,k+1]}} |\Omega_K| < \epsilon \\ \mathbf{d}_i^s & \text{otherwise} \end{cases}, \quad (17) \\
 \forall s &\in [0, \dots, s_{\max} - 1] \\
 \widetilde{\Delta \mathbf{x}}_i^{[k+1]} &= \mathbf{d}_i^{s_{\max}}
 \end{aligned}$$

356 We stress again that since the piecewise patches depend on both node positions and
 357 unit normals, the position update is always accompanied by the re-evaluation of the
 358 unit normal vectors through the analogously defined model $\eta_\tau^{[k,k+1]}$ (cf. (16)). This is
 359 omitted from (17) to keep a lighter notation.

360 *Ridges.* The displacement check and projection on boundary ridges is handled exactly
 361 in the same way as for manifold surfaces. The main difference is that now the parametric
 362 space is replaced with a curve parametrisation which is one-dimensional $\Sigma \subset \mathbb{R}$. Thus
 363 all operations previously performed on the tangent plane are performed by projection
 364 on the tangent line, and normal vectors of both the manifold surfaces joining at the
 365 ridge are stored and updated in the geometrical model.

366 *Corners.* These are the only allowed Dirichlet nodes, thus corners verify exactly the
 367 boundary condition, and are not included in the discrete variational form 3.1. In this

368 specific case, displacement is not allowed as they are already on the exact geometry, and
 369 the condition imposed is

$$\mathbf{x}_i^{[k+1]} = \boldsymbol{\xi}_i \quad (18)$$

370 3.5. Unsteady mesh adaptation through restarted iterations

371 Following [39, 10], dynamic mesh adaptation during the time evolution of a fluid
 372 flow simulation is performed by repeating the steady adaptation procedure described in
 373 the previous section at each time step, without the explicit formulation of a differential
 374 equation in time for mesh motion. This simplifies the coupling with existing flow solvers.

375 In this case of fixed boundary domains, the reference mesh $\boldsymbol{\xi}$ is constant in time,
 376 while the computational mesh $\mathbf{x}(t^{(n+1)})$ is the r-adaptation of the (fixed) reference mesh.
 377 Thus, the displacement at each time step $n + 1$ is initialized with the value achieved at
 378 the last Jacobi iteration K achieved in the previous time step n

$$\boldsymbol{\delta}_i^{[0](n+1)} = \boldsymbol{\delta}_i^{[K](n)} \quad (19)$$

379 so that successive Jacobi iterations during time evolution are effectively accumulated on
 380 the nodes positions.

381 4. Validation via adaptation on analytical functions

382 We consider here a series of analytical tests allowing to measure the effectiveness
 383 of the method. As shown in section 2, we recall here that the mesh adaptation model
 384 can be governed by the number of iterations n_{it} plus the three parameter pairs (α, γ_α) ,
 385 (β, γ_β) , (τ, γ_τ) , representing the intensity and the normalization constant of the solution
 386 gradient, the solution Hessian, and the solution itself in the definition of the monitor
 387 function. In this work, we have not seen specific benefits in mixing all three param-
 388 eter pairs, so we will explicitly report only the values for the used pairs, while values
 389 not shown are assumed to be zero. As elucidated in [10], since the reference domain
 390 Laplacian model in multiple dimensions is not derived from an error equidistribution
 391 principle, its numerical solution until convergence is not strictly required to reach satis-
 392 factory mesh adaptation and, in practice, a number of Jacobi iterations in the order of
 393 $\mathcal{O}(10)$ are generally sufficient to reach the desired adaptation. The number of iterations
 394 n_{it} will be reported for each case.

395 In section 4.1 adaptation is performed on a steady Gaussian-like function, in order
 396 to test the convergence order on the interpolation error. In section 4.2 adaptation is
 397 performed on an unsteady analytical moving front passing over a sphere, in order to
 398 assess the capability of the model to preserve the validity of the mesh over intersecting
 399 curved boundaries throughout the time simulation.

400 4.1. Steady adaptation in a square and a cube

401 We consider the approximation of the function

$$\rho = e^{\theta\psi^2}, \quad \psi = \|\mathbf{x}\|^2 - R^2 \quad (20)$$

402 with $\theta = 40$, $R = 0.75$. We consider both a two and three dimensional variant of the
 403 problem, the first defined on a square domain $[-2, 2] \times [-2, 2]$, the second on the cube
 404 $[-2, 2] \times [-2, 2] \times [-2, 2]$. This solution is plotted in figures 4a and 4b. In both cases we
 405 consider a series of simplicial meshes with a uniform mesh size distribution, and different
 406 average edge size h , whose details are shown in tables 1 and 2. The above function is
 407 chosen in order to test capability of the models to adapt on a circle represented by
 408 a smooth solution field, before their application to solutions with sharp/discontinuous
 409 features. The mesh PDE parameters are set to $(\tau, \gamma_\tau) = (5000, 1.0)$ in 2D, and to
 410 $(\alpha, \gamma_\alpha) = (500, 0.1)$ in 3D. Also note that the a-posteriori limiter for the displacement is
 411 only applied in 3D, which is the case in which tangling is more often occurring.

412 On these meshes, we measure the L^2 -error convergence of the \mathbb{P}^1 interpolation $\Pi\rho$

$$\|e\|_{L^2} = \left(\int_{\Omega} |\rho - \Pi\rho|^2 d\Omega \right)^{\frac{1}{2}} \quad (21)$$

413 We plot the observed trends in figures 3a and 3b. It can be seen that in two dimensions
 414 it is easier to preserve, quite independently from the number of iterations n_{it} performed,
 415 the second order convergence rate of the \mathbb{P}^1 interpolation, with an error reduction for
 416 a given number of nodes shown in table 3, but a high number of iterations on a coarse
 417 mesh can actually increase the error.

418 In three dimensions, while the error on the adapted meshes is considerably lower
 419 (table 4), the number of Jacobi iterations has to be increased to preserve the second
 420 order rate. Some adapted meshes obtained from the $h = 0.1$ and $h = 0.05$ initial
 421 meshes are visualized in figures 4 to help understand these two phenomena. Taking
 422 as example the three-dimensional case, as the initial mesh is refined from $h = 0.1$ to
 423 $h = 0.05$ in figure 4, it can be appreciated that the displacement produced by the
 424 same number of iterations and the same adaptation parameters is smaller. This has
 425 two consequences. The first consequence is that a high number of iterations on coarse
 426 meshes can excessively stretch the mesh elements (as shown in figure 4g) in an orthogonal
 427 pattern, due to the uncoupling of the Laplacian model in the coordinate directions,
 428 possibly increasing the approximation error on the adapted mesh (as seen in table 3 for
 429 the 2D case for the coarsest meshes). The second consequence is that more iterations
 430 are needed on fine meshes to preserve the second order rate, as shown in figure 3b. In
 431 three dimensions, the a-posteriori limiter also contributes to this effect by constraining
 432 the allowed displacement of each node inside its ball at each iteration.

433 These effects can be appreciated by observing the trend for the tetrahedron quality

$$Q = \frac{\left(\sum_{j=1}^6 l_j^2 \right)^{3/2}}{\alpha |\Omega_K|} \quad (22)$$

434 where l_j is the length of each edge of the element, $|\Omega_K|$ its volume, and α the normal-
 435 ization factor to get $Q = 1$ on a regular tetrahedron with unit edges. Since r-adaptation
 436 inevitably introduces some anisotropy which is not taken into account in our quality
 437 measure, we expect the quality to be somewhat degraded in the adapted regions. Any-
 438 way, a too high percentage of bad quality elements, when sharp solution fronts are quite

h	0.0125	0.025	0.05	0.075	0.1	0.15
Nb. of nodes	135550	34310	8560	3993	2213	1015
Nb. of elements	271098	68618	17118	7984	4424	2028

Table 1: Mesh data for the 2D square convergence analysis.

h	0.0375	0.05	0.075	0.1	0.15
Nb. of nodes	319830	140264	44521	20604	6727
Nb. of elements	1844811	802080	237458	106130	32308

Table 2: Mesh data for the 3D cube convergence analysis.

