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# Coarsening kinetics and the envelope theorem

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ABSTRACT

The scaling properties of microstructural coarsening are studied by means of the envelope theorem, which connects structural features of the projections of an evolving size distribution function in size space and time space. This is made possible by extending the envelope treatment of [P. Streitenberger, D. Zöllner, Acta. Mater. 88 (2015) 334–345] to the time domain, thus establishing a new method of the scaling analysis. An important new finding is that there exists a duality between the pictures of the family of distribution functions in size and time space, according to which the envelope in size space equals to the location of the maxima in time space, and vice versa. For self-similar coarsening the scaling properties are completely reflected by the associated envelopes and maxima in the two complementary representations. The analysis of cumulative size distribution functions for the determination of the growth path of individual particles or grains is extended to the time space. The construction of the envelope curves both, in size space as well as in time space, allows a new and efficient numerical determination of the coarsening kinetics from large four-dimensional datasets of experiments and simulations. This is demonstrated by numerical studies of the results of Monte Carlo Potts model simulations of grain growth, which confirm and complement the analytical results.



## 1. Introduction

Coarsening is a ubiquitous and for technical applications important phenomenon of late-stage phase transformations, where diffusive transport processes lead to irreversible long-time changes of the microstructure of materials. The kinetics of such long-time changes is described by growth laws or evolution equations for typical length scales of the microstructure as, for example, the particle radius, grain size, interface curvature radius or other relevant structural lengths. An important quantity associated with these length scales is the size or probability distribution function characterizing the spatial and temporal statistical distribution of structural lengths in the material. The time dependence of the microstructure finds its prominent expression in the scaling properties of the size distribution function (SDF)—the subject of many studies in recent years. In a recent paper published in this journal [1] we have investigated the scaling properties of the SDF by considering one of its properties that had not been examined in this context before—namely the envelope curve of a set of temporally developing size distribution functions. This approach is different from the standard procedure of scaling [2–6] used by many studies in recent years, especially for Ostwald ripening (e.g. [7–10], and the literature within) and grain growth (e.g. [11–15], and the literature within). The approach does not replace the standard procedure but complements it by new aspects and results. In particular, for a self-similar family of size distribution functions, where the particle or grain size is treated as variable and the time as family parameter, we've shown in Ref. [1] that the envelope is uniquely determined by the growth exponent and an envelope parameter, where the latter is a new characteristic quantity of the coarsening system associated with the scaled size distribution function.

However, the envelope analysis in Ref. [1] was restricted to the size domain by considering the SDF only as a function of the size variable with the time as the family parameter. In the present paper, this restriction is removed by treating alternately size and time as equal variable and family parameters, respectively. This opens up the possibility to apply the envelope theorem, which puts the envelope analysis of coarsening started in Ref. [1] on a new and systematic basis. The envelope theorem connects the structural features of the different projections of the evolving size distribution function onto size space and time space, which are complementary to each other. As an important new finding it is shown that there

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exists a duality between the pictures of the family of distribution functions in size and time space according to which the envelope in size space equals to the location of the maxima in time space, and vice versa. For a self-similar family of size distribution functions, it will be shown that the scaling properties are completely reflected by the associated envelopes and maxima in the two complementary representations, which are uniquely determined by growth exponents, envelope parameters and length scales as characteristic quantities of the coarsening system.

The presented approach of the scaling analysis, which is based on the envelope theorem with size and time as full and equal variables, may also be of particular interest with regard to the new four-dimensional measurement methods, as phase-contrast x-ray tomography and others, which allow to follow the evolution of the 3-D microstructure in-situ as a function of time [16]. Such 4-D experiments (cf., e.g., [16,17]) and related modern fast simulations (cf., e.g., [17,18]) of coarsening processes require also new methods of transforming large four-dimensional datasets into appropriate physical observables describing the coarsening kinetics. The construction of the envelope curves both in size space as well as in time space allows a new and efficient numerical determination of the coarsening kinetics from a high density of simulation and experimental data, respectively. This is demonstrated by numerical studies of the results of Monte Carlo Potts model simulations of grain growth, which corroborate and complement the analytical results.

The paper is organized as follows. In chapter 2 the envelope theorem is presented in a form, which is particularly suitable for our task and is applied to the treatment of the size distribution function of the coarsening process in chapter 3. In the next chapter the general equations of the complementary envelopes in size and time space for self-similar sets of SDFs are derived and used to characterize their scaling properties. In chapter 5, the analysis of the cumulative SDF for determination of the individual growth path of particles or grains is extended to the time space allowing an efficient reconstruction of the growth law. Finally, chapter 6 is devoted to the numerical treatment of the coarsening kinetics from Monte Carlo Potts model simulation data by means of the envelope method corroborating the theoretical results.

