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Body-Fitted Finite Element Discretizations for Moving Interfaces in Context of Microstructure Evolutions

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Résumé — The Level-set (LS) method [1] is used to model dynamic interfaces in the context of large deformations. This approach is used in simulations of microstructural evolutions [2–10] using a Finite Element (FE) framework where the interfaces are implicitly defined and captured by a refined mesh. This process can be very costly in terms of CPU-time and the presence of vacuum regions is inevitable. A new approach to discretize the interfaces given by the LS fields, which enables to treat these voids and to maintain the same accuracy with a reduced CPU-time will be presented.
Mots clés — Body-fitted, Moving Interfaces, Remeshing, Finite Element Method, Level-Set.

1 General Context

The simulation of microstructure evolutions as Grain Growth (GG) and Recrystallization (ReX) at the mesoscale [6, 8, 9, 11], can be very complex. Large displacements of interfaces and topology changes can occur during the evolution of the microstructure. The LS method is a well-known approach capable of managing this kind of phenomena during a simulation in a FE context. Interfaces between grains are then implicitly described in a Eulerian framework, as the zero-isovalues of the LS fields and their evolution are governed by convective-diffusive partial differential equations (PDEs).
In the context of the Finite Element Method (FEM), the LS approach circumvents the notoriously difficult problem of generating interface-conforming meshes for geometries subject to large displacements and to changes in the topology of the domains. However, in order to maintain high accuracy, moving interfaces are generally captured by a locally refined FE mesh with the help of mesh adaptation techniques. In a microstructural problem, the large number of interfaces and the fine mesh required in their vicinity make the mesh adaptation process very costly in terms of CPU-time, particularly in 3D [12]. Moreover, when using an implicitly defined interfaces, it is complex to describe the multiple junctions (namely interfaces between more than two grains) where the presence of numerical vacuums is inevitable.
In this work, a different adaptation strategy is used. It maintains the benefits of the classical Eulerian LS framework, while enforcing at all times the conformity of the FE mesh to implicit interfaces by means of local remeshing operations [13]. With this approach, the changes in properties between grains, such as the dislocation density, can also be represented by a genuinely discontinuous jump at the interface, instead of resorting to a smoothed field. Additionally, The remeshing algorithm employed can also treat the vacuum regions present at multiple junctions. Finally we will illustrate how the new method decreases the requirement in mesh density while maintaining the accuracy at the interfaces.

2 Numerical approach

The LS function used for the simulation of microstructure evolutions is a signed distance function to the interface :

$$\begin{cases} \phi(x) = -\mathrm{d}(x,\Gamma) & x \in \Omega_- \\ \phi(x) = +\mathrm{d}(x,\Gamma) & x \in \Omega_+ \\ \phi(x) = 0 & x \in \Gamma \end{cases}$$

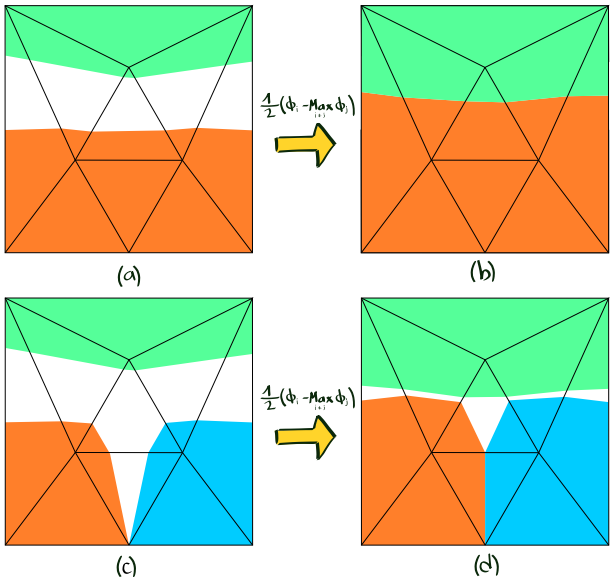

FIGURE 1 – Global treatment to eliminate non-physical vacuum regions on a FE discretization : two colored LSs (a) with no treatment of vacuum regions, (b) result after applying Eq. (1). Three colored LSs : (c) with no treatment of vacuum regions (d) result after applying Eq. (1).

