BACHELOR

Reconstructing single phase polycrystalline structures using linear interpolation of modified signed distance fields

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Reconstructing single phase polycrystalline structures using linear interpolation of modified signed distance fields

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Contents

1 Introduction **1**

2 Problem description **3**
2.1 Provided EBSD data . . . 3
2.2 Triple junctions . . . 3
2.3 Signed distance functions . . . 3
2.4 Test case construction . . . 5
2.5 Linear interpolation . . . 6
2.6 Interpolation of the test cases . . . 8

3 Interpolation of Voronoi-like SDFs **10**
3.1 Voronoi-like fields . . . 10
3.2 Voronoi interpolation . . . 12
3.3 Conclusion . . . 13

4 Extrapolating lines **14**
4.1 SDF formulation and methodology . . . 14
4.2 Results . . . 15

5 Adapting extrapolated line structures to complex curvatures **18**
5.1 Adjusted methodology using polygon selection . . . 18
5.2 Interpolation results . . . 20
5.3 Less extreme curvature test case . . . 22
5.4 Discussion . . . 23

6 Conclusion **24**

7 Recommendations **24**
7.1 Aligning interpolation . . . 24
7.2 Shape morphing via hierarchical interpolation . . . 24
7.3 Commercial software and other scientific fields . . . 24

1 Introduction

Advanced materials often owe their good macroscopic properties to their complex heterogeneous microstructures. Being able to model the complex microstructure of a material could allow for more realistic, in-depth analysis to optimize the design and manufacturing of advanced materials. Several materials such as metals fundamentally consist of crystallographic grains, of which multiple phases can exist. The performance of the material owe their properties to the grain size, structure and orientation [*Crystalline material grain structure* 2020].

To be able to model such grain structures, experimental data has been collected in the form of Electron Backscatter Diffraction (EBSD) maps. These maps are based on the top and bottom surface of a thin experimental sample of material. The thin samples are intended to make the top and bottom surface look relatively similar, making it easier to approximate what is between the top and bottom layers. An example of EBSD maps is shown in Figure 1.

Figure 1: EBSD maps of the top (left) and bottom (right) layers

The focus of this project is to determine and to create a full 3D micro-structure based on the data of the top and bottom surfaces. The final 3D geometry can serve as an input for FEM simulations. The simulation results can directly be compared to experiments, and be used as a more accurate representation of a material.

Previous methods to determine the unknown sub-surface grain structure were attempted, though found to contain critical errors and anomalies [Verheijen 2022]. Explicit and implicit descriptions were previously used to attempt to fill in the space between the two layers of grain boundaries. Explicit descriptions of geometry refer to defining a region to a set of points (e.g. a square formed by two corner points, (2,2) to (4,4)), whereas an implicit description describes the geometry using an isocontour of some function [Antman, Marsden, and Sirovich 2003].

The geometric descriptions used in former research required multiple exceptions to be able to define the correct grain boundaries. The implicit description of geometry had previously shown to be most promising of the two types of geometric descriptions [Verheijen 2022]. Therefore, the goal of this project is to further develop the use of implicit descriptions whilst avoiding the exceptions and problems that previous methods ran into.

The implicit description is defined by a Signed Distance Field/Function (SDF). A function is made so that it returns a distance to the nearest part of a specific boundary, from a pre-defined point [Antman, Marsden, and Sirovich 2003]. The grain boundaries of the top and bottom serve as a reference for linear interpolation to obtain an accurate 3D representation of each grain. Each grain can then be represented in the form of a level set function, that describes the position and the boundary. Furthermore, some small grains are only present on one side of the sample. It is desirable that the algorithm handles this problem in a systematic way.

For this report, the first sections detail the provided data, new geometry theory and problems that relate to the selected new geometry theory. After discussing these problems, a first novel solution is discussed, known as the "voronoi-like" signed distance fields. These "voronoi-like" fields were a first step to understand the necessary improvements to create the proposed solution, discussed in Chapter 5. The proposed solution referred to as both Extrapolating lines and as "Infinitely-long" lines utilizes modified signed distance fields that resolves the problems found in previous work. The final chapter of this report extends the solution to complex geometry, where the solution was found to be functional, with certain limitations when considering too severe boundary curvatures.

