A flexible 3D finite element simulation of grain growth

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ABSTRACT. *The finite element approximation of a grain growth model based on the variational formulation of Lagrange equations is presented. The specific developments needed to implement it into the flexible finite element software Zset are detailed. These are mainly the topological transformations due to geometry changes, and the associated remeshing. Finally, the evolution of a typical microstructure of 20 grains is simulated.*

RÉSUMÉ. *L'approximation par éléments finis d'un modèle de croissance de grains basé sur une formulation variationnelle des équations de Lagrange est présentée. Les développements spécifiques pour l'implémentation de ce modèle dans le code de calcul aux éléments finis Zset sont détaillés. Il s'agit principalement des transformations topologiques liées au changement de géométrie, et du remaillage associé. Finalement, l'évolution d'une microstructure typique de 20 grains est simulée.*

KEYWORDS: *grain growth, grain boundary, finite elements, remeshing, topological transformations, Z-set.*

MOTS-CLÉS : *croissance de grain, joints de grain, éléments finis, remaillage, transformations topologiques, Zset.*

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1. Introduction

Polycrystalline materials are composed of grains, characterized by different crystallographic orientations. The transition region between two neighbouring grains is called a grain boundary. Due to local atomic disorder, grain boundaries possess a surface free energy γ, which depends on crystallographic misorientation. The microstructure thus evolves to reduce the total grain boundary free energy (Burke *et al.*, 1952). The motion of each point on the boundary is along the local normal, and the velocity v_n is proportional to the local curvature κ (Turnbull, 1951). The proportionality coefficient is the product of γ and the grain boundary mobility m, $v_n = m\gamma\kappa$. The mobility characterizes the velocity of atoms in crystallographic lattices.

Many numerical methods can be employed to simulate grain growth, in two or three dimensions. Stochastic approaches using Monte Carlo techniques (Anderson *et al.*, 1984; Ono *et al.*, 1999; Kim *et al.*, 2005) or cellular automata are very popular. However, they may lead to biased results due to anisotropic discretization (Weygand, 1998), and physical entities such as time, local geometry…, are not clearly defined. Phase field and Level Set techniques are also used (Russo *et al.*, 2000; Adalsteinsson *et al.*, 1995), although time consuming and thus difficult to apply to 3D analyses. Finally, Finite element based methods (Bergheau *et al.*, 2004) are used to simulate grain growth (Weygand *et al.*, 1998; Kuprat, 2000; Couturier *et al.*, 2003; Brakke, 1992; Wakai *et al.*, 2000). In this case, dedicated software are often developed.

The aim of this paper is to present an implementation of the grain growth equations into a commercially available finite element software Zset (Besson *et al.*, 1997). After giving the main physical equations, we focus on remeshing and topological transformations, which were specifically developed for this purpose. Finally, we give an application example, which validates the implementation. It should be noted here that the use of a commercial code facilitates further developments linked to crystal growth like recrystallization, influence of second phase particles…

2. Finite element method applied to grain growth

The grain evolution is modeled according to the Kawasaki assumptions (Kawasaki *et al.*, 1989; Sun *et al.*, 1997), which describe the movement of grain boundaries through a viscous fluid medium. The Kawasaki formulation states the free energy decrease is entirely dissipated during the grain boundary motion. It is based on two terms:

– a free energy $L = \int_S \gamma ds$

– a Rayleigh's dissipative potential $D = \int_S \frac{v_n^2}{2m} ds$

In these equations, integration is carried out over the total area of grain boundaries S. The two terms are used to write the variational formulation of the Lagrange equation for a structure composed of N nodes:

$$\sum_{i=1}^{N} \left(\frac{\partial D}{\partial \vec{v}_i} + \frac{\partial L}{\partial \vec{x}_i} \right) . \vec{x}_i^* = 0 \qquad [1]$$

In this equation, $\vec{x}_i$ is the current position of node i and $\vec{v}_i$ its velocity. The vector $\vec{x}_i^*$ is a virtual position associated with the node i.

