



## Full length article

# Analytics on large microstructure datasets using two-point spatial correlations: Coarsening of dendritic structures



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## ABSTRACT

We extend the existing framework [1–4] of two-point spatial correlations to allow for the quantification, analyses, interpretation and visualization of microstructure coarsening measured by time-resolved X-ray computed tomography. Specifically, extensions were made to facilitate (i) the incorporation of nonconventional local attributes such as solid-liquid interface, interface curvature, and interface velocity in the description of the local state, and (ii) the efficient computation of bulk spatial correlations when the local attributes are sparsely defined only at special locations in the three-dimensional volume (e.g., solid-liquid interfaces). We have explored multiple variants of spatial correlations, including Pearson correlation coefficients and two-point joint probabilities, and examined their relative merits in providing useful new insights into the coarsening process. Algorithmic enhancements needed to carry out these computations on the large datasets produced in the experiments are also described. The results demonstrate the remarkable ability of these new protocols in automated (unbiased) capture of the four-fold symmetry of the dendritic microstructure, and in providing quantitative and reliable estimates of the characteristic lengths associated with the dendritic microstructure (including the secondary and tertiary dendrite arm spacings, secondary dendrite arm diameter, and the solute diffusion length). These estimated quantities agree well with the direct measurements from the microstructure. The results also indicate that interfaces with high negative and near-zero mean curvature ( $H$ ) have long range spatial auto-correlations, whereas all values of the interfacial normal velocity ( $V$ ) are only auto-correlated in the short range in space. For mid-range (positive) values of  $H$  and non-extreme values of  $V$ , the spatial distributions are essentially random.

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## 1. Introduction

Microstructures, which arise from inhomogeneities in composition or structure, are ubiquitous in materials ranging from condensed matters, to hydrodynamic systems, and to biological soft matters. Microstructures of materials can often have deterministic impacts on the properties of the materials on the macro-scale. Dendrites are one of the most frequently seen

microstructures during solidification of metals and alloys. The morphologies of these dendritic microstructures can strongly affect the physical, chemical and mechanical properties of the subsequent products of many metallurgical technologies, such as casting [5]. This makes the study of the evolution of dendritic microstructures a crucial part in predicting and controlling the properties of metallic materials.

However, like many other microstructures present in nature, dendrites are complex structures. They have irregular shapes, and are often highly interconnected. Moreover, as most real problems demand three-dimensional or even four-dimensional (including time) considerations, it makes it practically difficult to visualize the data, and even more so to analyze it. As a result, two-dimensional sections of the data are usually made in order to obtain salient

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attributes of the three-dimensional dataset, such as the secondary and tertiary arm spacings ( $\lambda_2, \lambda_3$ ) of the dendrite [6]. As the system size grows larger, the dataset may become unwieldy to handle as a whole, and hence data processing and interpretation must be done in a piece by piece manner. This adds significantly to the challenges in arriving at meaningful global (bulk) descriptors of the microstructure that are also of high value in correlating to its performance characteristics.

A number of statistical quantities have been defined to serve as microstructure descriptors. For example, the interface shape distribution (ISD) [7–9] and the interface normal distribution (IND) [10–15] have been used to capture the statistical distribution of the shapes and orientations of the interface areal elements. However, these descriptors capture the desired information in a grossly simplified manner by treating each measurement at a randomly selected point in the microstructure as a completely independent sample (generally referred as one-point statistics). In other words, they do not capture information on the spatial distribution of the selected features in a representative domain (volume) of the microstructure. Genau et al. [8,16,17] have developed a method that captures the two-point spatial correlations between the interface attributes of interest. However, their method only computed angularly averaged spatial correlations (i.e., the spatial correlations were not resolved directionally).

A rigorous statistical framework that can capture efficiently and systematically the directionally resolved higher-order microstructural features (i.e., spatial correlations) is necessary for aggregating and curating the core materials knowledge in the form of process-structure-property (PSP) linkages [18,19]. Towards this end, we develop and demonstrate for the first time, a new and efficient set of protocols for the computationally efficient quantification of the spatial correlations between microstructural features defined on the interfaces. These new protocols are built on the existing framework of two-point statistics that have been used previously to quantify the spatial correlations between local attributes defined in the bulk of the microstructure (as opposed to the attributes defined only on the interfaces in this work). Additionally, the new protocols are demonstrated using a scalable algorithm suitable for large and high-dimensional datasets.