2 Problem description

2.1 Provided EBSD data

The basis of this project is to reconstruct the layers between the top and bottom surface of a thin material samples. By using thin sample it can be ensured that the top and bottom grain structures appear similarly, with no hidden grains found between the two surfaces. Twin-jet electropolishing [*TEM Specimen Preparation* 2022] [Zaki, Gilchrist, and Zhang 2022] is used to thin the material until the grain structures closely resemble each other on either surface. Afterwards, the electron back scatter diffraction (EBSD) maps are created, scanning the grain structures of the top and bottom surfaces. The grain structure along with its size and specific boundaries can be represented visually after using data processing techniques [*Displaying EBSD Data* 2022]. An example of an EBSD map is shown in Figure 1.

2.2 Triple junctions

In a typical grain structure (shown alternatively in Figure 2), multiple grains are connected with each other. The regions between grains are referred to as the grain boundaries. An important feature of the grain boundaries is the triple junction, where three neighboring grains meet each other. The modelling triple junction is of key importance, as it was found to be a reoccurring issue in previous works [Verheijen 2022].

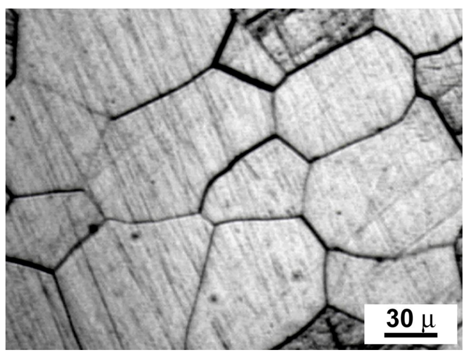


Figure 2: Polycrystalline grain structure [Pleshakov 2008]

Therefore a large focus is held in the triple junction interactions. Additionally, within each layer of EBSD maps, various shapes, angles and curvatures may exist around the triple junction. These will need to be accurately modelled to describe the 3D structure of the grains in crystalline materials.

2.3 Signed distance functions

Building on from previous work [Verheijen 2022], implicit geometry such as signed distance fields (SDFs) are sought after to avoid exceptions in calculating the middle layers.

For any given point, a SDF function will return a positive or negative distance to the nearest part of the specific boundary. If the point is found outside of the contour, it is a positive distance away. If it is negative, it will be inside of the contour. For points found on the contour, the value is zero. These SDF functions can be created for a variety of polygon shapes. An example of a square SDF is provided in Figure 3.

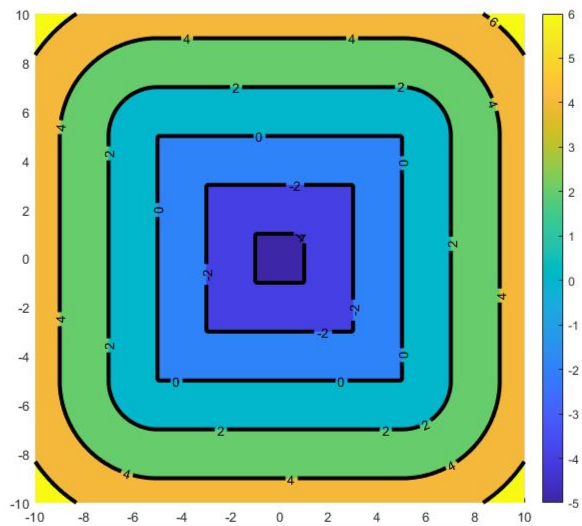


Figure 3: Visualization of a basic square SDF

In Figure 3, the square is defined by a zero contour. Points outside the contour are a positive distance away, whilst inside points being at a negative distance from the contour.

With the introduction of a new implicit geometry, several different manipulations exist that allow combining SDF's [Ronja 2018]. The main three operators are as follows:

$$DF_{Union} = min(DF_1, DF_2) \tag{1}$$

$$DF_{Subtract} = max(-DF_1, DF_2) \tag{2}$$

$$DF_{Intersect} = max(DF_1, DF_2) \tag{3}$$

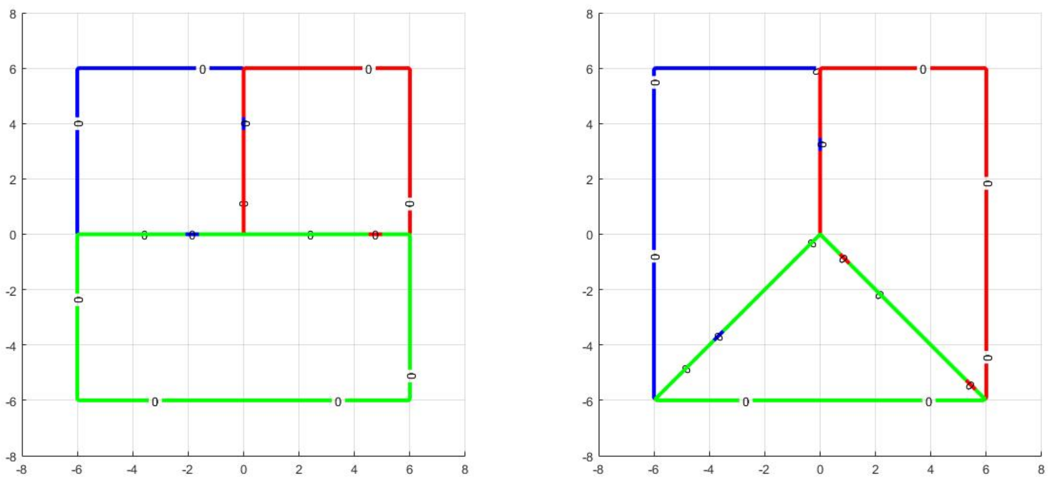
The union operator allows "adding" several fields together, while the subtract operator removes a specified field from another. The intersect operator takes any overlapping region of two fields. All three boolean operators are especially useful when manipulating SDFs. The union operator provides the most utility in various situations, as combining nearby shapes is a crucial step in the various methods discussed later in this report.

2.4 Test case construction

To test and evaluate the accuracy of various interpolation solutions a number of test cases with elementary microstructures were created. An emphasis is placed on testing a solution on a simpler case, facilitating the development of a solution that also applies for a complex geometry. When successful, the complexity can be increased to further analyze for any limitations with the proposed method.

For all test cases, a default arrangement was created, with the opposite layer being the same arrangement with different levels of modification. Complexity is introduced via increasing the shift or angle change of the grains, with a combination of both at the end of testing. If no failure occurs, the proposed solution is effective and the next test case used.

The most basic test case consists of a triple junction between three square grains, representing a 90 degree angle. Using the rectangle SDF function [Quilez n.d.], three rectangles are placed accordingly, as shown in Figure 4a.



(a) Basic triple junction test case

(b) Varying angle test case

Figure 4: Triple junction test cases

The first test case is simplified by eliminating the varying angles that could exist in the triple junction. Naturally, the next test case (show in Figure 4b) is constructed such that these angles are present. Each grain boundary can be modified to connect at the triple junction at varying angles.

2.5 Linear interpolation

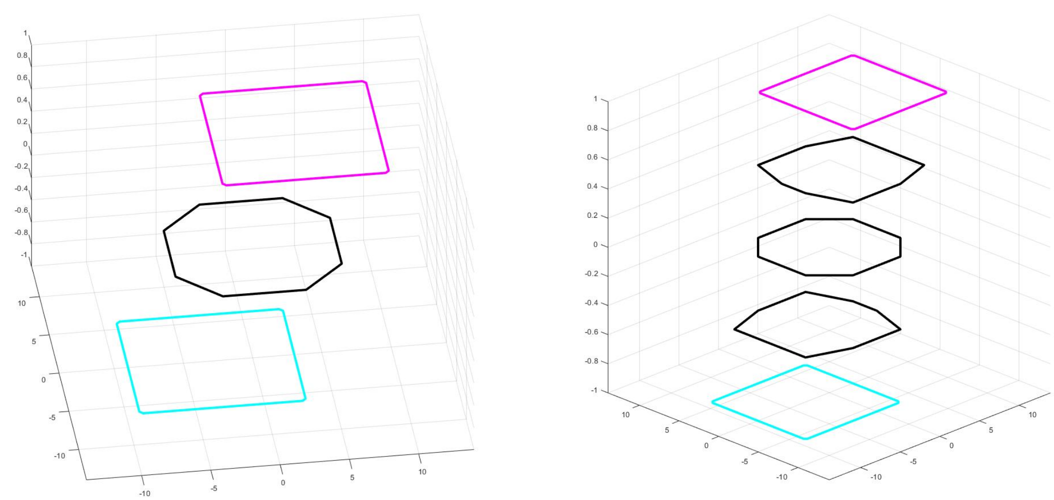
Linear interpolation is used to define new data points using the coordinates of two reference points. In the case of SDF's, the same applies for implicit geometry fields. The following equation is used for interpolation:

$$DF_{volume}(x,y,z) = (\frac{1}{2} + \frac{z}{h})DF_{top}(x,y) + (\frac{1}{2} - \frac{z}{h})DF_{bottom}(x,y) \quad (4)$$

where z denotes the height ($-\frac{1}{2}h$ bottom layer, 0 halfway, $\frac{1}{2}h$ top layer), h denotes the thickness of the material, and DF denotes the signed distance field of the respective top or bottom layer.

