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High performance computing of sintering process at particle scale

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Abstract. *In this work, a numerical framework for the simulation of solid state sintering at particle scale is proposed. During the sintering process, different diffusion mechanisms, thermally activated, lead to the consolidation of the compact powder. The physics behind the different diffusion mechanisms is embedded into an Eulerian finite element framework, where the Level-Set method is used to cope with the microstructural evolution. Several results obtained with the proposed method are presented.*

Keywords: Sintering, diffusion phenomena, surface tension, finite elements, level-set method.

1 INTRODUCTION

Sintering is nowadays a very important industrial manufacturing process and is used for the fabrications of high performance materials and parts in a wide -and still growing- range of domains. Since the 50's a large amount of work has been dedicated to the theoretical and experimental study of this process. However, and despite this large amount of research, the understanding of the underlying physical phenomena is still a field of active research.
Diffusion phenomena are considered to be responsible for the microstructural evolution that takes place during sintering [6]. This work is mainly concerned by the surface, volume and grain boundary diffusions, which are considered to be the most important diffusion paths. Those diffusion mechanisms can be modeled by using the *Fick*'s first law, which establishes a relationship between the matter flux $\underline{j}$ and the gradient of the chemical potential μ :

$$\underline{j} = m\,\underline{\nabla \mu} \tag{1}$$

where m is the mobility associated with the diffusion path considered. According to the region of the compact powder (surface, volume, grain-boundary, etc.) that is being considered, the mobility and the chemical potential present different expressions, as it can be seen in Table 1.

Property		Diffusion path		
		Surface	Volume	Grain Boundary
Mobility	m	$D_s\delta_s/kT$	D_v/kT	$D_{gb}\delta_{gb}/kT$
Chemical potential	μ	$\Omega\gamma_{sf}\kappa$	$(1-f)\Omega\,p$	$\Omega\,\sigma_{nn}$

Table 1: Chemical potential and mobility for each diffusion path.

In table 1 D_s, D_v and D_{gb} are, respectively, the surface, volume and grain boundary diffusion coefficient, δ_s and δ_{gb} the thickness of the layer through which the material diffuses, k the Boltzmann's constant, T the absolute temperature, Ω the molar volume, κ the mean curvature, γ_{sf} the surface tension at solid/fluid interface, p the pressure, σ_{nn} the normal stress and f a constant of the material representing the ratio between the volume of a vacancy and the volume of an atom [5].

The mass flux leads to a deposition of mass at the surface and at the grain boundary. This deposition induces a normal velocity which should satisfy the following mass conservation equation:

$$v_n = -\Omega \underline{\nabla} \cdot \underline{j} \qquad \text{For surface and grain boundary diffusions} \tag{2}$$

$$v_n = \Omega \underline{j} \cdot \underline{n} \qquad \text{For volume diffusion} \tag{3}$$

where v_n is the normal velocity due to the mass flux $\underline{j}$ at a given point.
The previous equations are integrated into a continuum finite element Eulerian approach using the numerical strategy presented in Section 2. The results are presented in Section 3 and finally the conclusions and perspectives are discussed in Section 4.

2 NUMERICAL STRATEGY

All the simulations are performed by using the finite element method within an Eulerian framework. The computational domain, containing the compact powder as well as the surrounding medium, is discretized by simplexes. All the different fields are interpolated by piecewise linear continuous functions. The evolution of the particles are described by using the level-set method. One of the main advantages of using the level-set method is related to its capability of handling strong topological changes. Additionally it is possible to compute the outward normal ($\underline{n} \propto \partial\phi$) and the curvature ($\kappa \propto \partial^2\phi$) [2, 8, 9].
Considering the surface diffusion, the associated velocity (Table 1 and Equation (2)) is related to the fourth derivative of the level set function ϕ : $\underline{v^s} \propto \partial^2\kappa \propto \partial^4\phi$, which means that this velocity cannot be computed directly out of ϕ. For this reason a stabilized mixed formulation curvature / curvature surface laplacian has been developed in [1], where a linear velocity field $\underline{v^s}$ is obtained in such a way that the unphysical oscillations of the velocity and the curvature remain negligible.
Concerning the volume diffusion, according to Table 1 and Equation (3) the volume diffusion velocity is related to the gradient of the pressure and therefore the momentum conservation equation should be solved. At the particle scale, the effect of the surface tension cannot longer be considered as negligible. This surface tension, present at the interface between the particles and the surrounding medium, induces a discontinuity of the normal stress. The numerical resolution of this problem within an Eulerian approach leads to unphysical oscillations of the pressure field which does not allow to properly compute the volume diffusion velocity. For this reaon a numerical approach for the computation of the pressure field has been proposed in [9], where different methods for the computation of the surface tension term are proposed. Additionally, two different stabilization methods have been tested (P1+/P1 and a multiscale method) and different methods for the computation of the curvature have been studied. See [9] for further details concerning the proposed formulation and the different methods developed.
Even if the methods presented in [9] allow to obtain a pressure field with almost no oscillations, the pressure field is still discontinuous across the interface between the particles and the surrounding medium. For this reason, the computation of volume diffusion velocity is not straightforward. Two methods for the computation of this velocity field where developed [2, 8]. The main idea behind this velocity computation is to use the velocity over a layer slightly below the particles surface where the pressure field is continuous, and then this velocity is convected to the interface.