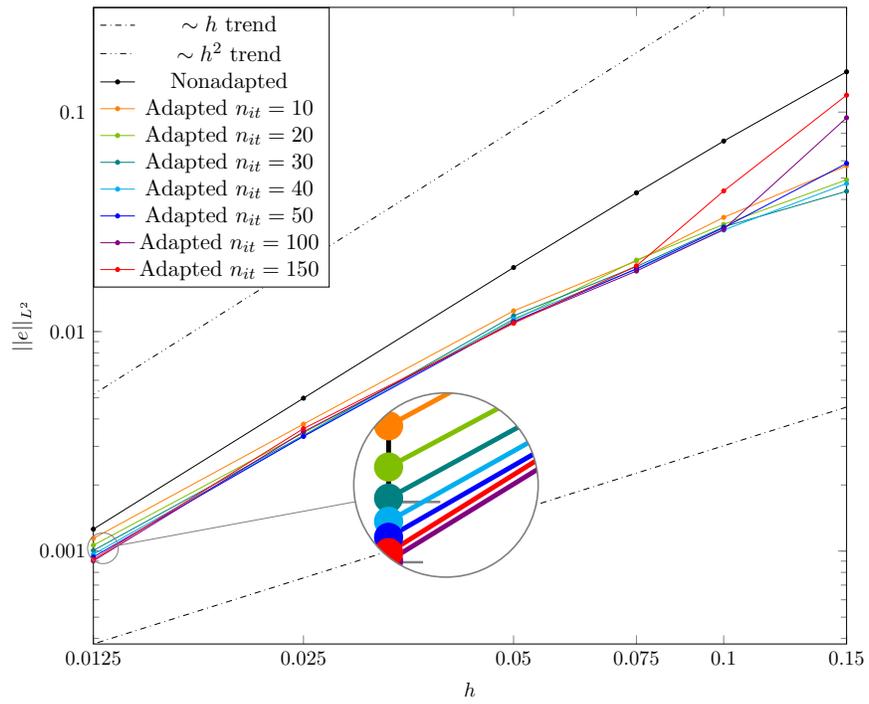
h	$\mathcal{E}^{[0]}$	$\mathcal{E}^{[10]}$	$r^{[10]}$	$\mathcal{E}^{[150]}$	$r^{[150]}$
0.15	1.525974e-01	5.693340e-02	62.6905 %	1.194055e-01	21.751 %
0.1	7.379553e-02	3.313339e-02	55.1011 %	4.372964e-02	40.742 %
0.075	4.288518e-02	2.097308e-02	51.0948 %	1.991813e-02	53.555 %
0.05	1.958636e-02	1.243068e-02	36.5340 %	1.090836e-02	44.306 %
0.025	4.974168e-03	3.788809e-03	23.8303 %	3.614722e-03	27.330 %
0.0125	1.258864e-03	1.142442e-03	9.2482 %	9.152757e-04	27.294 %

Table 3: Interpolation errors $\mathcal{E}^{[k]} = \|e^{[k]}\|_{L^2}$ for the 2D square convergence analysis, for 10 and 150 iterations, and reduction $r^{[k]} = (1 - \mathcal{E}^{[k]}/\mathcal{E}^{[0]})$ with respect to the nonadapted case.

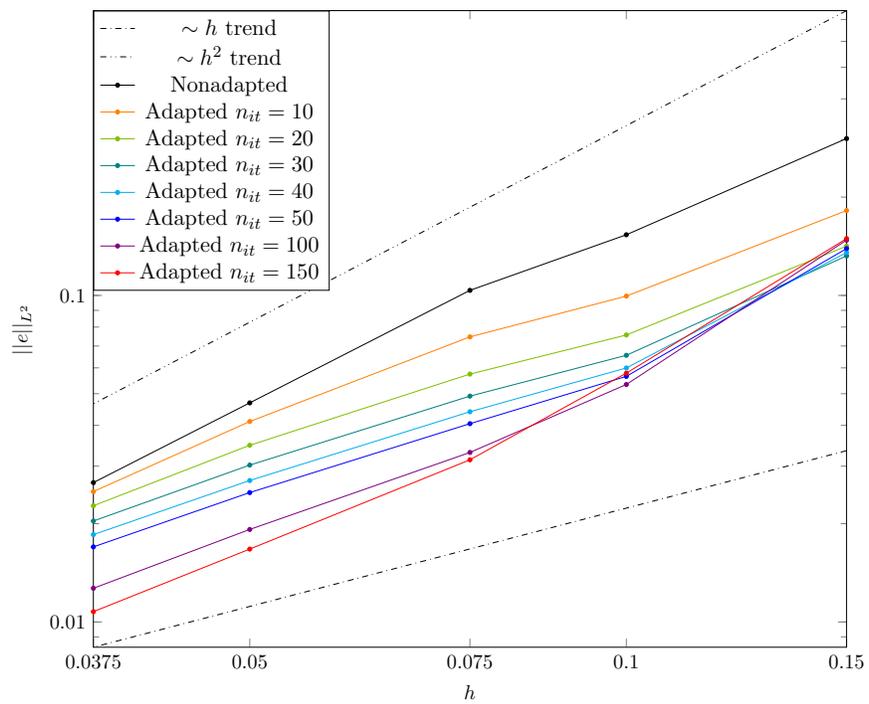
h	$\mathcal{E}^{[0]}$	$\mathcal{E}^{[10]}$	$r^{[10]}$	$\mathcal{E}^{[150]}$	$r^{[150]}$
0.15	3.023667e-01	1.693936e-01	43.9774 %	1.450969e-01	52.013 %
0.1	1.533983e-01	9.494413e-02	38.1061 %	5.919961e-02	61.408 %
0.075	1.036390e-01	7.284977e-02	29.7082 %	2.832881e-02	72.666 %
0.05	4.687948e-02	4.084946e-02	12.8628 %	1.424675e-02	69.610 %
0.0375	2.671484e-02	2.499870e-02	6.4239 %	9.579343e-03	64.142 %

Table 4: Interpolation errors $\mathcal{E}^{[k]} = \|e^{[k]}\|_{L^2}$ for the 3D cube convergence analysis, for 10 and 150 iterations, and reduction $r^{[k]} = (1 - \mathcal{E}^{[k]}/\mathcal{E}^{[0]})$ with respect to the nonadapted case.

439 localized in the domain, can be a sign that the mesh is stretched also in smooth solution
440 regions, possibly worsening the error reduction performances. In figure 5 we plot the
441 evolution of the histograms of the elements quality with the number of iterations for the
442 $h = 0.1$ and $h = 0.05$ meshes. The excessive stretch observed in figure 4g corresponds to
443 a significantly degradation of the elements quality for the $h = 0.1$ mesh, especially when
444 increasing the number of iterations, with more than 24% of elements having $Q < 0.2$ for
445 150 iterations, much higher than for the $h = 0.05$ (less than 10%).

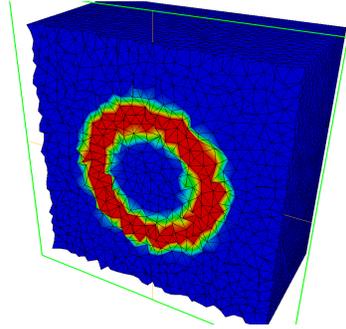


(a) Interpolation error trend for the 2D square test case.

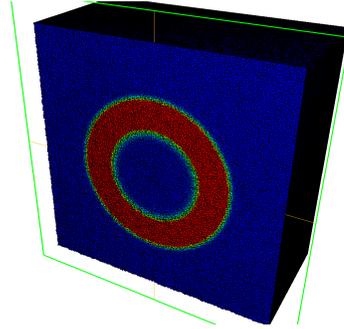


(b) Interpolation error trend for the 3D cube test case.

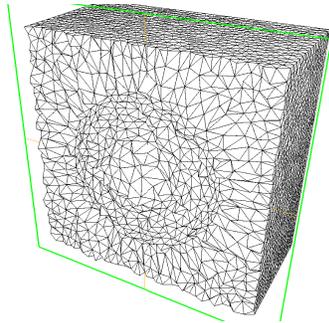
Figure 3: Interpolation error convergence with mesh adaptation for the square and cube analytical test cases.



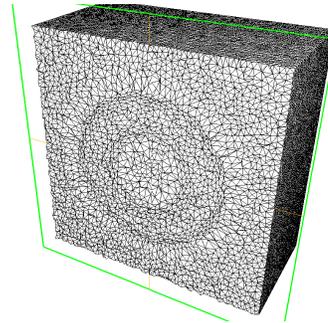
(a) Monitor function, $h = 0.1$ mesh.



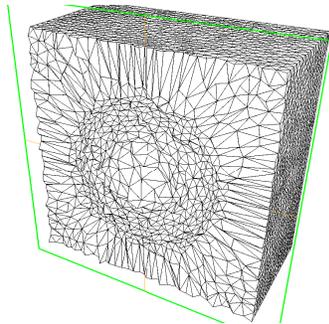
(b) Monitor function, $h = 0.02$ mesh.



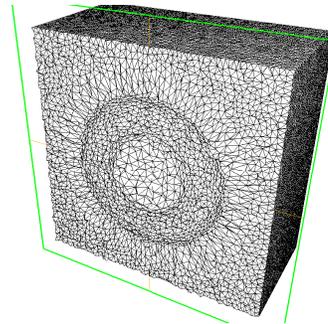
(c) Adapted mesh $h = 0.1, n_{it} = 10$.



