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Topology-faithful nonparametric estimation and tracking of bulk interface networks

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ABSTRACT

The main focus of this paper is a nonparametric filtering technique for the estimation of interface geometry in bulk materials obtainable from modern imaging measurements. The filtering methodology relies on an assumed hierarchy of topological features present in a typical interface network, such as foam interfaces and grain boundary networks in polycrystalline materials. Each type of topological feature is treated in order of rank in the hierarchy, with the lower-level feature being filtered subject to the positional constraints imposed by the higher-level features. Such a scheme is an alternative to existing surface smoothing/estimation techniques in microstructural materials science, in which the explicit treatment of different elements of the network topology is absent, or at best arbitrarily parameterized. We describe the ramifications of this technique in the usual microstructural applications in which the computation of important physical quantities is predicated on the precise estimation of the interface features. As an additional application, we describe a novel front-tracking algorithm for quantifying the transport of such interfaces.

1. Introduction

The morphology of surfaces and interfaces has garnered great interest in many fields of scientific and engineering research. Such studies have implications in applied physics, materials science, biology, pharmacology, chemical engineering and computer vision [1–3]. A vast part of this research is predicated on the proper imaging of interfaces in the medium of interest. Interfacial networks are composed of two-dimensional, possibly curved interfaces that separate two distinct regions of homogeneous matter, such as gas in bubble foams, or phases or crystalline orientations in solids. We use in this paper language relevant to interfaces in polycrystalline materials but the methods described are equally applicable in other fields by straightforward adaptation of the terminology. The three dimensional entities with more or less uniform crystalline characteristics henceforth will be referred to as 'grains'.

A particular type of grain boundary can be specified by five parameters on the mesoscale where 'meso-' refers to a length scale that is large compared to interatomic distances but small compared to a typical grain size. Among the several possible parameterizations; we choose the set of three specifying the relative crystal orientations of the grains, and two specifying the local normal direction relative to the crystal axes in one of the grains. The normal direction in the other crystal frame can be computed from these five parameters. This parameterization ignores a microscopic relative translation on the atomic scale and thereby atomic-level faceting of the interface, a feature addressed explicitly in molecular statics and dynamics simulations. The set of these five parameters is said to specify the grain boundary character [4–7]. Note that the character between two grains can vary over the two-dimensional boundary between them because, while the misorientation is fixed, the local normal typically varies significantly over a curved grain surface. Similar characterizations can be made for triple lines (two misorientations and a tangent line) and quad points (three misorientations). Finally, we note that crystal symmetry is typically exploited to reduce these specifications to unique 'fundamental zones' that span physically distinct ranges of orientations or misorientations.

Whether from a basic or applied science viewpoint, the importance of characterizing grain boundaries in this manner cannot be overstated. In polycrystalline materials, the local interfacial energy density and mobility are known to be sensitive to the five grain boundary parameters at each location [8,9,7,10]. It also informs applications like grain boundary engineering whose eventual goal is to precisely manipulate bulk material properties through the

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tuning of the grain boundary character distributions [11,12,4,13]. Further, it is well-known that the topological elements of a grain boundary network like triple junctions and quad points are hotbeds of activity with respect to precipitate diffusion [14–16] and strain accumulation [17,18]. Real grain boundary networks are usually the starting point for atomistic and continuum simulations of microstructure evolution, the physics of which is most difficult to model at triple lines and quad points.

All these applications are predicated upon measurements of the various topological features of a grain boundary network, which are inevitably subject to noise, whether through experimental resolution or image gridding. Given the generally accepted assumption of mesoscopically smooth interfaces, this necessitates the use of a smoothing estimator prior to any further analysis. Owing to the diverse roles of topological elements such as triple lines and quad points in microstructure phenomenology, an important motivation for this novel filtering technique and other recent ones [19] is to give them their due importance through explicit treatment.

Other factors motivating this work are:

- Unlike voxelized images of most everyday objects, there exists no general intuition for the shape of a grain in a sample, and therefore a grain boundary. In the former case, iterative smoothing algorithms such as Laplace and Taubin smoothing [20] yield an acceptable result that is partially helped along by the user's advance knowledge of the object in question. However these methods can suffer from under- or over-smoothing if the number of iterations or step size are not chosen properly.
- Explicit modeling techniques [21] more often than not belie the sheer variety in the observed structure of grain boundaries and network topologies.
- Existing nonparametric techniques [22] require the use of a smoothing window of a user-defined size.

The methodology described here internally optimizes a compromise between fidelity to the input data points and a constrained Laplacian smoothing. An objective function is minimized with respect to this compromise. The algorithm requires no user input in terms of filter parameters, only that the connectivity of the nodes be specified in advance, in the form of a graph. We distinguish the type of kernel resulting from graph-connectedness to a given node from a fixed-size window centered on that node since the former, which we rely upon, does not take into consideration the physical distance between neighboring nodes, and only keeps track of the connectivity.