3 NUMERICAL RESULTS

The numerical simulation of the sintering process at the particle scale is an active and a very challenging research field. All the developments have been implemented in the finite element library *CimLib*. *CimLib* is a highly parallel C++ library developed at *Center for Material Forming* (Mines ParisTech, CNRS UMR 7635) by the team of Professor Coupez [3]. As in [2], the simulations presented in this work have been performed by using a mesh adaptation strategy aiming to obtain accurate results while keeping a “reasonable” number of mesh elements. The mesh is refined over a narrow band around the surface of the particles, the detailed strategy is presented in [7]. The element size is computed as a function of the second derivative of a primal variable such as a filtered level-set function or the pressure field. This approach has successfully been applied within the sintering simulation context by Bruchon et al. in [1, 2, 9].
The validation of numerical approaches dealing with the simulation of sintering at particle scale is very difficult since it is very complex to gather enough information from experimental setups. Therefore the most useful tool for the validation of numerical approaches consists in using theoretical models developed to study the growth of the

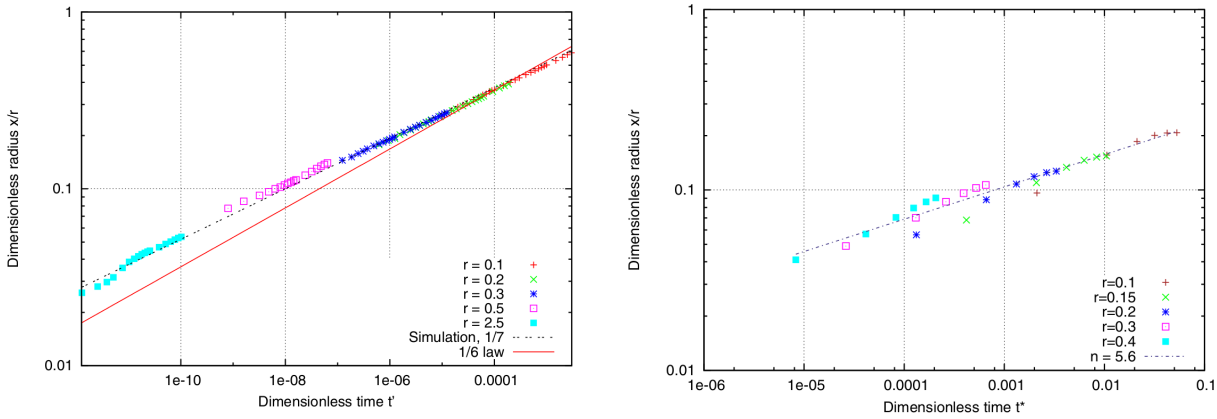
neck between two particles of the same size. Those models are mainly based on some geometrical hypotheses of the evolution of the neck and the particles, and in general can be written as follows:

$$\left(\frac{X(t)}{r}\right)^n = A\,t \tag{4}$$

$$\left(\frac{X(t)}{r}\right)^n = A't^* \tag{5}$$

where r is the radius of the particles, A and n are some parameters depending on the radius of the particles and the diffusion path being considered, and t is the time. Equation (4) is slightly modified in order to introduce the dimensionless time t^* in such a way that the evolution of the dimensionless neck (X/r) matches the same slope for different particle radii.

Figure 1a presents the evolution of the dimensionless radius X/r as a function of t^* during sintering by surface diffusion for particle radii between 0.1 and 2.5. According to Exner et al. [4], the exponent n on equation (5) ranges between 3 and 7 for surface diffusion, which is in agreement with the simulations performed here.



a. Surface diffusion. b. Volume diffusion.

