Adaptive mesh refinement for the numerical modelling of complex microstructural evolution applications

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1. Introduction

The objective of this note is to demonstrate the necessity of using an appropriate automatic adaptive meshing technique so as to handle complex microstructural evolutions. Examples of such microstructural evolutions include the deformation and recrystallization of polycrystalline aggregates or the growth of dendrites occurring during the solidification of metallic alloys. In such applications, it is required to track and/or capture accurately the interface between two or several domains having different mechanical behaviour. Also, the interface is a region where strong physical and/or kinematic incompatibilities, stemming from the heterogeneity of the mechanical response, occur. Gradients of the various mechanical fields develop across the interface and are expected to be significant in the direction perpendicular to the boundary. For these reasons, anisotropic mesh refinement along the interface, with a smaller mesh size in the perpendicular direction to it, is needed. This strategy represents a good compromise between accuracy and computation time as the mesh refinement is performed only where it is necessary. The level set framework used in our approach to represent and follow the boundaries is fully compatible with this meshing technique and allows for the remeshing to be handled quite easily throughout the evolution of the microstructure as often as needed.

After presenting briefly the basis of the anisotropic meshing and remeshing tool, two illustrative applications are presented.

2. Anisotropic meshing and remeshing based on the level set framework

In order to construct an anisotropic mesh, an appropriate anisotropic metric has to be defined. In our approach, the construction of the metric is based on the level set framework which is used for domain representation. The level set is defined as a signed distance function \( \phi \) with a zero level corresponding to the interface \( \Gamma \):

\[
\begin{cases}
\phi(x) = d(x, \Gamma), x \in \Omega \\
\Gamma = \{x \in \Omega, \phi(x) = 0\}
\end{cases}
\]  

(1)

The direction of mesh refinement is the normal to the interface which is defined by the gradient of the level set function \( \nabla \phi \). Figure 1 illustrates the concept in 2D. Let \( h_1 \) be the desired mesh size far from the interface where isotropic mesh is needed and \( h_2 \) the desired mesh size in the direction of \( \nabla \phi \) in the region close to the interface where anisotropic mesh is needed. As seen on figure 1, \( h_1 \) is also the mesh size in the direction perpendicular to \( \nabla \phi \) in the region surrounding the interface.
The metric $M$ is defined as follows:

$$M = C(\nabla \phi \otimes \nabla \phi) + \frac{Id}{h_i^2}$$  \hspace{1cm} (2)

where $Id$ is the identity tensor, $C$ a scalar parameter which is equal to $\frac{1}{h_2^2} - \frac{1}{h_1^2}$ in the anisotropic region and 0 in the isotropic region. One can verify that such a common definition for the metric leads to an isotropic mesh far from the interface and an anisotropic mesh near a specified region around the boundary.

The metric $M$ is fed into MTC [1] which builds the corresponding mesh. Most importantly, the level set description is fully compatible with automatic remeshing. The values of the level set function are directly interpolated from the old mesh to the new one and the corresponding anisotropic metric and mesh are reconstructed. Thus, periodic adaptive automatic remeshing can be easily performed, thereby always ensuring appropriate refinement near the interface.

3. Application 1: deformation and subsequent primary recrystallization of polycrystalline aggregates

Recrystallization phenomena inevitably occur during thermal and mechanical processes and have a major impact on the final in-use properties of the polycrystalline metallic materials [2]. The objective of this study is to model the deformation of 3D grain structures subjected to important strains in an attempt to provide reliable quantitative data to be used for the modelling of the recrystallization.

3D polycrystalline volumes are constructed using random Voronoï tessellation or based on voxelized experimental data. When dealing with a polycrystalline aggregate, an individual level set function is used for each grain: $\{\phi_i, 1 \leq i \leq N_G\}$, with $N_G$ the total number of grains in the aggregate. One can also define a global level set function as $\phi_{glob} = \max\{\phi_i, 1 \leq i \leq N_G\}$ with a zero value corresponding to the interface between all grains. The obtained digital microstructures are meshed anisotropically and adaptively, with refinement close to the grain boundaries as seen on figure 2. Digital mechanical testing then takes place using classical crystal plasticity constitutive law [3] coupled to a non-linear finite element solver in an updated Lagrangian framework. In this context, the level set function of each grain moves according to the material velocity, which corresponds here to the mesh velocity. The large deformation of the aggregate is responsible for strong mesh distortion as seen on figure 2, hence the need for frequent remeshing.
Fig. 2. 1000 grains polycrystal. Left: Anisotropic mesh before deformation (2 125 688 nodes, 12 385 889 elements); right: mesh after 70% thickness reduction