where $\mathrm{d}(x,\Gamma)$ is the Euclidean distance between a point and the interface Γ.
The presence of non-physical vacuum regions with the LS method is well known [2] and the following treatment has been used in previous works [2, 6, 14–16] to treat it :

$$\forall i = 1 \dots N, \hat{\phi}_i = \frac{1}{2}\left(\phi_i - \max_{j \neq i} \phi_j\right), \tag{1}$$

where $\hat{\phi}_i$ is then used as LS function. The effect of this treatment is illustrated in Fig. 1. If this treatment is applied between two LS functions as in Fig. 1.(a), no node nor mesh edges will contain a vacuum (Fig. 1(b)). However, when applying the same procedure on three level-sets as in figure Fig. 1.(c) it can be seen that this treatment does not totally remove vacuum regions on mesh edges or elements (Fig. 1.(d)).

2.1 Grain Growth : Diffusion Equation

GG by capillarity has a pure advective nature where the velocity $\vec{v}$ at every point on the interfaces can be expressed as a function of its local mean curvature :

$$\vec{v} = -M\gamma\kappa\vec{n}, \tag{2}$$

where M is the mobility of the interface, γ the grain boundary energy, κ the local mean curvature (curvature in 2D and sum of the main curvatures in 3D) and $\vec{n}$ the outside unitary normal to the grain interface.

When M and γ are assumed isotropic, Eq. 2 can be used to establish the following advection equation for the migration of the grain boundaries :

$$\frac{\partial \phi_i}{\partial t} - M\gamma\kappa(\vec{n} \cdot \vec{\nabla}\phi_i) = 0 \tag{3}$$

Generally, the solution of Eq. 3 requires time steps extremely small in order to obtain a solution without instabilities, this is why it is preferred to re-write Eq. 3 as a diffusive equation by adding an additional hypothesis : the LS fields remain signed distance functions ($|\vec{\nabla}\phi_i| = 1$) around their 0-isovalues. Finally, the following diffusive equations of the LSs are solved in a FE context :

$$\frac{\partial \phi_i}{\partial t} - M\gamma\Delta\phi_i = 0 \tag{4}$$

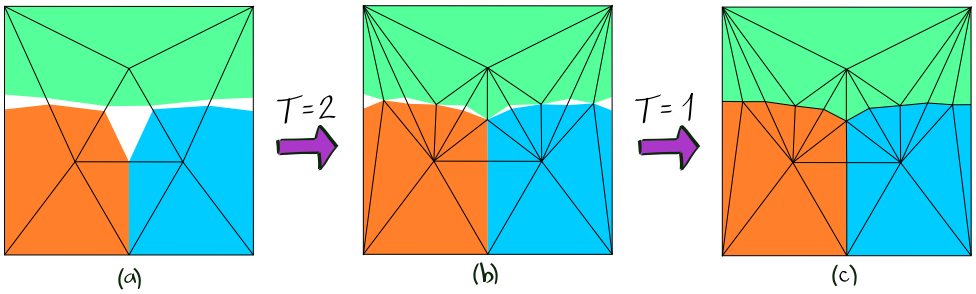

FIGURE 2 – Solution of the three grains 2D problem : (a) result after using Eq. (1), (b) result after the first iteration of the joining algorithm, (c) result after the second and last iteration of the joining algorithm.

Eq. 4 is in general much more stable than Eq. 3 and enables avoiding a direct calculation of κ but requires an additional step. LS functions need to be maintained as signed distance functions, the process used to do so is called reinitialization [16]. Of course this reasoning can be extend to the context of an anisotropic nature of γ or M [10] but will not be considered here.