Before applying any interpolation solution to the test cases, it is important to understand the basic principles and some limitations of standard linear interpolation of an SDF field.

When applying linear interpolation to SDFs, the shape of one SDF will morph to the other. The generated SDF of a middle layer assigns more weight to the layer it is closest too. As an example, the interpolation is applied to two squares, slightly offset from each other in Figure 5.



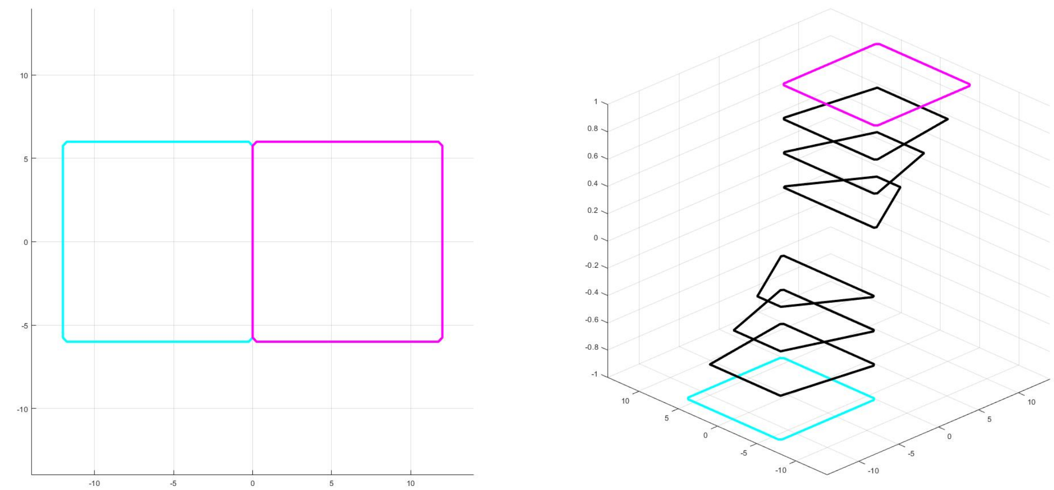
(a) Linear interpolated result at height zero (black)

(b) Multi-layer plot of interpolating a minor shift

Figure 5: Mesh refinement validation

The zero contour clearly morphs from one shape to the other, while losing the corners of the original shape (See Figure 5). The loss of corners is the first major issue found with interpolating shifted SDFs, which was outlined in previous work [Verheijen 2022].

The complication of corners being lost in the middle layers is more dramatic in larger shifts. If the shift is too large, causing no overlap, an even more detrimental result arises as illustrated in Figure 6b.



(a) Top view of top and bottom grain

(b) Multi-layer plot of interpolating a translated geometry

Figure 6: Mesh refinement validation

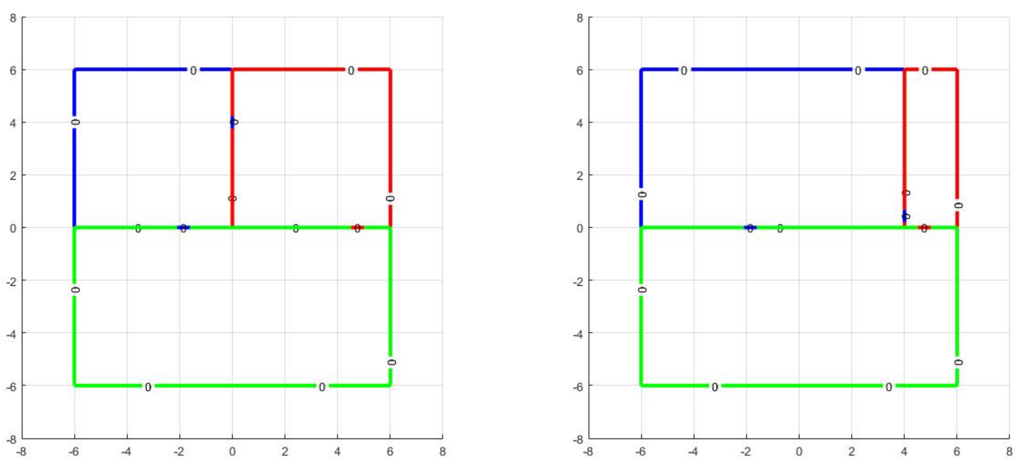
As illustrated in Figure 6b, the middle layer will disappear entirely when the shift is too large. Additionally the corners are dramatically shaped, which do not correspond well to the original geometry. The reason as to why the corners are clipped is that when the square is shifted, the gradients of the SDFs in the top and bottom layers do not point in the same directions. In other words, the two SDFs then measure distances to different edges of the square, which is where interpolation creates an incorrect missing ”corner”.