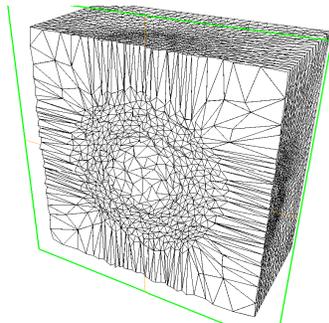
(d) Adapted mesh $h = 0.05, n_{it} = 10$.



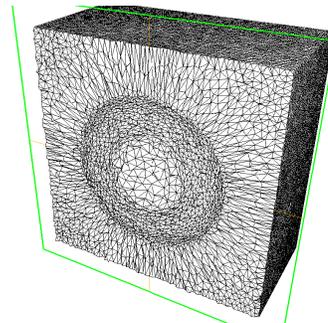
(e) Adapted mesh $h = 0.1, n_{it} = 30$.



(f) Adapted mesh $h = 0.05, n_{it} = 30$.



(g) Adapted mesh $h = 0.1, n_{it} = 100$.



(h) Adapted mesh $h = 0.05, n_{it} = 100$.

Figure 4: Monitor function (top row) and volumic cuts in the adapted meshes (second to last row) for the cube test case, for different number of iterations, on the $h = 0.1$ and $h = 0.05$ initial meshes.

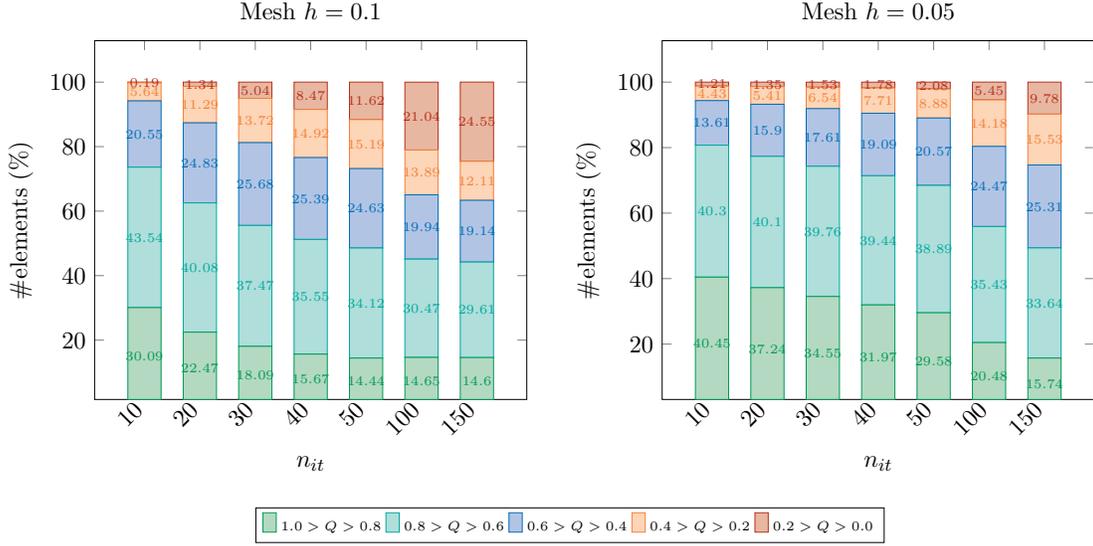


Figure 5: Evolution of mesh elements quality Q with the number of iterations n_{it} for the 3D cube test, for the $h = 0.1$ and $h = 0.05$ meshes.

446 4.2. Moving front passing over a spherical boundary

447 The algorithm was tested by adapting over a moving front defined as

$$\rho(X(x, t)) = \begin{cases} 1 & \text{if } X(x, t) < 0 \\ 0.5 \cos(s\pi X(x, t) + 1) & \text{if } X(x, t) \in [0, \delta] \\ 0 & \text{if } X(x, t) > \delta \end{cases} \quad (23)$$

448 with

$$X(x, t) = s(x - x_0 + vt) \quad (24)$$

449 and scaling $s = 20$, initial position $x_0 = 0.7$, speed $v = 0.2$, front thickness $\delta = 0.005$.
 450 Unsteady mesh adaptation is performed on this analytical solution every $\Delta t = 0.25$.

451 The setup is shown in figures 6a and 6b. The domain is a quarter cylinder of radius
 452 1.5 along the x-axis with $x \in [-1.5, 1.5]$, surrounding a quarter sphere centered at the
 453 origin with radius 0.5. This case is designed to test as many geometrical sources of mesh
 454 tangling as possible before the application to fluid flow simulations, as it contains at the
 455 same time curved surfaces, ridges (the intersection of the sphere with each symmetry
 456 planes) and corners (the intersections of the sphere with both the symmetry planes),
 457 and a sharp solution moving over the geometry. Adaptation is performed with $(\alpha, \gamma_\alpha) =$
 458 $(40, 0.1)$, with 30 Jacobi iterations, on an uniform mesh with edge size $h = 0.05$. The
 459 number of nodes and elements is reported in table 5, as this is the same base mesh that
 460 will be used for the shock-sphere interaction simulations in the next section.

461 The obtained meshes are shown in figure 6 showing in particular that the method
 462 is able to preserve a valid mesh both when the front is passing over the surface of
 463 the sphere (figures 6e, 6f) and most importantly when it hits and leaves the sphere

464 (figures 6c, 6d and 6g, 6h respectively). Without the a-posteriori limiter, that effectively
 465 blocks excessive deformation near the corners and in the first layer of elements above
 466 the curved surface, it was impossible to complete the simulation without the occurrence
 467 of tangled elements.

468 *Remarks on mesh folding and the purpose of the a-posteriori limiter.* As discussed in
 469 section 1, there is no analytical proof for the validity of the meshes produced by our
 470 model neither in the continuum nor in the discrete setting. Examples of folded meshes
 471 have indeed already been reported in the literature for several other methods [15, 30].
 472 Mesh folding has not been reported for the variable-diffusion Laplacian in the reference
 473 domain in two dimensions [9, 38, 10], but in [9] the authors themselves remark that there
 474 is no theoretical reason against its occurrence. In three dimensions, we have found that it
 475 is quite frequent to produce folded elements for too strong adaptation parameters or on
 476 concave boundaries when the limiter presented in the previous section is not applied. An
 477 example of the first situation is given in figure 7a, where an inverted element is produced
 478 just outside of the most refined region. An example of tangling on a concave boundary is
 479 given in figure 7b, where two points on the surface are blocked and cannot move without
 480 folding the adjacent elements (the volume limiter is not applied, but displacement on the
 481 surface is limited on the surface ball in order to allow the projection on Bézier patches),
 482 and one element near the lower circle is folded.

483 In the numerical simulations presented in the next section, all of which have con-
 484 cave boundaries, tangling was observed whenever a shock wave hit or developed on the
 485 front of the object, without limiter. Since this happened in the first **instants** of the
 486 simulations, we have found that the straightforward three-dimensional extension of the
 487 original variable-diffusion Laplacian method in the reference domain [9] would simply
 488 be unpractical on those cases without an additional limiting or correction step to avoid
 489 mesh folding.

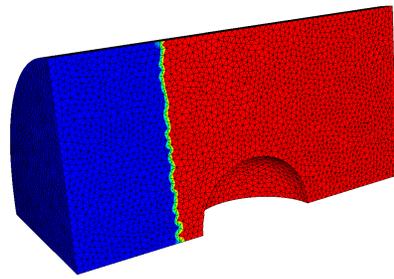
490 5. Adaptation for unsteady compressible flows

491 We consider the simulation of unsteady inviscid compressible flows in a time depen-
 492 dent frame of reference. In particular, we couple the **Fmg** library we developed to the
 493 **Flowmesh** solver [21, 28, 36], based on a node-centered second order, total variation-
 494 diminishing finite volume scheme for the Euler equations, written in an Arbitrary-
 495 Lagrangian-Eulerian (ALE) form [13]

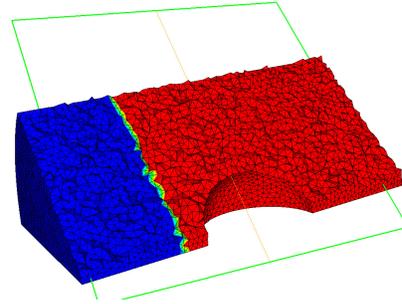
$$\frac{d}{dt} \int_{\Omega(t)} \mathbf{u} \, d\Omega + \oint_{\partial\Omega(t)} \hat{\mathbf{n}} \cdot (\mathbb{F}(\mathbf{u}) - \mathbf{v}\mathbf{u}) \, d\Gamma = \mathbf{0} \quad (25)$$