2.2 Fitting and Joining Algorithm

Only by using Eq. (1) it can not be ensured that the domain will be free of vacuum, hence another procedure needs to be established. A generalized version of the so-called interface fitting algorithm, introduced in a previous work [13], is proposed to remove these remaining vacuum regions while constructing a conform FE mesh of the interface. Compared to the existing literature, this algorithm is based on purely topological operations, and can be easily extended to 3D :

for all $T = d \dots 1$ **do**
  for all T-simplex S of the mesh **do**
    Compute all intersections between edges of S and any interface
    Insert the barycenter of these intersections in the mesh by splitting S
    Set the LS function associated to any interface that intersected edges of S to zero on the inserted node
  end for
end for

The value of d is 2 in 2D and 3 in 3D. A 3-simplex is a tetrahedron, a 2-simplex a triangle, and a 1-simplex a line segment. An example of the application of this this interface joining technique in 2D is shown in Fig. 2.

All elements of the mesh are colored, hence there is no vacuum. We can also observe that even if the element does not contain a junction (or at least three phases) the algorithm will also treat this element and close the vacuum present in it. The obtained mesh is of poor quality, hence this interface joining process will generally be followed by a mesh adaption step to restore a good element shape close to grain boundaries.

3 Tests and results in a 2D 1000 grains case

The Fitting and Joining Algorithm is going to be compared with a more classic method of mesh adaptation during calculations where the interfaces are captured with a non-conform local refined mesh as detailed in [3, 6, 11, 14] and described as the Classic Meshing Adaptation (CMA) technique in the following instead of tracked with a body-fitted mesh adaptation algorithm. Both cases will be compared to the convergence of the evolution of the mean grain size (equivalent radius in number) when using a homogeneous refined static mesh. When a homogeneous static mesh is considered transport errors are not present. In addition, if the mesh size is small, errors on the reinitialization procedure become less important as the distance functions are better described and finally vacuum regions become smaller. Hence the case with the homogeneous refined static mesh will be treated as the better solution in terms

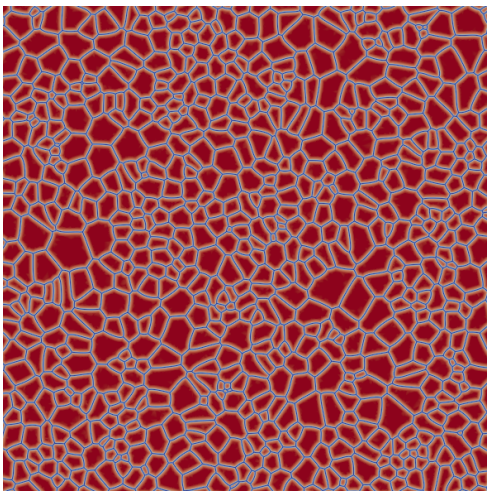

FIGURE 3 – Initial state of the microstructure composed of 1000 grains and builded thanks to a Laguerre-Voronoï algorithm.

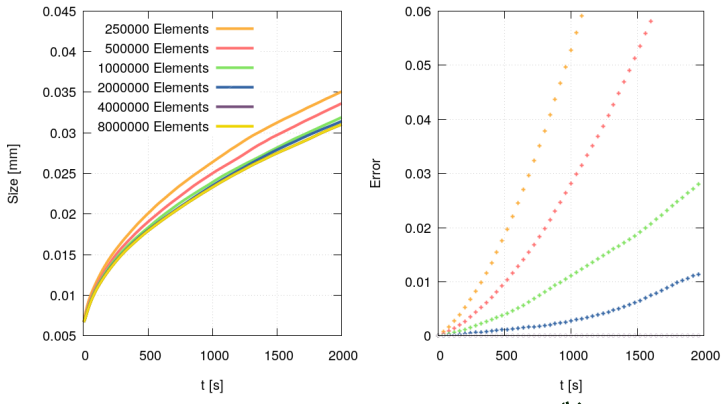

FIGURE 4 – Convergence analysis when a homogeneous static mesh is considered, left : evolution of the mean grain size of the microstructure, right : cumulated $L2$ error in time comparatively to the 8-million elements case. These results illustrate that the 8-million elements case can be considered as the reference case.

of precision and errors of the two other cases will be computed thanks to its evolution.

