C. R. Mecanique 338 (2010) 127–131

Contents lists available at ScienceDirect

Comptes Rendus Mecanique

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Enhancement of the accuracy of numerical field computation using an adaptive three-dimensional remeshing scheme

Schéma adaptatif de remaillage tridimensionnel pour l'amélioration de la précision numérique de calcul de champs physiques

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A R T I C L E   I N F O

Article history:
Received 17 November 2009
Accepted after revision 17 March 2010
Available online 13 April 2010

Presented by Jean-Baptiste Leblond

Keywords:
Waves
Adaptive meshing
Riemannian metric
Error estimates
Mesh optimization
Numerical approximation and analysis
Electromagnetics

Mots-clés :
Ondes
Maillage adaptatif
Metrique riemannienne
Estimation d'erreur
Optimisation de maillages
Approxiamation et analyse numérique
Eléctromagnétisme

A B S T R A C T

We present an improved adaptive remeshing strategy based on the unit remeshing concept to control the accuracy of the numerical solution of partial differential problems. Such an adaptive remeshing is applied in computing and in representing the strong variation of the physical fields in the space of solutions. We show that, the precision of the solution being controlled, this improved scheme permits to decrease drastically the computational time as well as the memory requirements by adapting the number and the position of nodes where high variations of gradients of the solution are present.

R É S U M É

Nous présentons une méthode de remaillage adaptatif, basée sur le concept de remaillage unité, pour contrôler la précision de la solution numérique lors de la résolution d'un problème d'équations aux dérivées partielles. Une telle méthode est appliquée au calcul et à la représentation des fortes variations des champs physiques dans l'espace des solutions. Nous montrons que, avec une précision contrôlée, cette méthode de remaillage permet de diminuer fortement le temps de calcul et l'espace mémoire en adaptant le nombre et la position des nœuds de calcul là où de fortes variations des gradients de la solution sont présents.

Version française abrégée

Un prérequis essentiel pour la simulation de problèmes physiques par une méthode aux éléments finis est la construction d'un maillage adéquat du domaine de calcul [1]. La qualité de la solution dépend fortement de la qualité des éléments de ce maillage. En particulier, la solution optimale peut être obtenue sur la base d'un maillage régulier du domaine. La solution numérique obtenue sur un tel maillage est généralement analysée en utilisant un estimateur d'erreur a posteriori, lequel permet de renseigner si la solution est, ou non, précise. Cette qualité de la solution est étroitement reliée à la

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1631-0721/$ – see front matter
doi:10.1016/j.crme.2010.03.006

correspondance du maillage à la solution du phénomène physique, laquelle est quantifiée en terme de taille des éléments ou la dimension des fonctions de formes éléments finis. Ceci nécessite donc la génération d'un maillage adapté. L'adaptation de maillage basée sur une h-méthode ajuste le maillage sur la solution en raffinant ou déraffinant localement le maillage, tandis que la p-méthode ajuste localement les fonctions de formes en augmentant la dimension de leur espace. Une méthode d'adaptation combinée, hp-méthode, pourrait être aussi envasigée [2]. Dans ce papier, on s'intéresse à l'adaptation basée sur une h-méthode. L'estimateur d'erreur a posteriori, basé sur l'erreur d'interpolation et dépendant du hessien de la solution, est quant à lui bien adapté au problème de d'adaptation de maillage basée sur une h-méthode [3–5].

Si le remaillage adaptatif à deux dimensions semble être pratiquement résolu ([6] pour une synthèse), sa généralisation au problème à trois dimensions paraît être encore ouvert. Pour ce faire, deux approches peuvent être proposées : le remaillage global et le remaillage local. Dans l'approche de remaillage local, un maillage donné est modifié en accord avec sa carte de taille. Plusieurs méthodes ont été proposées pour le remaillage local ([7] pour une synthèse), lesquelles peuvent être rangées en deux catégories : raffinement et déraffinement des éléments, et subdivision et suppression des arêtes. Dans la première approche, chaque élément ne respectant pas la carte de taille prescrite est raffiné ou déraffiné. Des éléments respectant la carte de taille sont également raffinés pour assurer la conformité du maillage. Le raffinement et la suppression des arêtes consistent à casser les arêtes trop longues et à éliminer les arêtes trop courtes par rapport aux spécifications de tailles données.