All grain boundaries are meshed with 2D surface elements in 3D space. The mobility and the surface free energy are assumed to be constant in each element. Element quantities are built from the analytical computation of the partial derivatives in Equation [1]. The first term appears as a product between a viscosity matrix and a velocity vector, whereas the second acts as a loading vector.

Element viscosity matrix

A mobility m^e is defined for element e with surface S^e. The element viscosity term then reads:

$$\frac{\partial D^e}{\partial \vec{v}_i^e} = \int_{S^e} \frac{v_n}{m^e} \frac{\partial v_n}{\partial \vec{v}_i^e} ds \qquad [2]$$

In this equation, $\vec{v}_i^e$ is the velocity of node i in element e. In an isoparametric element, the velocity of each point can be written as a linear combination of the node velocities. It turns out that the normal velocity and its derivative with respect to $\vec{v}_i^e$ can be expressed as follows:

$$v_n = \sum_{i=1}^{k} N_i \vec{v}_i^e . \vec{n}^e \quad \text{and} \quad \frac{\partial v_n}{\partial \vec{v}_i} = N_i \vec{n}^e$$

where k is the number of nodes in element e, N_i the shape function associated with node i and $\vec{n}^e$ the local normal vector.

The above equations lead to the following element viscosity term:

$$\frac{\partial D^e}{\partial \vec{v}_i^e} = \sum_{j=1}^{k} \left[\int_{S^e} \frac{1}{m^e} N_i N_j \vec{n}^e \otimes \vec{n}^e ds \right] . \vec{v}_j^e \qquad [3]$$

where $\otimes$ denotes the tensorial product.

Finally, we can write Equation [3] for all nodes in the element e as a product of an element viscosity matrix $[A^e]$ and a vector $\{V^e\}$ containing the all nodal velocities:

$$\frac{\partial D^e}{\partial \vec{v}_i} = [A^e].\{V^e\} \qquad [4]$$

Element load vector

The derivative of element free energy $L^e = \gamma^e S^e$ with respect to the position $\vec{x}_i^e$ of node i in element e gives the element load $\vec{f}_i^e$:

$$\vec{f}_i^e = -\frac{\partial L^e}{\partial \vec{x}_i^e} = -\gamma^e \frac{\partial S^e}{\partial \vec{x}_i^e} \qquad [5]$$

The surface variation with respect to node position is derived in appendix A. Finally, Equation [5] is equivalent to:

$$\vec{f}_i^e = -\gamma^e \int_{S_0} \left[\left(\frac{\partial N_i}{\partial \eta} \vec{a}^\xi - \frac{\partial N_i}{\partial \xi} \vec{a}^\eta \right) \times \vec{n}^e \right] d\xi d\eta \qquad [6]$$

This allows the definition of an element load vector $\{F^e\}$, whose components are nodal load vectors $\vec{f}_i^e$.

Assembly

The above element terms are directly derived from geometry, mobility and surface free energy of the grain boundary. The corresponding vectors and matrices $\{V^e\}$, $\{F^e\}$ and $[A^e]$ are assembled respectively into two global vectors $\{V\}$ and $\{F\}$ and one viscosity matrix $[A]$. This typical task is assigned to the finite element code Zset, which has finally to solve the following global system:

$$[A].\{V\} = \{F\} \qquad [7]$$

Dof assignment and resolution

In the computation of element quantities, no assumptions are made on the kinematic conditions for grain boundaries displacement. However, nodal motion depends on its connectivity with grain boundaries and grains. If a node belongs to only one grain boundary, its displacement is collinear to the local normal vector. In this case, only one degree of freedom (dof) is affected to the node, namely its normal velocity. If the node is on a triple line (*i.e.* intersection between three grains), then its displacement is collinear to each grain boundary normal, and thus must be orthogonal to the

triple line. Two degrees of freedom are affected to this type of node. Lastly, if a node is a quadruple point (*i.e.* intersection between four grains), three degrees of freedom are assigned to it because there is no particular kinematic condition.

A substitution method is applied to incorporate these conditions in the system [7]. Classic implementations of this method require a reduction of the global matrix and a recalculation of common terms for each increment. Our approach avoids redundant calculations by taking into account node connectivity during the construction of the system. This allows us to directly obtain the reduced matrix. It should be noted here that, according to this approach, non dissipative motions, like displacement within the grain boundary, are automatically excluded.