Therefore, the drawbacks of linear interpolation need to be taken into account when applying a viable solution. Making sure that the corners are preserved, as well as maintaining a middle layer result, is especially important to creating the correct plot.

2.6 Interpolation of the test cases

Modelling the grain structure with SDFs based on linear interpolation has major limitations as described in previous work [Verheijen 2022]; Grain structure shifts result in clipped grains in the triple junction areas. In addition, when a shift is too large, the calculated grain SDF of the middle layer disappears.

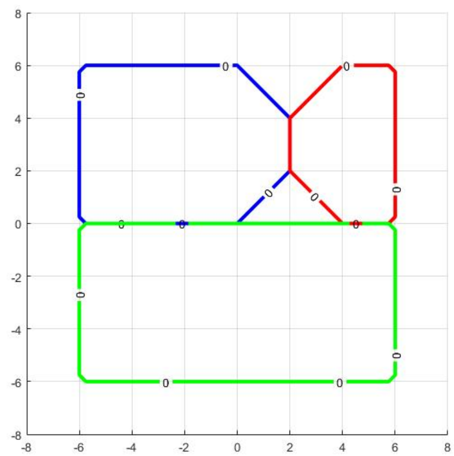
The issues surrounding this problem were evaluated in a test case using different top and bottom layers. At the top layer the triple junction was placed at the origin while the triple junction was shifted to the right for the bottom layer (See Figure 7).



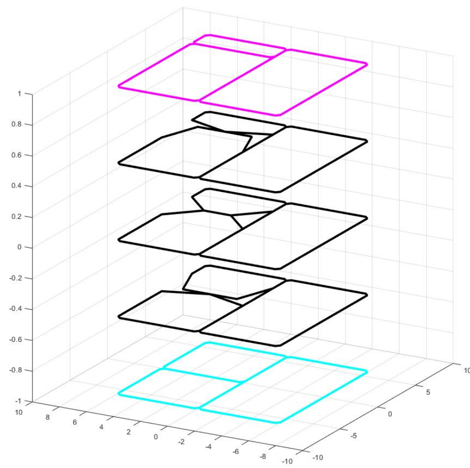
(a) Bottom layer test case with triple junction at the origin (b) Top layer test case, with shifted upper grains

Figure 7: Setup of the top and bottom SDF layers

The grains can then be processed to generate a middle layer, through the the use of standard linear interpolation (see subsection 2.5). Each SDF of a grain is interpolated between its associated top and bottom layer pair. The result of this SDF interpolation is presented in the multi-layer plot Figure 8b.



(a) Middle layer plot (z=0) with missing corners at triple junction



(b) Multi-layer plot of interpolated SDFs

Figure 8: Resulting SDF interpolation

In reference to Figure 8a, the corners are lost due to the linear interpolation. Furthermore, the corners that are missing are at varying angles throughout the layer height (see Figure 8b). If the same method is applied throughout an entire grain structure, multiple regions would be empty while there is an expectation for material to be present. In the next section new methods will be described to improve the reconstruction of the middle layer while at the same time conserving the shape of the corners.