Nous proposons une nouvelle méthode de remaillage local basée sur le raffinement et la suppression des arêtes, combinée avec une procédure de modification topologique afin d'améliorer la qualité du maillage.

1. Introduction

An essential prerequisite for the numerical finite element simulation of physical problems expressed in terms of PDEs is the construction of an adequate mesh of the domain [1]. One can show that the quality of the solution strongly depends on the shape quality of the mesh of the domain. In particular, the optimal solution at this stage can be obtained with a regular mesh of the domain. The numerical solution obtained with the initial mesh is generally analyzed using an appropriate a posteriori error estimate which, based on the quality of the solution, indicates whether or not the solution is accurate. The quality of the solution is closely related to how well the mesh corresponds to the underlying physical phenomenon which can be quantified by the element size of the mesh or the dimension of the finite element trial functions. To this end, an adapted mesh needs to be generated. An adaptive h-method adjusts the mesh to the solution by locally refining or coarsening the mesh. An adaptive p-method adjusts the trial function spaces on selected elements by increasing the dimension of the local spaces. Finally, an adaptive hp-method combines the h- and p-method by refining or coarsening the mesh locally in some parts of the domain and enlarging the trial function spaces in other parts [2]. Here, we focus on the adaptive h-method. An a posteriori error estimate based on the interpolation error depending on the Hessian of the solution seems to be well adapted to the purpose of adaptive h-method. Various works are related to such error estimates [3–5]. Let u be the exact scalar solution field, u_h the computed field from a given mesh and $\Pi_h u$ the interpolated field from the same mesh. For elliptic problems, the Cea's lemma $\|u - u_h\| \leqslant C\|u - \Pi_h u\|$ where C is a constant depending on the computational domain, is verified. In other words, by controlling the interpolation error, one can control the finite element error. Let K be a mesh element and h_K be its size, on can show that [5]:

$$\forall x \in K, \quad \big\|u(x) - \Pi_h u(x)\big\|_\infty \leqslant \frac{9}{32} M h_K^2 \tag{1}$$

with $M = \max_{x\in K}(\max_{\|v\|=1} |v^T H_u(x) v|)$, where v is any unit direction and $H_u(x)$ is the Hessian of u at x. This relation allows us to bound the interpolation error by controlling the mesh size:

$$h_K \leqslant \frac{4}{3}\sqrt{\frac{2}{M}}\varepsilon \quad \Rightarrow \quad \forall x \in K, \quad \big\|u(x) - \Pi_h u(x)\big\|_\infty \leqslant \varepsilon \tag{2}$$

The Hessian of the exact solution u is approximated by the Hessian of the computed solution u_h, which is calculated using discrete derivatives obtained from a local reconstruction of a smooth approximation of the solution.

The adaptive remeshing in two dimensions seems to be almost solved ([6] for a survey). However, its generalization to three-dimensional case is a great challenge. There are two approaches to deal with this, global remeshing and local remeshing. In the local remeshing approach, a given mesh is modified with respect to the prescribed size map. Several methods have been proposed for local remeshing ([7] for a survey) which can be classified in two categories: element-based refinement and edge-based refinement. In the first approach, each element violating the prescribed size map is refined using templates. To ensure the conformity of the overall mesh the refinement must be applied to elements which verify the size map, resulting to unnecessary refined elements. The edge-based refinement consists in splitting all the elements sharing an edge without propagation to adjacent elements.

We propose a new local remeshing method based on edge removing and edge-based refinement combined with a Delaunay-based topology modification procedure to construct, from a given mesh, a new mesh conforming to a given size map.

2. Unit remeshing strategy

Let h be a size function defined on a domain Ω in R^3. We define a Riemannian metric tensor $\mathcal{M}$ from h by $\mathcal{M} = \frac{1}{h^2} I_3$ which transforms the size h to unity in all directions. The mesh of Ω respecting size h is a mesh of Ω equipped with the metric $\mathcal{M}$ in which all edge lengths are of unity measure. Recall that if $e = AB$ is a mesh edge, the length of e with respect to the metric $\mathcal{M}$ is:

$$l_{\mathcal{M}}(e) = \|\overrightarrow{AB}\| \int_0^1 \frac{1}{h(A + t\overrightarrow{AB})} \, \mathrm{d}t \tag{3}$$

We propose a new remeshing method resulting in the construction of a unit mesh of a domain Ω in R^3, by modifying a given mesh of Ω equipped with a Riemannian metric $\mathcal{M}$ defined from a specified size map h associated to the mesh vertices. The general scheme of our method includes two main steps (mesh edge processing and mesh element optimization) and can be written as:

- *Mesh edge processing loop*
  - "small" edge removal and "large" edge splitting,
  - topology modification with shape quality improving modification.
- *Mesh element optimization loop*
  - vertice relocation and topology modification with shape quality improving.