An explicit time integration scheme is used to determine node displacement from velocity. The time step Δt is automatically adjusted to avoid too large displacements. Finally, to prevent singularities in the system for particular geometries (e.g. flat grain boundary), the diagonal terms of the viscosity matrix are slightly penalized by a factor p: $[A] \rightarrow [A] + p \max_{i,j} |A_{ij}|[I]$.

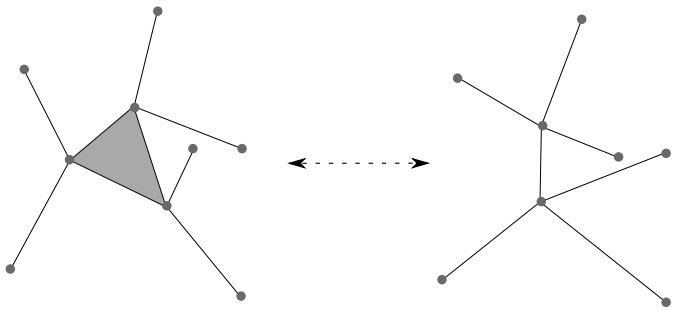
3. Topological transformations and remeshing

3.1. *Topological transformation*

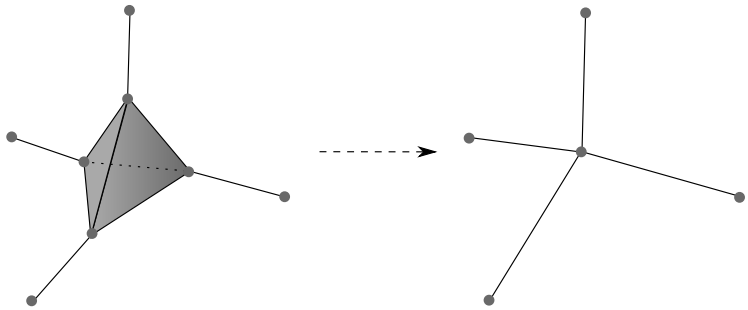
During grain growth, microstructure evolution involves geometrical transformations. Theses transformations follow some rules on grain connectivity (Kinderlehrer *et al.*, 2004; Wakai *et al.*, 2001). For example, a quadruple point must be connected to four grains, six grain boundaries and four triple lines. Two types of transformations (Figure 1) exist in three dimensions: a reversible transformation between a line and a grain boundary, and a grain shrinking to a quadruple point.

The transformation of an entity involves removing, creating and modifying geometrical objects such as triple lines, grain boundaries, grains and vertices. These topological transformations are treated before the remeshing step. A critical length l_c is used: a line with length smaller than l_c, a grain boundary with surface less than l_c^2, and a grain with volume less than l_c^3, are to be transformed. However, connectivity conditions are also used to determine if the transformation is allowed. For example, only triangular grain boundaries and tetrahedral grains can be transformed.

The transformation algorithm begins by transforming grains, followed by grain boundaries and lastly triple lines. This order is established because grains contain grain boundaries and grain boundaries contain lines. In addition, for each entity group, the transformation order is done from smallest to largest. In the case of a transforming grain, the grain is replaced by a quadruple point localized at the grain barycenter. For grain boundary transformation, the boundary face is converted into a triple line orthogonal to the boundary. The middle of the created triple line coincides with the barycenter of the transformed grain boundary. When a triple line has to be transformed, the above procedure is reversed.