The initial microstructure considered is composed of 1000 grains generated using the concept of Laguerre-Voronoi cells [17–19]. Fig. 3 illustrates its initial state. The values for M and γ are chosen as representative of a 304L stainless steel at 1050° celsius (with $M = M_0 * e^{-Q/RT}$ where M_0 is a constant $M_0 = 1.56e11[mm^4/Js]$, Q is the thermal activation energy $Q = 2.8e^5[J/mol]$, R is the ideal gas constant, T is the absolute temperature T=1323 [K] and $\gamma = 6e^{-7}[J/mm^2]$). The thermal treatment is realized at a constant temperature during 2000 seconds.

Figure 4 describes the evolution of the mean grain size when different static meshes are considered. We assume that convergence is reached when the cumulated $L2$ error in time remains lower than 1% at 2000s. Hence, the 8-million elements case can indeed be considered as a reference case in the following.

Figure 5 shows the evolution of each case, the one using the CMA technique for the capturing of the interfaces and the New Fitting and Joining Algorithm (NFJA).

4 Discussion, conclusion and perspectives

Figure 5 illustrates that the evolution of each one of the methods have almost the same accuracy. It is also clear that the curve of CPU-time is not linear, this is due to the fact that the number of grains is

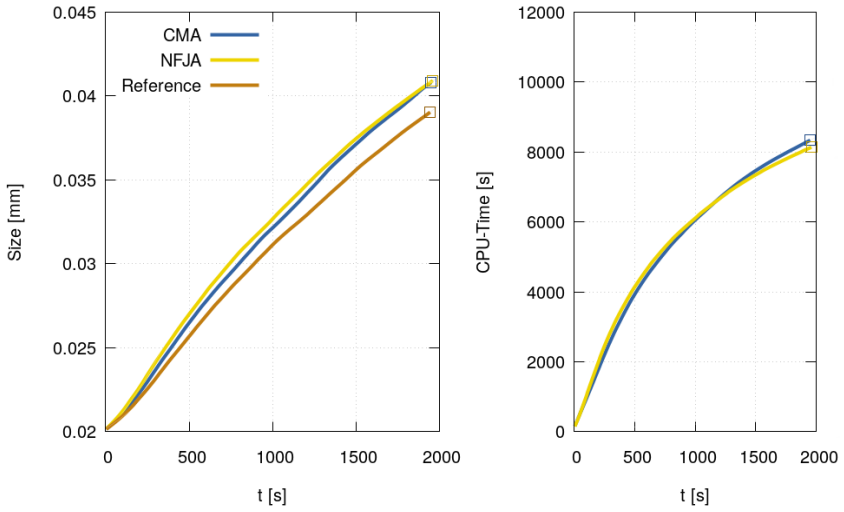

FIGURE 5 – Results for each case : using a Classic Meshing Adaptation (CMA) technique, using the New Fitting and Joining Algorithm (NFJA) and the reference curve. Left : evolution of the mean grain size and right : CPU-time of simulation, the reference case is not plotted.

also changing during the simulation, the less grains there are, the smaller the zone needed to maintain with a refined mesh hence the smaller the time of computation by increment. CPU-time for both cases (CMA and NFJA) are very near, however they represent very different processes. The time needed to remesh with the NFJA for a fixed number of elements is higher as in addition to the mesh adaptation process, the fitting needs to be done. On the other hand, the NFJA needed less mesh elements to define the interface and to maintain the same accuracy. Thus the propose new front-tracking approach appears already as competitive comparatively to the existing LS front-capturing approach used in the state of the art in context of unstructured FE mesh [8–10, 20].

Furthermore improvements could be made with the use of the NFJA that could result in a diminution of the CPU-time that could not be possible to make by employing more classical approach. Indeed, with this approach, geometrical data such as interface normals and curvatures can be computed directly from the body-fitted mesh using the position of the interface nodes only, instead of relying on the costly and inaccurate approximation of the LS field derivatives which could lead to the direct use of Eq. 3 in a stabilized framework. These perspectives will be described in a forthcoming publication.

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