A small edge is an edge with a length with respect to the metric smaller than unity. In practice, we consider an edge to be small if its length is smaller than $1^- = 1/\sqrt{2}$. The edge removal operation consists in contracting the edge to its midpoint or one of its extremity (if it is an internal edge with an extremity belonging to the boundary). Let us denote by *Shell*(e) (shell of edge e) the set of elements sharing edge e, by *Ball*(e) (ball of edge e) the set of elements sharing an end point of e, and by q_e the shape quality of *Ball*$(e) \setminus$ *Shell*(e) which represents the worst quality of elements of *Ball*$(e) \setminus$ *Shell*(e). The removal operation is applied if the shape quality of the resulting set of elements (the worst element quality) is greater than αq_e where α is a threshold factor to control the quality worsening (for example $\alpha = 0.95$). If the edge belongs to the boundary, the resulting configuration after edge removal must preserve the boundary shape or geometry. If the kernel of *Ball*$(e) \setminus$ *Shell*(e) is empty or does not contain the midpoint of e (in the case where e is internal), the edge removal operation fails. The topology modification with shape quality improvement allows us to grow these kernels in order to ensure the efficiency of the edge removal operation. Similarly, a large edge is an edge whose length with respect to the metric is greater than unity, or in practice $1^+ = \sqrt{2}$. The edge splitting operation consists in splitting in two parts all the elements of the shell of the edge from its midpoint.

Edge removing and edge splitting are well-known operations allowing us to construct a mesh with edge lengths smaller than unity. Therefore, these operations must be combined by mesh topology modification with shape quality improvement, in order to construct a unit mesh in which all edge lengths are equal to unity. Generally, the mesh topology modification includes edge and facet flipping. The latter is a simple transformation of two elements into three elements. The edge flipping consists in removing the edge by retriangulating the shell of the edge (set of elements sharing the edge). There is an exponential number of possible configurations depending on the number of elements of the shell. In practice, one can limit the edge flipping operation to the case of shells containing at most 7 elements. We propose a new mesh topology improvement based on a modified Delaunay kernel. The idea is to modify locally the mesh topology using the Delaunay kernel, in order to improve the shape quality. Let us recall the Delaunay kernel.

The Delaunay kernel is a procedure allowing us to insert a point in a triangulation. Let us denote by T a triangulation and by P a given point. Inserting P in T using the Delaunay kernel can be written as (cf. [6]): $T = T - C(P) + B(P)$ where $C(P)$ is the cavity associated with point P, and $B(P)$ is the re-meshing of $C(P)$ based on P. For robustness purpose, the cavity $C(P)$ is defined by $C(P) = C_1(P) \cup C_2(P)$ with:

$$C_1(P) = \{K \text{ element of } T \text{ including } P\} \tag{4}$$

and

$$C_2(P) = \left\{K, K \in T, \ \exists K' \in C(P), \ K \text{ adjacent to } K', \ d(O_K, P) < r_K\right\} \tag{5}$$

where O_K (resp. r_K) is the center (resp. radius) of the circumsphere of K. Set $C_1(P)$ is constituted by all the elements containing P. Set $C_2(P)$ is assembled by adjacency from the elements of $C_1(P)$ and is composed of elements with a circumsphere containing point P. By this way, it is obvious that cavity $C(P)$ is starshaped with respect to P and set $B(P)$ which is composed of elements defined by P and external facets of $C(P)$ is well defined.

We modify the Delaunay kernel in order to take into account the shape quality. The modified Delaunay kernel consists in redefining $C_1(P)$ and applying a new cavity correction procedure by controlling the shape quality change. It is iteratively

Table 1
Number of nodes, number of tetrahedra, minimal mesh size h_{min}, the minimum value, the mean value and the maximum value of the interpolation error ε and the computational time (remeshing + intensity) for remeshing step during the adaptive remeshing process.