496 where \mathbf{u} is the array of the conservative solution, $\mathbb{F}(\mathbf{u})$ its flux, ρ denotes the mass
 497 density, $\rho\mathbf{U}$ the momentum, and ρe^t the total energy density. The moving domain
 498 velocity is represented by the vector field \mathbf{v}

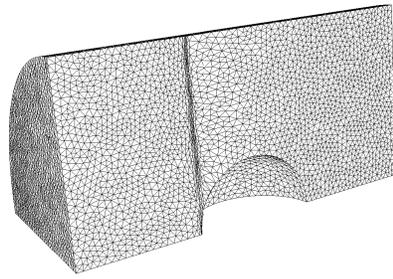
$$\mathbf{u} = \begin{pmatrix} \rho \\ \rho\mathbf{U} \\ \rho e^t \end{pmatrix}^T, \quad \mathbb{F}(\mathbf{u}) = \begin{pmatrix} \rho\mathbf{U} \\ \rho\mathbf{U} \otimes \mathbf{U} + P\mathbb{I} \\ \rho e^t\mathbf{U} + P\mathbf{U} \end{pmatrix}^T \quad (26)$$



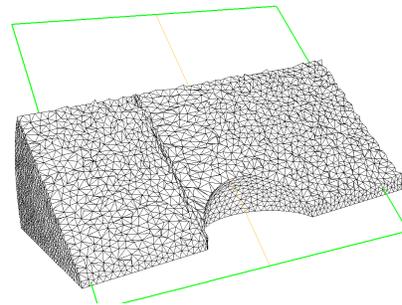
(a) Solution on input mesh boundary.



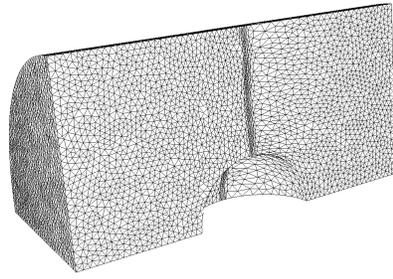
(b) Solution on input mesh volumic cut.



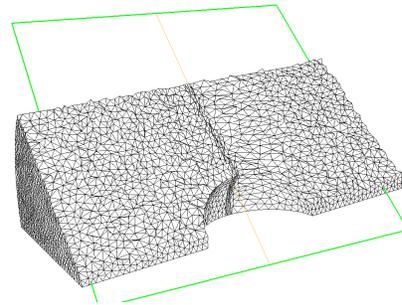
(c) Output mesh boundary at $t = 1.0$.



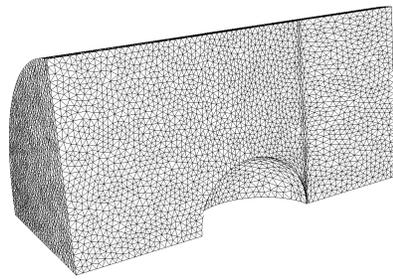
(d) Output mesh volumic cut at $t = 1.0$.



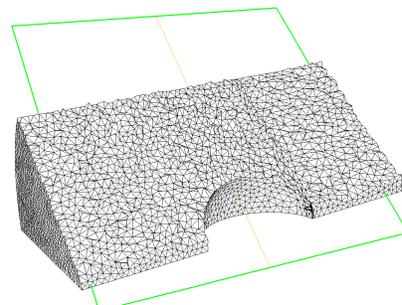
(e) Output mesh boundary at $t = 3.5$.



(f) Output mesh volumic cut at $t = 3.5$.



(g) Output mesh boundary at $t = 6.0$.



(h) Output mesh volumic cut at $t = 6.0$.

Figure 6: Moving front test case, meshes from $t = 0.0$ to $t = 6.0$.

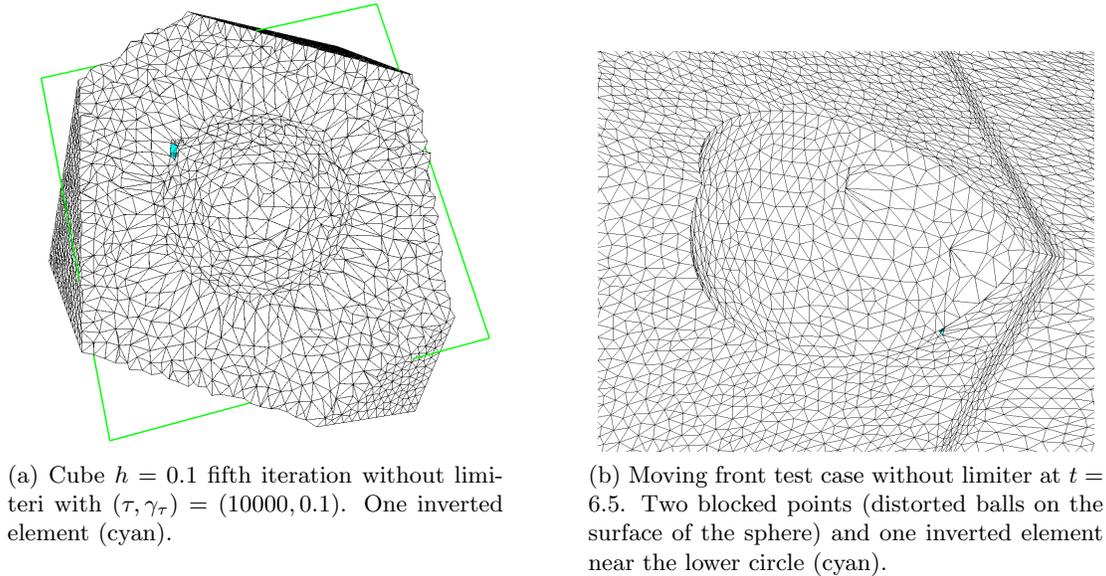


Figure 7: Examples of folded meshes with no limiter applied.

The pressure P is computed using the ideal gas equation of state for ideal gases

$$P = (\gamma - 1) \left(\rho e^t - \frac{1}{2} \rho |\mathbf{U}|^2 \right)$$

499 Within the code, a local conservative solution transfer procedure at each time step is
 500 guaranteed by the ALE formulation.

501 Unsteady mesh adaptation is performed according to the scheme shown in section 3.5.
 502 At each time step, the flow solution is predicted on the previous computational mesh,
 503 then the computational mesh is adapted, and finally the flow solution is recomputed
 504 on the adapted mesh. To this end, `Flowmesh` makes use of a conservative ALE-remap
 505 exactly matching the volumes swept by cell faces during mesh displacements and nodal
 506 volumes, and automatically fulfilling a Discrete Geometric Conservation Law (DGCL)
 507 [22, 18, 53]. The code also includes the support of topological mesh modifications like
 508 edge split, edge collapse, barycentric node insertion, and Delauney node insertion, not
 509 used in this work.

510 To apply mesh adaptation at each time step, a low order computation of the solution
 511 at the next time step on the current mesh is used to provide a monitor function to the
 512 mesh PDEs.

513 5.1. Case 1: two-dimensional forward facing step

514 As a preliminary validation, we reproduce the results shown for the same method
 515 without a posteriori relaxation in [10] for the two-dimensional forward facing step [17,
 516 48, 52]. Our initial mesh is a Delauney triangulation made of 10946 elements, 5474
 517 nodes, with an average edge length $h = 0.0025$. Note that this unstructured mesh has

	Base mesh		Refined mesh	
	# nodes	# elements	# nodes	# elements
Step 2D	5474	10946	21639	43276
Step 3D	47445	277655	555026	3217351
Shock-sphere	35379	209142	488963	2872845

Table 5: Number of nodes and elements for the simplicial meshes employed for the unsteady compressible flow cases.

	Base (nonadapted)	Base (adapted)	Refined (nonadapted)
Step 2D	31m 32s	44m 43s	2h 52m 21s
Step 3D	1h 39m 55s	2h 21m 28s	45h 37m 18s
Shock-sphere	40m 12s	1h 32m 48s	12h 5m 12s

Table 6: Computational times comparison. The overhead due to solution prediction and adaptation is important, but negligible if compared with an uniform refinement strategy.

518 a higher edge size with respect to the one proposed in [52], which had an edge size
519 $h = 0.00125$. The initial condition is a uniform Mach 3 flow towards the right of the
520 domain.

521 All simulations are run on 4 cores of a Intel Xeon E5-2690 (2.6 GHz), mesh adaptation
522 is serial. We perform mesh adaptation on the base $h = 0.0025$ mesh, and compare results
523 with those obtained without adaptation on the refined $h = 0.00125$ mesh. Adaptation
524 is performed on mass density, with $(\alpha, \gamma_\alpha) = (40, 0.1)$ and $(\beta, \gamma_\beta) = (10, 0.5)$. Mesh
525 data are shown in table 5, while contour lines for mass density are compared in figures 8
526 and 10. Contour lines range and spacing for each time instant is the same as in [52].
527 **The adapted meshes are shown in figures 9 and 11.** Shock waves are resolved better
528 on the coarse adapted mesh than on the refined nonadapted mesh, while resolution on
529 rarefaction fans and contact discontinuities is comparable. Computational times are
530 shown in table 6. While mesh adaptation produces a significant overhead if compared
531 to the base nonadapted case, this overhead is negligible if compared to the refined
532 nonadapted calculation.