(a) Reversible transformation of a grain boundary into a line



(b) Loss of grain

Figure 1. *Available topological transformations in 3D during grain growth*

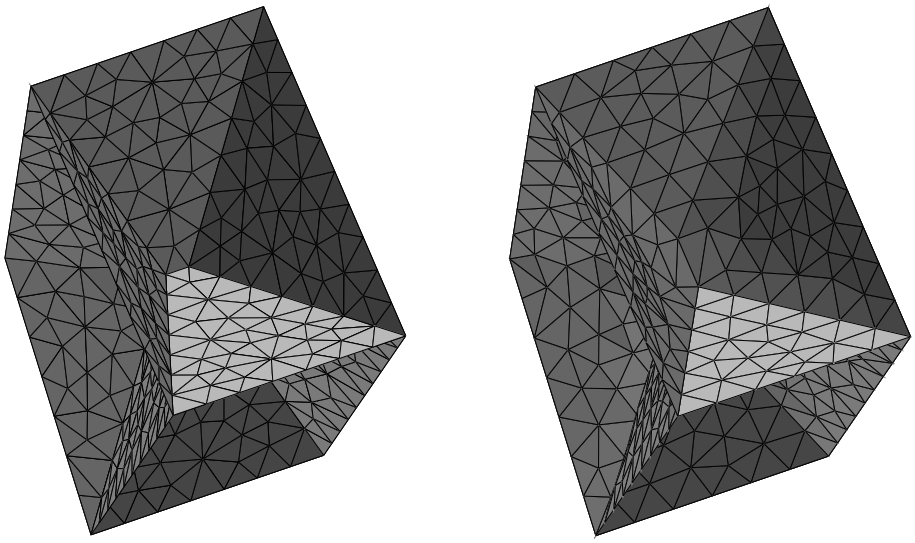
3.2. *Remeshing*

Evolution of the microstructure may require remeshing. This task is accomplished by coupling the free mesher GMSH[1] with meshing tools in Zset. Topological transformations automatically lead to remeshing. However, Remeshing can also be triggered by other criteria such as element quality and a predetermined remeshing frequency. The Figure 2 is an example of topological transformation followed by remeshing.

The first remeshing step treats triple lines as splines in order to prevent the apparition of non conform elements. Indeed, the connection between lines is easily guaranteed since intersections only exist at line extremities. The second step is the remeshing of grain boundaries. Each grain boundary is first projected onto its mean plane, then remeshed using Delaunay triangulation developped by J. R. Shewchuk

1. http://www.geuz.org/gmsh

(Shewchuk, 1996) and available in GMSH, and finally projected back to the initial geometry. The algorithm keeps node positions on the triple lines during meshing.



(a) Initial mesh (b) Final mesh

Figure 2. *Example of the transformation of a line: the horizontal central line is transformed into an orthogonal grain boundary*

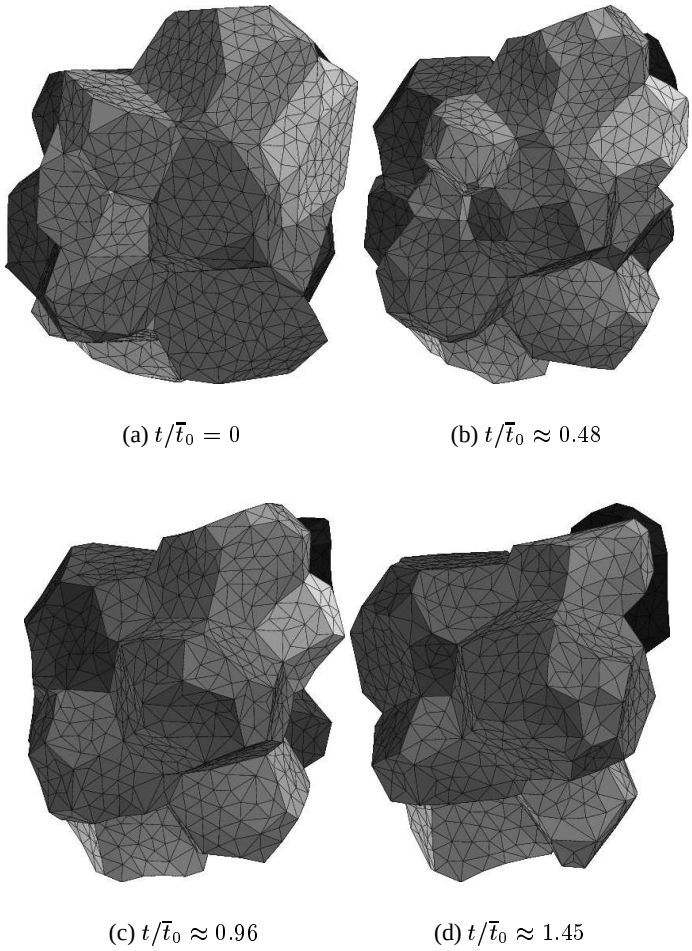
A direct method is used to project nodes and elements from the initial mesh to the mean plane and from the mean plane to the final mesh. This simple and efficient method is appropriated because of the low curvature of grain boundaries. Element and node groups are updated in the last step. Since grain interiors are empty, no further operation is requires for their remeshing.