While the grains in polycrystals can take on essentially arbitrary shapes, the topological features typically encountered, and which are explicitly dealt with here, can be demonstrated with children's (or adult's) building blocks. Place two, say, cubic blocks (grains) together on a surface with edges aligned (blocks 1 and 2). The two blocks meet at a two dimensional interface (grain boundary 1-2). Now place a third block on the same surface so that it forms boundaries with both blocks 1 and 2 (boundaries 1-3 and 2-3). These boundaries meet at triple line 1-2-3. Now, place block 4 on top of these three so as to form boundaries with all three below (boundaries 1-4, 2-4, and 3-4). One now has new triple lines 1-2-4, 1-3-4, and 2-3-4. Furthermore, triple line 1-2-3 now terminates at a quadruple point, 1-2-3-4, where all four grains meet. Unless one makes special arrangements to again align edges, these are the topological features that will characterize an extended group of similarly stacked blocks.

In this paper, all line junctions of interfaces in a network are referred to by the generic term 'triple line' in allusion to the fact that energetically stable junctions in 3D are shared between exactly three interfaces. The incidental existence of a 'n-tuple line' in a polycrystalline material where $n > 3$ interfaces intersect is known to be energetically unstable, forcing the interface topology to deform to a lower energy configuration [23,24]. Likewise, a node of termination of n' such triple lines is referred to as a 'quad point' irrespective of the value of n', alluding to the fact that $n' = 4$ is the physically stable configuration in bulk materials. The mathematical machinery developed in this paper is as appropriate for contrived interface networks that deviate from this topological rule as for digital images of real bulk microstructure, in which these deviations are almost never observed.

We first describe the topological hierarchy in general terms and then address the interface estimation procedure, which is a modification of Laplacian smoothing of a set of meshed surface points. This is followed by application to pixelated versions of easily parameterized geometric primitives, in particular circles, spheres and cylinders. Post-smoothing errors are quantified in terms of estimated sizes of these primitives as well as estimated normals for specific geometries. We then address specific cases of interest in mesoscale materials science: two- and three-dimensional grain boundary networks. The former finds relevance in the study of thin films and the latter in that of bulk material behavior (most prominently in the computation of grain boundary character distribution plots, a common characterization of materials microstructure). We demonstrate how the user is freed from the largely intuitive choices of smoothing parameters that is characteristic of iterative or windowed techniques. We then describe in some detail the applicability to finite element methods in materials science as well as interface velocity estimation, which is made possible with data obtained from modern non-destructive imaging techniques. A new nonparametric algorithm to achieve the latter is described.

2. General formalism

Consider a set of N noisy sample points $\mathbb{X} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}$ in $\mathcal{D}$-dimensional Cartesian coordinates that sample an imaged grain boundary. A subset $\mathbb{X}_S \subset \mathbb{X}$ of these points is tagged as a 'perimeter' that samples the edges of the grain boundary feature, with the same grid resolution as the interior. For example, in three dimensions, these points could represent a two-dimensional boundary including all edge points, or a one-dimensional triple line with its terminating quad points. We also specify a connectivity for every point in $\mathbb{X}$, described by a graph Laplacian matrix $L^{(0)}$:

$$L^{(0)}_{ij} = \begin{cases} N(i) & \text{If } i = j \\ -I(j;i) & \text{if } i \neq j \end{cases} \tag{1}$$

where $N(i)$ is the number of points connected to $\boldsymbol{x}_i$ and $I(j;i)$ is an indicator function that is 1 if point j is connected to point i and 0 otherwise. We require that all $\boldsymbol{x}_i \in \mathbb{X}_S$ remain constrained to their initial positions while the $\boldsymbol{x}_i \in \mathbb{X} - \mathbb{X}_S$ are smoothed, all the while adhering to the same node connectivity. We denote this smoothing operation by $SMOOTH(\mathbb{X}, \mathbb{X}_S)$.

As a general rule, we enter points $\boldsymbol{x}_i$ into our hierarchy such that all $\boldsymbol{x}_i \in \mathbb{X}_S$ are at one level above all $\boldsymbol{x}_i \in \mathbb{X} - \mathbb{X}_S$. Notationally the hierarchy level or 'rank' is denoted by a function $H(\boldsymbol{x}_i)$ such that $H(\mathbb{X}_S) = 1 + H(\mathbb{X} - \mathbb{X}_S)$; the sole purpose of H being to distinguish points of different ranks and the actual returned value being a matter of choice.

Fig. 1 visualizes two common systems with different hierarchy sizes. Keeping in mind that in an interface network in $\mathcal{D}$-dimensional space there exist in general objects of dimensionality $d = 0, 1, \ldots, \mathcal{D} - 1$, we define the rank function $H(\boldsymbol{x}_i) \equiv \mathcal{D} - d$, where d corresponds to the lowest-dimensional object in the network to which $\boldsymbol{x}_i$ belongs. For example, a triple point in a