Nodes	Tetrahedra	min[ε]	mean[ε]	max[ε]	h_{min}	Times (s)
			Adaptive 3D remeshing process			
8074	47 161	4.2×10^{-10}	5.6×10^{-4}	2.9×10^{-2}	1.00	$0 + 2$
1 055 728	6 380 319	9.3×10^{-12}	4.3×10^{-5}	0.9×10^{-3}	0.25	$297 + 264$
			Classical mesh in spherical coordinates			
25 000 000					0.25	6252

applied to all the vertices to locally improve the mesh quality. Since point P is already a mesh vertex, $C_1(P)$ is redefined by:

$$C_1(P) = \{K, K \in T, K \text{ having } P \text{ as vertex}\} \tag{6}$$

Let us denote by q_{C_1} the worst shape quality of elements of $C_1(P)$. Cavity $C(P)$ (being $C_1(P) \cup C_2(P)$), is iteratively modified by the following step:

– if there is an element of $B(P)$ sharing a boundary facet f of $C(P)$ with a shape quality worse than q_{C_1}, remove from $C(P)$ the element of $C_2(P)$ containing facet f.

After this new cavity correction procedure, the shape quality of $B(P)$ will be better than that of $C_1(P)$. Thereby, the topology modification consists in replacing $C(P)$ by $B(P)$ which locally improves the shape quality of elements sharing P. In the case where P is a boundary vertex, the resulting configuration $B(P)$ must also preserve the boundary geometry. The cavity definition and the correction cavity procedure can easily be modified to include this new constraint.

The vertice relocation step is a classical iterative procedure which consists in moving each mesh vertex in order to improve the shape quality of its sharing elements.

3. Numerical example

The proposed remeshing scheme is applied to compute the interaction of an illuminating vectorial monochromatic field **E** with a spherical metallic particle of relative radius $R/\lambda = 1/60$. The complete problem can be written in the 3D space [8]:

$$\nabla \times \left(\frac{1}{\mu_r} \nabla \times \mathbf{E}\right) - k_0^2 \varepsilon_r \mathbf{E} = \mathbf{0} \quad \text{and} \quad \nabla . \mathbf{E} = \mathbf{0} \tag{7}$$

where k_0^2 is a constant of the problem, which is related to the wavelength in vacuum λ: $k_0 = 2\pi/\lambda$, μ_r and ε_r being the complex relative permeabilities and permittivities of the materials depending on the spatial coordinates. Basically the complex vectorial field is not of interest as only its square modulus can be detected practically. Therefore, in the following, the square modulus of the total field will be plotted $I_r = \|\mathbf{E}\|^2$. The use of a non-regular non-Cartesian adaptive mesh is necessary to reproduce the curvature of the intensity around the spherical particle.

For the present case, the metric governing the remeshing process is based on the Hessian of I_r. Fig. 1 shows the initial and the final solution field I_r associated with the initial coarse mesh (at left) and the final adapted mesh (at right). Such an adaptive mesh will be particularly efficient in the spatial zone where such a strong field intensity distribution occurs.

Table 1 shows the number of mesh nodes and mesh elements for a specified minimal mesh size h_{min} and a relative interpolation error ε related to the initial and final adapted meshes. The final mesh is compared to a generic mesh in spherical coordinates. We can remark that the adapted remeshing process permits to drastically decrease the number of computational nodes (here in the order of 25 times from 25 000 000 to 1 055 728). Such an adaptive remeshing process ensures a maximum error in the whole computational domain to be limited by the threshold $\varepsilon = 0.001$, excepted in the zone where h_{min} is reached (i.e. at the discontinuity interface between the two materials). The latter defines the maximum width of the discontinuity of the solution at the interface of the material.

4. Conclusion

In this Note we have presented an improved adaptive 3D remeshing strategy based on the unit mesh concept. This approach can be used in connection with the analytical or numerical Finite Element method for the computation of the solution in context of high variation field solution. Based on a classical problem in electromagnetism, we have verified that a sufficient grid size refinement must be considered to ensure the convergence and stabilization of the solution, particularly in the regions where a strong confinement of the solution around the structure takes place. The proposed adaptive remeshing allows us to control the accuracy of the solution field. This improved procedure considerably accelerates the convergence of the solution and minimizes both the memory requirement and the computational time, by keeping a control on the accuracy of the solution.