533 5.2. Case 2: three-dimensional forward facing step

534 We propose a three-dimensional extension of the classical supersonic forward facing
535 step. The impulsive start of a Mach 3 flow in a 3 length units long and 1 length unit
536 wide/high wind tunnel, with a 0.2 length unit wide/high step located at 0.6 length units
537 from the inlet (see figure 12a). Adaptation is performed on the mass density (figures ??
538 and ??), with $(\alpha, \gamma_\alpha) = (40, 0.02)$ on a base mesh with an overall edge size $h = 0.04$
539 (slightly refined on the step front plane, $h = 0.02$). Results are compared with those
540 obtained without adaptation on a refined mesh with uniform edge size $h = 0.015$. The
541 number of elements and nodes in the meshes are shown in table 5. Contour lines for
542 mass density on the same diagonal cut plane are shown in figures 13 and 15, for 50
543 equispaced lines between the values 0.715867 and 6.03154. To obtain a comparable
544 resolution on shocks between the coarse adapted and the refined nonadapted meshes,

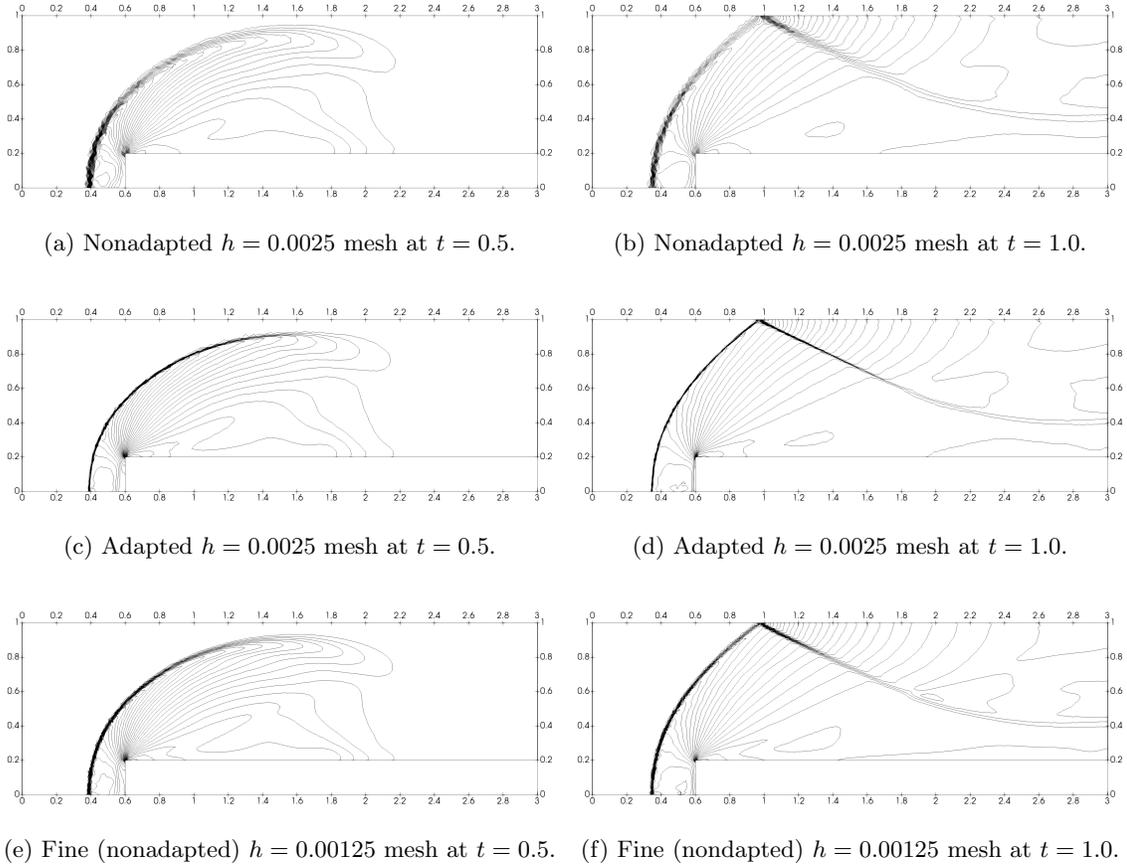


Figure 8: Two-dimensional forward facing step mass density contour lines at $t = 0.5$ and $t = 1.0$.

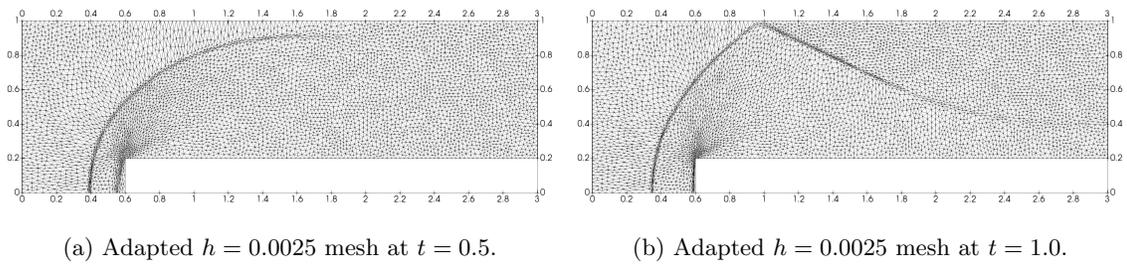


Figure 9: Two-dimensional forward facing step adapted meshes at $t = 0.5$ and $t = 1.0$.

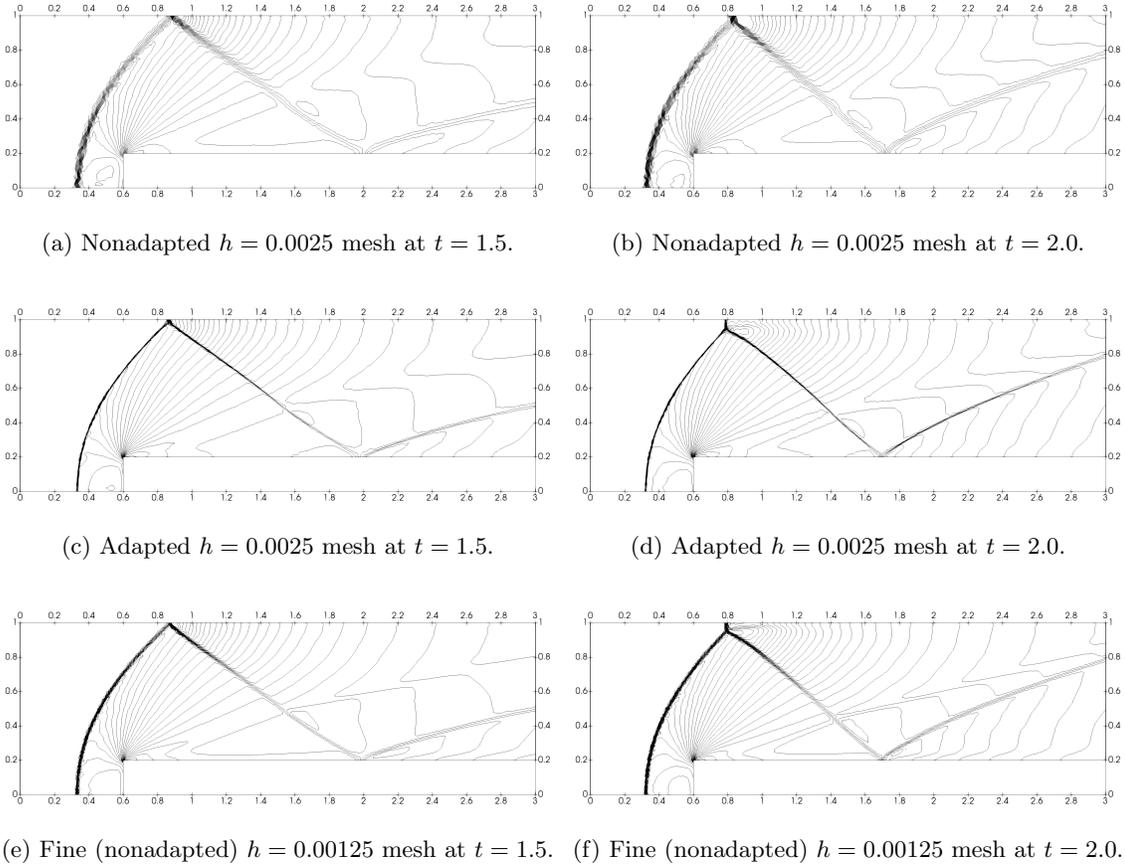


Figure 10: Two-dimensional forward facing step mass density contour lines at $t = 1.5$ and $t = 2.0$.