The deformation simulation provides an estimate of the spatial distribution of strain energy within the polycrystalline aggregate. The latter quantity is used as input for modelling subsequent primary recrystallization as seen on figure 3. As in the deformation stage, level set functions are used to represent grains during the recrystallization stage. The microstructure obtained at the end of the deformation step is used as input to the recrystallization simulation. New nuclei are introduced in the simulation by creating new level set functions based on the gradient of the stored energy.

Fig. 3. Left: stored energy at the grains interface after deformation; right: the gradient of the stored energy

Fig. 4. From left to right and top to bottom: evolution of the recrystallized part in blue
As opposed to the deformation step, the microstructure evolution during the recrystallization stage is performed in Eulerian context. Thus, the level set function of each grain is convected throughout the mesh. In order to correctly evolve the fronts, several issues need to be addressed. The main problem is the development of vacuum and/or overlapping regions. A highly refined mesh is needed near the interfaces of the grains so as to ensure a good accuracy in the computation of the interface velocities. The adaptive meshing technique described previously has proved to be an efficient tool in achieving this objective [4]. Frequent remeshing is needed as the microstructure evolves as seen on figure 4.

4. Application 2: dendritic growth

Dendritic growth occurs during complex heat/solute diffusion processes associated to curvature effects and all at their own length and time scale. First numerical results concerning the simulation of dendritic growth of a single dendrite in two dimensions is presented in this section. Material parameters and geometry were taken from [5]. The initial solid grain is a circle with an initial concentration corresponding to the equilibrium liquid concentration of the phase diagram and is inserted in a square domain. As with recrystallization simulation, the level set framework is used in an eulerian context for the evolution of the microstructure. Frequent remeshing is needed and for the case presented here the frequency of remeshing was 20, for several thousands of time steps. Figure 5 illustrates the evolution of the different computed variables during dendritic growth. One can observe a logical anisotropic growth, as well as the solute’s migration between phases and the different thermal and solutal diffusion layers. Even though these first results are promising, dendrite final shape is not quite well achieved: due to curvature effects, dendrite's tip should be rounded and instabilities occurring at the interface should vanish with time. If we look at the mesh during growth (figure 6) we can see that although a relatively fine adaptation near the interface was performed, it may not be sufficient to capture the anisotropic curvature correctly. Moreover, we may also need to enlarge the adaptation to the whole solutal diffusion layer (due to the abrupt concentration's pattern in this zone). Perspectives of this work include the use of a posteriori error estimators both on level set and concentration solutions to better guide the meshing procedures.

Fig. 5. Growth of one dendrite. From left to right and from top to bottom: representation of the adimensional concentration, of a normalized $[0,1]$ function of the level set, of the real concentration and of the adimensional temperature.
5. Conclusion

It has been shown that an adaptive anisotropic automatic meshing and remeshing technique coupled to a level set framework is a promising tool to describe complex phenomena such as the deformation and subsequent primary recrystallization in polycrystalline materials and dendritic growth during solidification of metallic alloys. Indeed, in the case of polycrystalline aggregates, large plastic deformation is achieved on a representative volume element of 1000 grains and for primary recrystallization modelling, full kinematic compatibilities are enforced, and nucleation and growth phenomena are implemented. Perspectives for recrystallization modelling include simulations with a statistical number of grains, the prediction of recrystallization kinetics and the comparison with other models. Concerning dendritic growth, perspectives include a better guidance of the adaptive meshing procedure using error estimators. Furthermore, a local level set method can also be adopted, to avoid advection of the function over the whole computational domain.

It should be noted that this research note presents a first promising step in the simulation of complex phenomena at the microscale. The adaptative meshing technique presented here seems to be an unavoidable tool if we wish to simulate microstructural evolutions at even smaller scales.

References