No vectorial values are projected in the new mesh because the grains evolution is purely geometrical. In our case studies, structures have geometrical periodic conditions. A periodic mapping is performed to ensure that two periodic boundaries will have same mesh. This modification is done after a remeshing step.

4. An evolution example

A structure composed of 20 grains with geometrical periodic conditions was generated with a Voronoï tessellation. After a first transformation and remeshing step where all small objects are suppressed, the initial structure contained 283 vertices, 496 triples lines and 234 grain boundaries. A mobility m and a surface free energy

γ were selected for all grain boundaries. Based on the initial average grain boundary area $\overline{S}_0$, we defined an average energy $\overline{E}_0 = \gamma \overline{S}_0$ and a reference time $\overline{t} = \frac{\overline{S}_0}{m\gamma}$.



(a) $t/\overline{t}_0 = 0$ (b) $t/\overline{t}_0 \approx 0.48$

(c) $t/\overline{t}_0 \approx 0.96$ (d) $t/\overline{t}_0 \approx 1.45$

Figure 3. *Evolution of structure initialy composed of 20 grains*

The average length between two neighbouring nodes is chosen as 20% of a characteristic length l_m, and the critical length l_c is equal to 3% of this length. In this example, the characteristic length l_m is the cube root of the mean grain volume. The initial mesh had 4806 elements for 2350 degrees of freedom. It should be noted here that the dof assignment described above leads to a reduction of the number of degrees of freedom from 6705 to 2350.

The Figure 3 shows the evolution of the microstructure from 20 to 7 grains. It shows the initial, two intermediate and the final configurations. The computation was

stopped due to periodic constraints in the last configuration: the next transformation would have involved two periodic grain boundaries in the same grain. The Figure 4 gives the evolution of energy, number of vertices, lines, boundaries and grains, as a function of time. Two major phases of energy evolution can be observed in this figure. The first phase is characterized by a strong non-linear variation of the energy. During this phase, initially plane shaped grain boundaries acquire a curvature in order to respect tension equilibrium at triple lines. During the second phase, the energy evolution depend linearly on time. This can be explained by the fact that the majority of the movement is controlled by grain boundary curvature, and thus energy decrease is controlled by a decrease of area. The evolution of the number of geometrical objects shown in this figure illustrates the fact that the main topological evolutions are controlled by grain disappearance. The number of topological entities is nearly constant between two grain shrinkages.

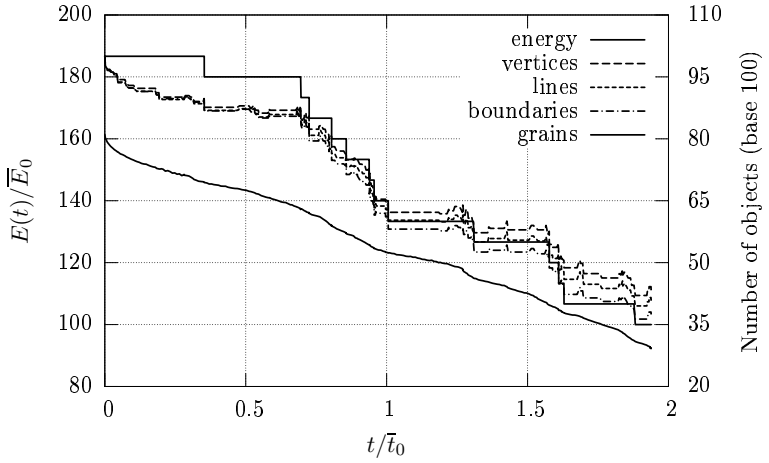


Figure 4. *Energy and topology evolution of structure initially composed of 20 grains*