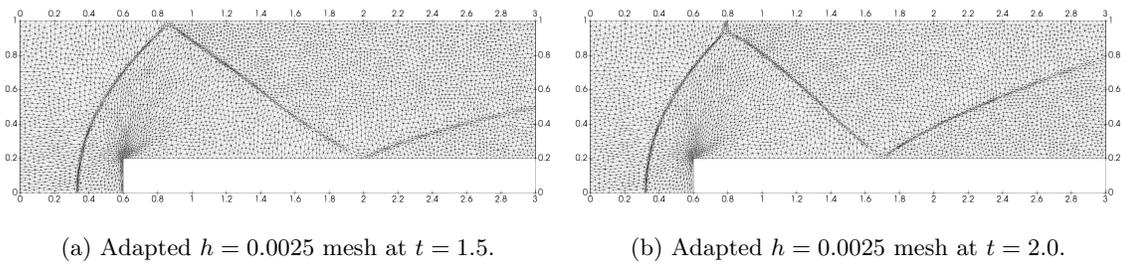
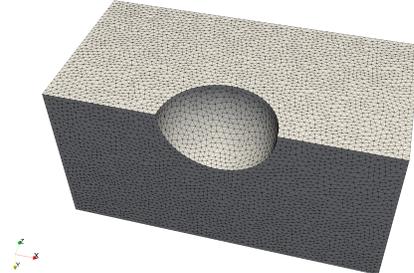


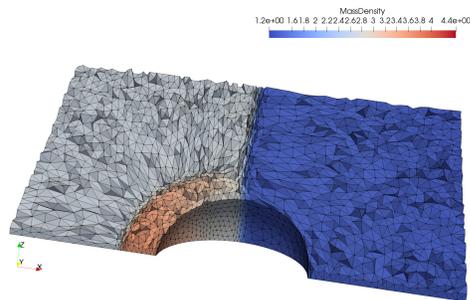
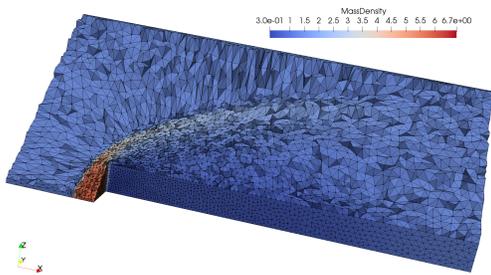
Figure 11: Two-dimensional forward facing step adapted meshes at $t = 1.5$ and $t = 2.0$.



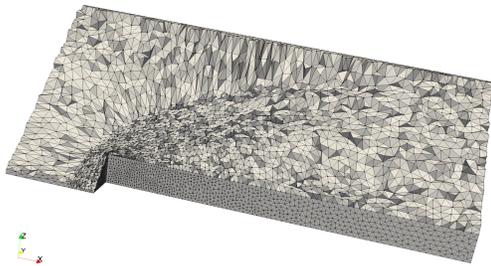
(a) Forward facing step test case.



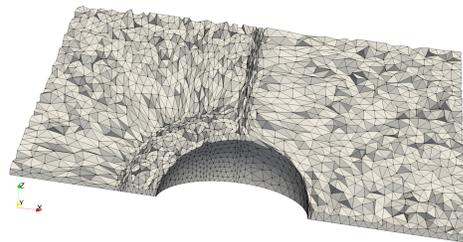
(b) Shock-sphere test case.



(c) Step, volumic cut and mass density at $t = 0.7$. (d) Sphere, volumic cut and mass density at $t = 90$.



(e) Step, volumic cut at $t = 70$.



(f) Sphere, volumic cut at $t = 90$.

Figure 12: Initial meshes, adapted meshes and solution for the three-dimensional forward facing step and shock-sphere interaction cases.

545 we had to produce a refined mesh that is more than ten times bigger (in terms of nodes
546 and elements) than the coarse one. Note that the diagonal cut is possibly the most
547 demanding plane on which results can be compared, as the Laplacian model is uncoupled
548 in multiple space directions, thus it tends to provide better results on cartesian planes, as
549 shown in section 4.1. Adapted meshes are shown in figures 14 and 16. Computational
550 times are shown in table 6. The benefits in terms of computational times in three
551 dimensions are greater than in two dimensions. Anyway, while in two dimension we
552 observed that mesh tangling was a rare occurrence with our Laplacian model, in three
553 dimensions it was impossible to continue the time simulation without the a-posteriori
554 limiter after the first few time steps, due to the strong deformation that quickly led to
555 tangled elements at the step front and around its corners, but also at the shock reflection
556 lines.

557 5.3. Case 3: shock–sphere interaction

558 In order to test the capabilities of the method to handle simultaneously shock waves
559 and curved boundary, we choose to simulate the interaction of a traveling shock wave
560 on a sphere. Some configurations for the diffraction of shock waves over cylindrical
561 and spherical obstacles have been studied experimentally for example in [7, 40]. An
562 early application of unstructured mesh adaptation to two-dimensional shock-cylinder
563 simulations can be found in [14], while structured grid adaptation on axisymmetric
564 shock-sphere simulations can be found in [37].

565 The simulation is limited to a quarter of a cylindrical domain (as for the analyti-
566 cally moving shock of the previous section, see figure 12b). We choose a planar shock
567 moving at $M_s = 1.5$. Adaptation is performed on the mass density (figures ?? and ??),
568 with $(\alpha, \gamma_\alpha) = (40, 0.1)$. Again, the aim is to compare the results obtained with mesh
569 adaptation on a base mesh with edge size $h = 0.05$ with those obtained on a uniformly
570 refined mesh with edge size $h = 0.02$. Mesh data are shown in table 5. Contour lines
571 for the mass density solution on a radial plane are shown in figures 17 and 19, for 50
572 equispaced lines between the values 1.36081 and 4.00883. Resolution on shock waves
573 with mesh adaptation is comparable with those obtained on a uniform mesh about ten
574 times bigger in terms on number of nodes and elements. Adapted meshes are shown in
575 figures 18 and 20. Computational times are shown in table 6.

576 In this case too it was impossible to complete the simulation over valid meshes
577 without the action of the a-posteriori limiter near the corners and the curved surface.

578 6. Conclusions

579 The proposed algorithm for dynamic r-adaptation extends to three dimensions the
580 method first proposed in [9, 10, 5] for two-dimensional flows. An iterative solver based
581 on diagonal Jacobi iterations for the discretized mesh PDEs with natural boundary con-
582 ditions allows a cheap, uncoupled solution in each space direction. A novel a-posteriori
583 relaxation scheme allows to prevent mesh tangling through the construction of a se-
584 quence of valid meshes also over curved boundary surfaces and corners, which is the
585 main concern of r-adaptation methods in multiple dimensions, and it is interleaved with