## 2. Current framework for microstructure quantification

### 2.1. Microstructure function

We start with a concise summary of the currently employed framework for microstructure quantification, which starts with a definition of the microstructure function denoted as [20]

$$m(u, x), \quad u \in \mathbb{U}, \quad x \in \mathbb{X}. \quad (1)$$

In this notation,  $x$  denotes a spatial point in the microstructure volume being studied,  $u$  denotes a potential local state (i.e., a local attribute of interest in the microstructure that could be defined using a combination of tensorial quantities of different ranks, e.g. interfacial curvature, interfacial velocity, etc.) that may or may not be found at any selected spatial point in the microstructure volume,  $\mathbb{U}$  denotes the local state space (the complete set of all local states  $u$  relevant to the phenomenon being studied), and  $\mathbb{X}$  denotes the spatial domain over which the microstructure is being defined (the complete set of all possible locations,  $x$ ). With these definitions,  $m(u, x)$  is the probability density associated with finding local state  $u$  at the spatial location  $x$ . Although this function is fully capable of mapping over continuous spaces, any practical implementation on either experimental or simulation datasets demands the adoption of one of the many discretized variants of this function. It is also

noted that the discretized versions are also better suited for computer programming. We examine next the details of these discretized variants.

It is assumed that the microstructure volume of interest occupies a rectangular parallelepiped space  $\mathbb{X}$  that can be uniformly tessellated into spatial bins (i.e., voxels)  $X_s \in \mathbb{X}$ , where  $s = 1, 2, \dots$  is the integer index enumerating the spatial bins. Note that  $s$  may be a vector in a high-dimensional space. In other words, for a three-dimensional volume, one might use a vector  $s = (s_1, s_2, s_3)$  to index each spatial bin  $X_s$  in the microstructure volume, where  $s_1, s_2$ , and  $s_3$  take integer values. In a similar way, we could tessellate the local state space  $\mathbb{U}$  in some suitable manner to identify discretized bins in the local state space. In other words, we can discretize  $\mathbb{U}$  into bins  $U_n \in \mathbb{U}$ , with  $n = 1, 2, \dots$  (could also be a vector index if needed) enumerating these local state bins. Building on the discretized representations, we can now invoke a discretized representation for the microstructure function as  $m[n, s]$ , which denotes the volume fraction in the spatial bin  $X_s$  occupied by local states identified by  $U_n$ . Specifically,

$$m[n, s] = \int_{u \in U_n} \int_{x \in X_s} m(u, x) dx du. \quad (2)$$

With this definition, it is easy to see that, at each spatial bin  $X_s$ , the volume fractions of all local states  $U_n$  have values between 0 and 1, and they sum up to 1. In mathematical form,

$$\sum_n m[n, s] = 1, \quad 0 \leq m[n, s] \leq 1 \quad \forall n. \quad (3)$$

When the discretization in space is fine enough, each spatial bin  $X_s$  will only contain local states belonging to one local state bin  $U_n$ . In that case, the microstructure function  $m[n, s]$  will be a binary function taking values of 0 or 1. In other words,

$$m[n, s] = \begin{cases} 1, & u(x) \in U_n \quad \forall x \in X_s \\ 0, & \text{otherwise} \end{cases} \quad (4)$$

It should be noted that the binning of the local state space occurs quite naturally in some situations. For example, if one is dealing with a multiphase material system, then each phase can be simply assigned a different value of  $n$ . In particular, in a two phase system,  $n$  could take on values of 0 and 1.

### 2.2. Two-point spatial correlations

Only the relative placement of the local states contains high value information in a given microstructure, as it captures effectively the statistical information on the neighborhoods encountered in the microstructure. This information can be captured systematically in a hierarchical set of microstructure descriptors called  $n$ -point spatial correlations (or  $n$ -point statistics) [1–3,18,21–23]. The most basic of these capturing morphological information come in the form of two-point spatial correlations (often referred simply as two-point statistics). The two-point spatial correlation of local states  $u$  and  $u'$  is mathematically expressed as [24]

$$f(u, u'|r) = \frac{1}{|\Omega(r)|} \int_{x \in \Omega(r)} m(u, x) m(u', x + r) dx, \quad (5)$$

where  $\Omega(r)$  is the ( $r$ -dependent) subset of the microstructure domain that allows evaluation of both  $m(u, x)$  and  $m(u', x + r)$ , and  $|\Omega(r)|$  is a measure of the size of  $\Omega(r)$  (i.e. the total volume occupied by  $\Omega(r)$ ).  $f(u, u'|r)$  captures the joint probability density associated

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