## 2. The envelope theorem

Let us consider the regular function $z = z(p,q)$ of the two independent variables $p$ and $q$, which can be treated alternately as endogenous variable and exogenous parameter, respectively. Consider first the family of curves $z(p,q)$ vs. $p$ with $q$ as the exogenous family parameter. This family represents the projection of the function $z = z(p,q)$ onto the $z$-$p$-plane of a three-dimensional Cartesian $p$-$q$-$z$-coordinate system. The family has an envelope $z_e = z_e(p)$. That is the curve, which touches all members of the given family of curves, if the following set of equations are fulfilled [19]:

$$\Psi(z_e,p,q) = 0, \tag{1a}$$

$$\frac{\partial}{\partial q}\Psi(z_e,p,q) = 0, \tag{1b}$$

where

$$\Psi(z_e,p,q) = z_e - z(p,q) \tag{2}$$

is the family of $z(p,q)$ vs. $p$ in the implicit form with $z_e$, $p$ and $q$ as variables. Eqs. (1a) and (1b) follow from the property that the tangent at any given point of the envelope is also a tangent to the curve $z(p,q)$ vs. $p$ that passes through this point [19]. Since Eq. (1b) is equivalent to the requirement of an unconstraint maximum of $z(p,q)$ with respect to the parameter $q$,

$$\frac{\partial}{\partial q}z(p,q) = 0, \tag{3}$$

the solution of Eq. (1b) can be written in the form

$$q_m(p) = \max_q z(p,q), \tag{4}$$

where $q_m(p)$ is the corresponding maximizer. Eliminating by means of Eq. (4) the parameter $q$ in Eq. (1a) yields the following equation for the envelope of the family of curves $z(p,q)$ vs. $p$:

$$z_e(p) = z(p,q_m(p)). \tag{5}$$

Conversely, considering now the family $z(p,q)$ vs. $q$, where $p$ is treated as the family parameter and $q$ as the variable, which represents the projection of $z = z(p,q)$ onto the $z$-$q$-plane. The envelope of this set of curves follows according to Eq. (1b) from the solution of the unconstraint maximum condition

$$\frac{\partial}{\partial p}z(p,q) = 0 \tag{6}$$

given by the maximizer $p_m(q) = \max_p z(p,q)$, which inserted into Eq. (1a) yields

$$z_e(q) = z(p_m(q),q). \tag{7}$$

From Eqs. (1)–(7) the envelope theorem can be summarized as follows: The envelope of the family of curves $z(p,q)$ vs. $p$ represents the maxima of the family of curves defined by $z(p,q)$ vs. $q$, while conversely the envelope of this family, $z(p,q)$ vs. $q$, represents the maxima of the family $z(p,q)$ vs. $p$. With other words, the existence of an envelope of the projection of curves $z = z(p,q)$ onto the $z$-$p$-plane is associated with the existence of maxima of the projection of the same curves onto the $z$-$q$-plane. It is this duality between the pictures of the two families of the function, which is used in the following sections to describe the coarsening kinetics.

It should be mentioned at this point that the first order derivative of the envelopes Eqs. (5) and (7) is equal to the partial derivative of $z(p,q)$ with respect to $p$ and $q$, respectively,

$$\frac{dz_e(p)}{dp} = \left.\frac{\partial z(p,q)}{\partial p}\right|_{q=q_m(p)}, \qquad \frac{dz_e(q)}{dq} = \left.\frac{\partial z(p,q)}{\partial q}\right|_{p=p_m(q)}. \tag{8}$$

This is a direct consequence of the envelope conditions Eqs. (3) and (6) and is an alternative formulation of the envelope theorem, which is mainly used in producer and optimization theory of economics [20].

## 3. Size distribution functions and the envelope theorem

In order to demonstrate the application of the above described envelope theorem to the coarsening theory we consider at first the size distribution function $F(R,t)$, which is defined as usual in such a way that $dN = F(R,t)dR$ denotes the number of particles or grains per unit volume in the size interval $R$ and $R + dR$ at time $t$ (cf., e.g., [8,21]). Consequently, the total number of grains at time $t$ is given by

$$N(t) = \int_0^\infty F(R,t)dR. \tag{9}$$