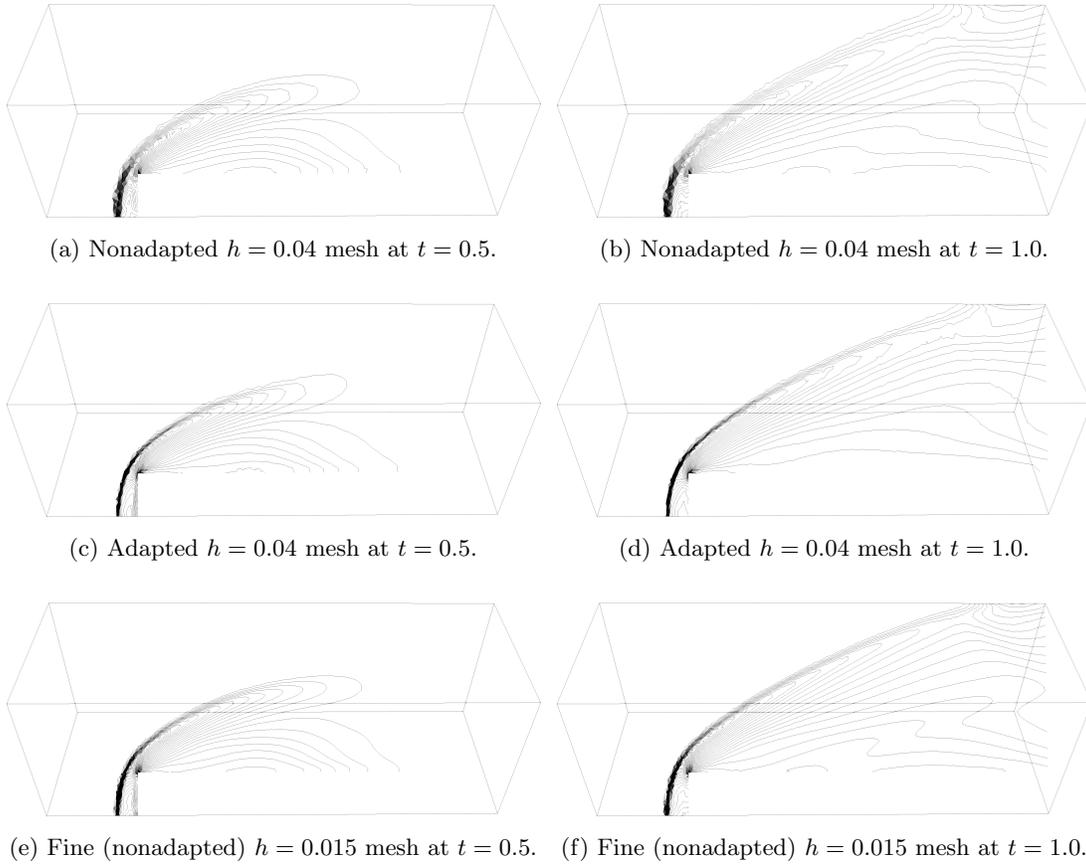


Figure 13: Three-dimensional forward facing step mass density contour lines at $t = 0.5$ and $t = 1.0$.

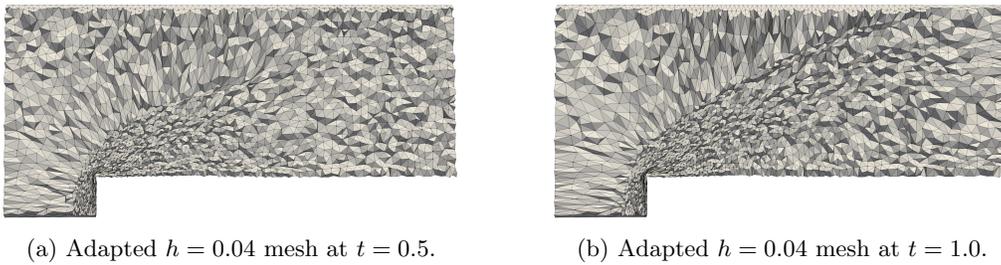


Figure 14: Three-dimensional forward facing step adapted meshes at $t = 0.5$ and $t = 1.0$.

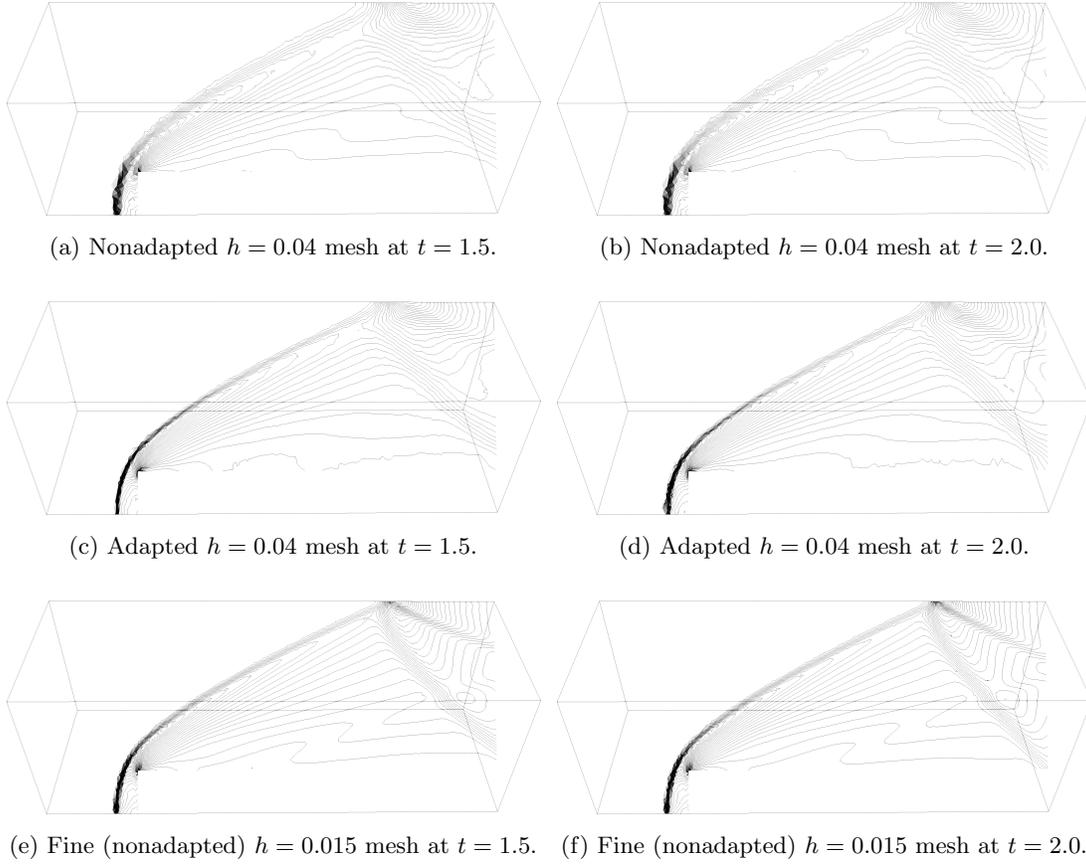


Figure 15: Three-dimensional forward facing step mass density contour lines at $t = 1.5$ and $t = 2.0$.

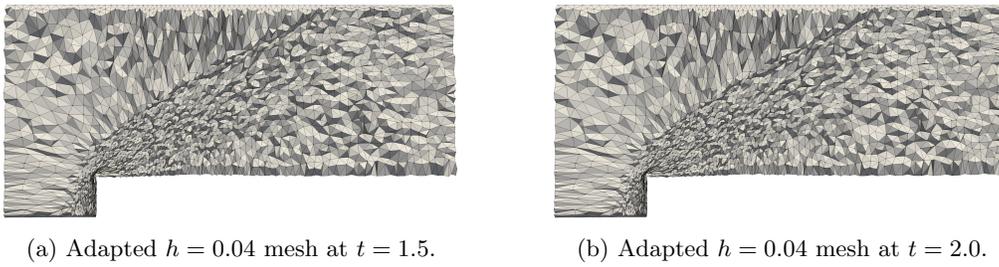


Figure 16: Three-dimensional forward facing step adapted meshes at $t = 1.5$ and $t = 2.0$.

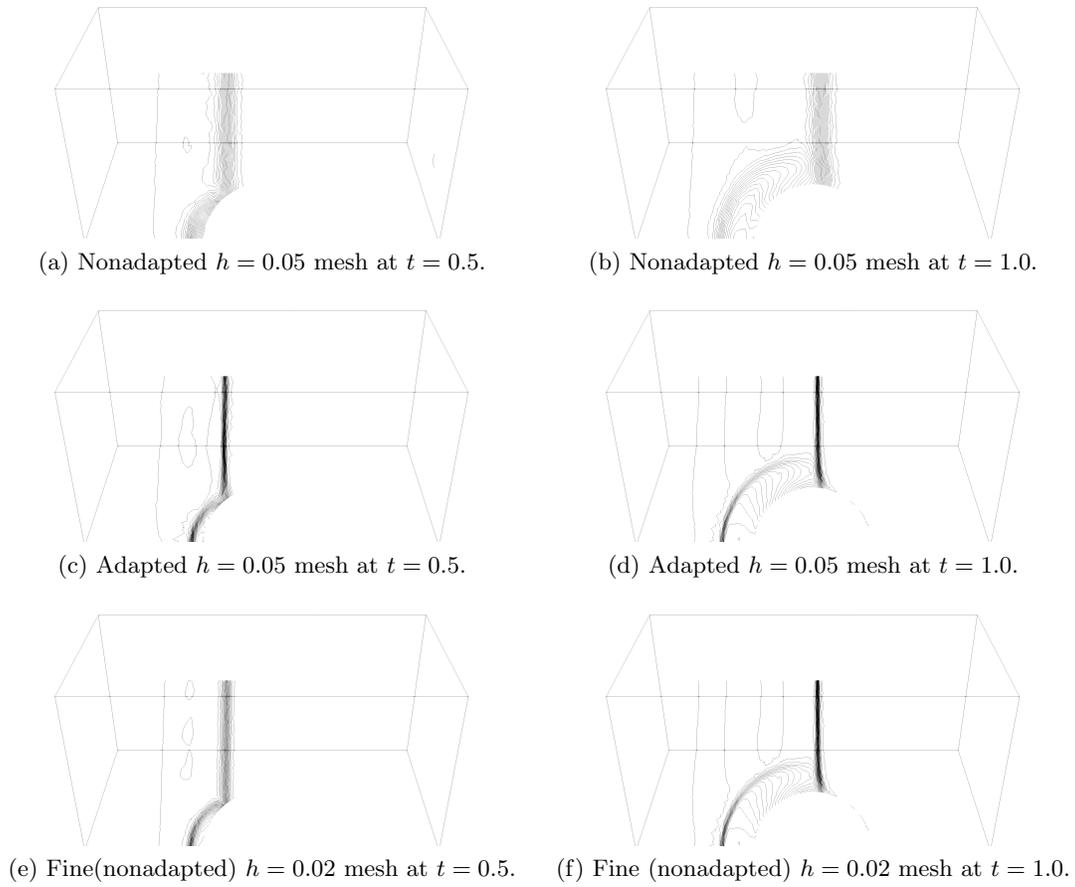


Figure 17: Shock-sphere interaction mass density contour lines at $t = 0.5$ and $t = 1.0$.