5. Conclusion

This paper gives an application of the finite element method to the simulation of grain growth. This includes the development of dedicated tools to remesh and transform a representative structure of polycrystalline materials. Our mathematical formulation is independent of the number of nodes per element. This allows a large flexibility on the choice of element type. By design, the size of the global system is reduced to the geometrically necessary number of degrees of freedom, leading to a significant reduction in computational time. A numerical example illustrates the evolution of a representative elementary volume made of 20 grains. It successfully demonstrates the application of this method to 3D structures with complex and periodic topological transformations. It is now possible to simulate the evolution of microstructures composed of a few tens of grains. The Zset software with our library allows to study the

influence of physical parameters such as surface free energy, the mobility or the initial grain size distribution. However, some optimization in the algorithms is still required to reduce the remeshing time. More representative microstructures will be simulated. The obtained results will be analyzed in forthcoming papers.

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A. Surface variation with respect to node position

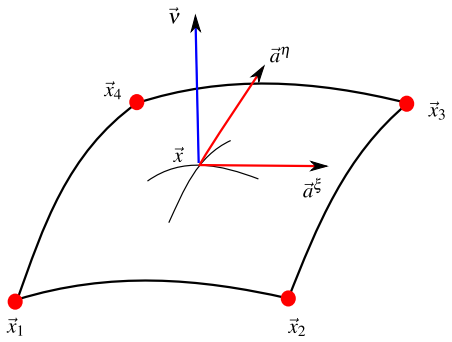

Figure 5. *Geometry of 2D element in a 3D space*

Calculations are performed in the reference element coordinate (ξ, η). The surface can be written as:

$$S^e = \int_{S_0} \|\vec{a}^{\xi} \times \vec{a}^{\eta}\| d\xi d\eta \quad \text{with} \begin{cases} \vec{a}^{\xi} & = \sum_{i=1}^{k} \frac{\partial N_i}{\partial \xi} \vec{x}_i^e \\ \vec{a}^{\eta} & = \sum_{i=1}^{k} \frac{\partial N_i}{\partial \eta} \vec{x}_i^e \end{cases}$$

where S_0 is the reference element area, and $\times$ denotes the cross product.

As shown in Figure 5, the vector $\vec{\nu}^e = \vec{a}^{\xi} \times \vec{a}^{\eta}$ is collinear to the element normal $\vec{n}^e$ at point $\vec{x}(\xi, \eta)$. The derivative of the element surface is obtained from the derivative of the norm of this vector:

$$\frac{\partial \|\vec{\nu}^e\|}{\partial \vec{x}_i^e} = \frac{1}{\|\vec{\nu}^e\|} \frac{\partial \vec{\nu}^e}{\partial \vec{x}_i^e} . \vec{\nu}^e = \frac{\partial \vec{\nu}^e}{\partial \vec{x}_i^e} . \vec{n}^e \qquad [8]$$

The $\vec{\nu}^e$ derivative can be divided in two terms:

$$\frac{\partial \vec{\nu}^e}{\partial \vec{x}_i^e} = \vec{a}^\xi \times \frac{\partial \vec{a}^\eta}{\partial \vec{x}_i^e} + \frac{\partial \vec{a}^\xi}{\partial \vec{x}_i^e} \times \vec{a}^\eta$$

The orientation tensor $\tilde{E}$ can be used to express the cross product: $\vec{a}^\xi \times \vec{a}^\eta = \vec{a}^\eta . \tilde{E} . \vec{a}^\xi$. This leads to:

$$\frac{\partial S^e}{\partial \vec{x}_i^e} = \frac{\partial \vec{\nu}^e}{\partial \vec{x}_i^e} . \vec{n}^e = \left(\frac{\partial N_i}{\partial \eta} \vec{a}^\xi - \frac{\partial N_i}{\partial \xi} \vec{a}^\eta \right) \times \vec{n}^e \qquad [9]$$