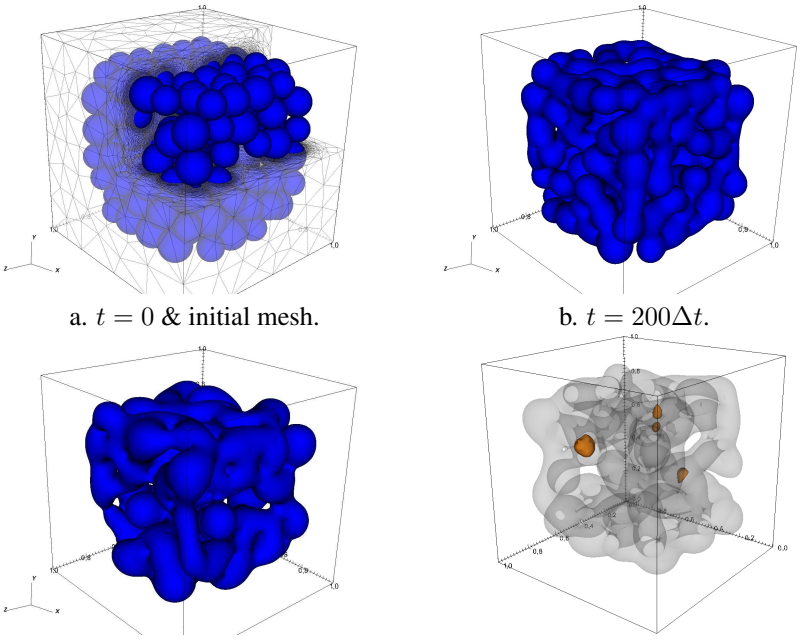
Figure 1: Dimensionless neck growth x/r vs. dimensionless time t^*. a. Surface diffusion and b. Volume diffusion.

In the same way, Figure 1b shows the kinetics of the growth of the dimensionless neck X/r by volume diffusion as a function of the dimensionless time t^* for particle radii ranging from 0.1 to 0.4. For volume diffusion, the exponent n in equation (5) ranges between 4 and 5 [4]. This time the best fitting curve in Figure 1b corresponds to an exponent n equal to 5.6 (referred to as "$n = 5.6$").

Surface and volume diffusions are coupled to simulate the sintering of a particles packing by these two diffusion mechanisms simultaneously. Figure 2 shows a sintering simulation by coupled volume and surface diffusions over a set of 154 particles with radii ranging from 0.0633 μm to 0.0797 μm. Figure 2a shows the initial particles packing as well as a cut of the refined mesh that is made up of about 2 millions nodes and about 11 millions tetrahedral elements.

The evolution of the structure is showed in Figures 2a to 2c. In the initial geometry (Figure 2a) particles are set to be quasi-tangent, and as diffusion takes place, the necks between the particles grow up to a point (Figure 2c) where the particles can not be distinguished any more. One of the most important advantages of the numerical approach developed in this work is related to its capability to supply information about the local state of the structure at any time step. As the structure evolves and after about 250 time steps ($t \approx 0.2$s) closed porosity appears. The structure keeps on evolving, and after $570\Delta t$ it is possible to identify multiple pores of different sizes inside the compact powder, as it can be seen in Figure 2d.

It is important to highlight that neither the mass nor the density of the particles change during the sintering process, therefore, the volume of the particles must remain constant. Considering the simulation shown in Figure 2, the change of total volume of the particles after 570 time steps is about 0.12%, which is negligible. This simulation involves 570 time steps and has been performed in about 245h by using a parallel computing strategy on 24 cores.



a. $t = 0$ & initial mesh. b. $t = 200\Delta t$.

c. $t = 570\Delta t$ d. Closed porosity ($t = 570\Delta t$).

Figure 2: Evolution of a particle packing through the time.

4 CONCLUSIONS

A numerical approach for the sintering simulation by surface and volume diffusion has been presented. The level-set framework adopted allows to handle all the different topological changes that can appear during sintering. The results obtained with the approach proposed are in agreement with the predictions given by the analytical models for the neck growth between two particles. A simple approach for the coupling of different diffusions mechanisms has been developed and the results seem to be in agreement with the kinetics observed in reality, but it is still very difficult to validate the results since there is no experimental data available for these two diffusion routes acting simultaneously. Regarding the sintering process, grain boundary diffusion is a very important diffusion mechanism and it should be included into the computational framework in order to obtain totally realistic sintering simulations. The numerical strategy proposed is suitable for the introduction of the grain boundary diffusion, however further developments are yet to be done. The global goal of this work is to simulate the sintering process of fully 3D granular packing, which would open huge perspectives regarding the digital materials design.

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