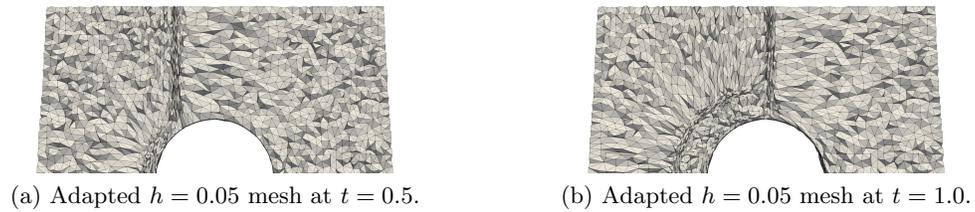


Figure 18: Shock-sphere interaction adapted meshes at $t = 0.5$ and $t = 1.0$.

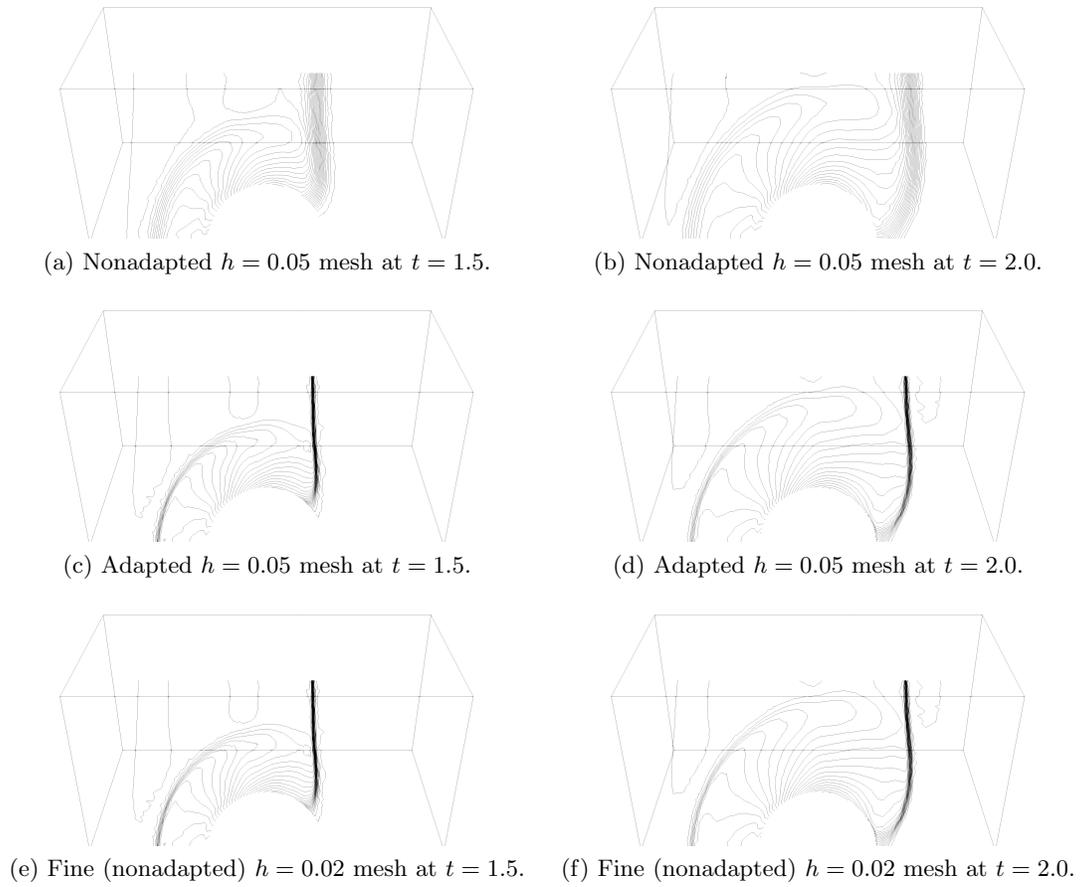


Figure 19: Shock-sphere interaction mass density contour lines at $t = 1.5$ and $t = 2.0$.

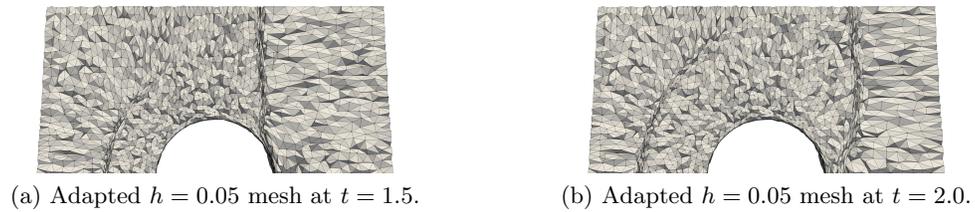


Figure 20: Shock-sphere interaction adapted meshes at $t = 1.5$ and $t = 2.0$.

586 a projection step on the curved boundary parametric model. The iterative correction
587 scheme allows to obtain valid meshes both in the volume and on the curved bound-
588 aries, and does not depend either on the specific choice of the mesh PDE model or the
589 boundary geometry representation.

590 The reference domain formulation for mesh movement produces sufficiently adapted
591 meshes in as few as ten Jacobi iterations per time step during an unsteady flow sim-
592 ulation. While the a-posteriori relaxation algorithm is akin to a forward substitution
593 algorithm, and thus formally dependent from the node ordering, this doesn't appear
594 to spoil the adaptation pattern in any of our tests. We show the successful genera-
595 tion of valid adapted mesh on three-dimensional cases with moving shock waves. While
596 the computational time overhead with respect to the original unadapted mesh is non-
597 negligible, it is more than acceptable when compared to the simulation times needed
598 to achieve the same accuracy on discontinuous flow features on uniformly refined mesh.
599 The attractiveness of the method rests in fact in its applicability on moving shocks,
600 where an off-line mesh refinement approach would require to refine the mesh in most of
601 the computational domain, and its easy coupling with ALE solvers, enabling solution
602 conservation on the adapted meshes.

603 Limitations of this r-adaptation method are the same of the original two-dimensional
604 formulation, namely the Laplacian models excessively pulls nodes towards non-convex
605 boundaries and the displacement uncoupling in the multiple space directions can create
606 sensible adaptation patterns for excessively strong adaptation parameters. Also, the
607 choice of the parameters of the monitor function appear to be application dependent.
608 possibly leading to excessive mesh stretching for same values of the parameters. In
609 these extreme situations, the effect of the novel a-posteriori relaxation scheme allows
610 nonetheless to recover a valid mesh by blocking mesh displacement in critical zones,
611 allowing to continue the mesh movement at successive time steps as the flow features
612 evolve away from the blocked mesh elements. We would like to remark that our limiting
613 procedure is targeted at preserving mesh validity throughout the adaptation procedure.
614 This means that a nodal displacement can be blocked if the volume of an adjacent
615 element falls below an user-defined threshold, but the mesh remains valid. Thus, the
616 vertex positions of the blocked elements can be relaxed either by a subsequent application
617 of r-adaptation at the next time step as the monitor function moves (as it is often the case
618 in the simulation of traveling waves), either by the application of standard smoothing
619 algorithms, which are fundamentally simpler than untangling methods.

620 While a linear finite element approximation is sufficient to model the nodal degrees
621 of freedom of straight-sided meshes, generalizations of the a-posteriori limiting method
622 to curved meshes can be envisaged by increasing the degree of the finite element ba-
623 sis. This would require the formulation of a volume positivity predicate for the curved
624 tetrahedron, which is outside the scope of this work.

625 Future research lines include the parallelization of the current method, for which no
626 specific problems are envisaged, and the study of r-adaptation as a tool to complement
627 h-adaptation in time-dependent simulations to somewhat reduce the overhead of the
628 adaptation strategy.

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