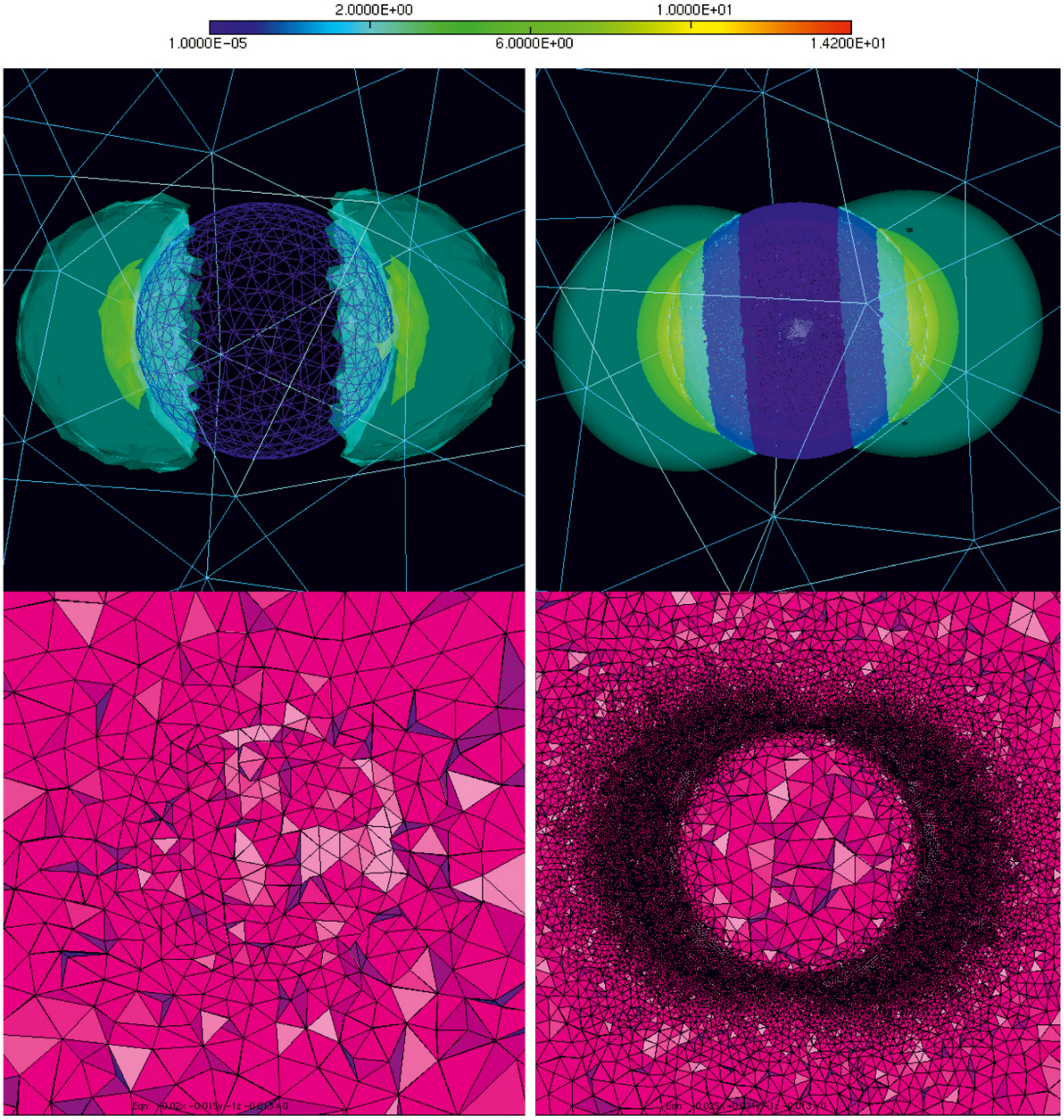

Fig. 1. The intensities of the solution field I_r (for $\varepsilon_r = -9.44 + j1.51$) associated with the initial mesh (at left) and the adapted mesh (at right).

Acknowledgements

Authors thank the Centre de Calcul Intensif ROMEO2 for computational facilities, the Région Champagne-Ardennes and the Conseil Régional de l'Aube for financial support.

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