3 Interpolation of Voronoi-like SDFs

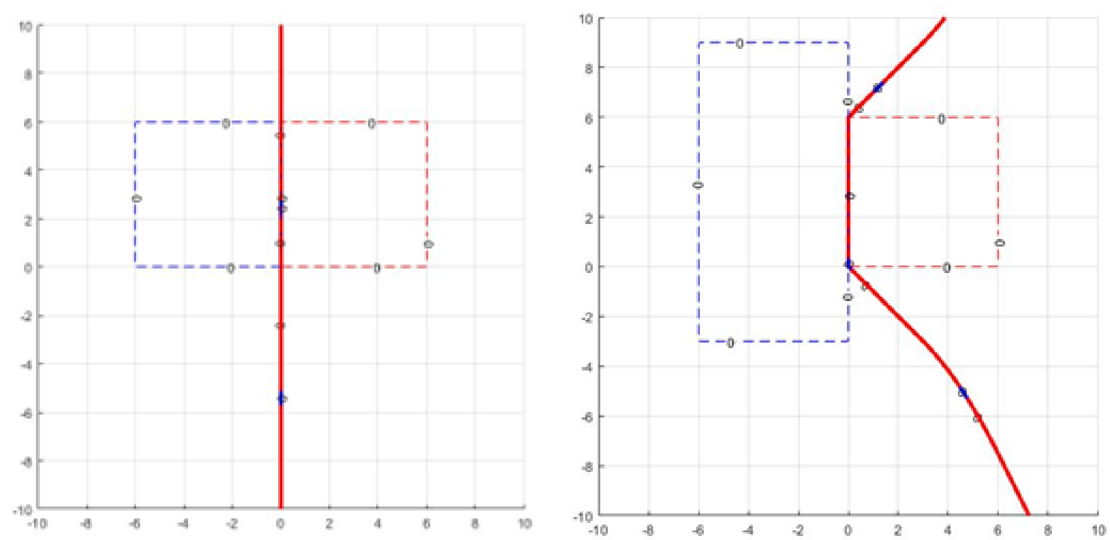
In the process of understanding and learning the result of calculating interpolations of SDF fields, several methods and approaches were utilised, through the process of attempting different solutions. Which in turn created multiple key understandings. The first method with improved success was based on ”voronoi-like” signed distance fields.

3.1 Voronoi-like fields

The ”voronoi-like” distance fields was an initial starting point to explore improved 3D structure modelling. Not to be confused with the subtract operator (Equation 2), the corresponding values of both fields are subtracted from each other. The basic function is as follows:

$$DF_V = DF_1 - DF_2, \tag{5}$$

where DF_V is the created voronoi-like field, and DF's are two neighboring grains. Figure 9a shows a result between two SDF shapes. The effect that is being caused is that the zero contour line is taking the middle distance from either distance field, which infinitely extends outwards. Therefore, if either neighboring grain is touching, a line will be formed on that boundary, and if one is larger than the other (Figure 9b), the zero contour will take the middle distance.



(a) Voronoi-like field generated from two SDF shapes, applied on top two grains of the simple test case

(b) Voronoi-like field behaviour when one SDF is larger than the other

Figure 9: Voronoi-like field behaviour

However, one detail that was discovered with voronoi-like fields is that the resulting distance field is not characteristically the same as a normal SDF. Contours other than the zero contour are warped and tend to be far from being the correct distance to each other. See Figure 10.

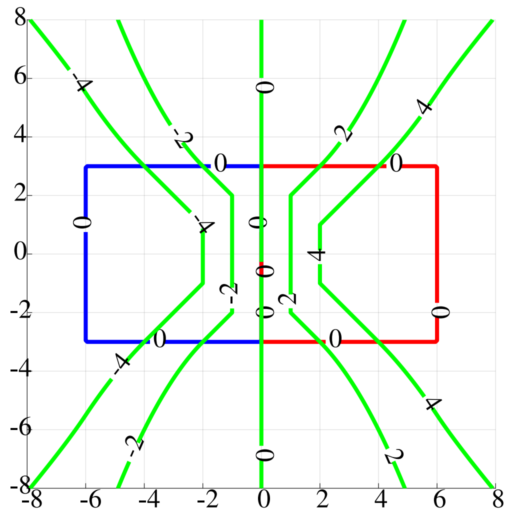
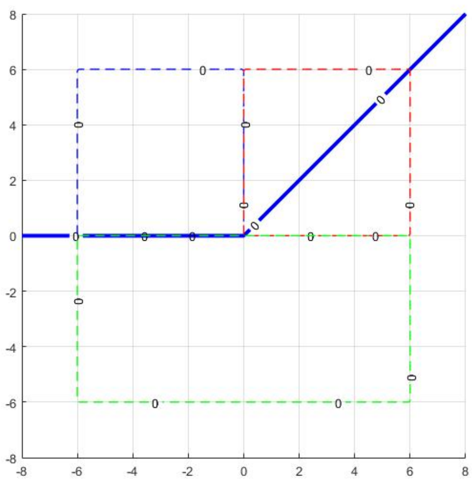


Figure 10: Warped contours as present in the voronoi-like distance field

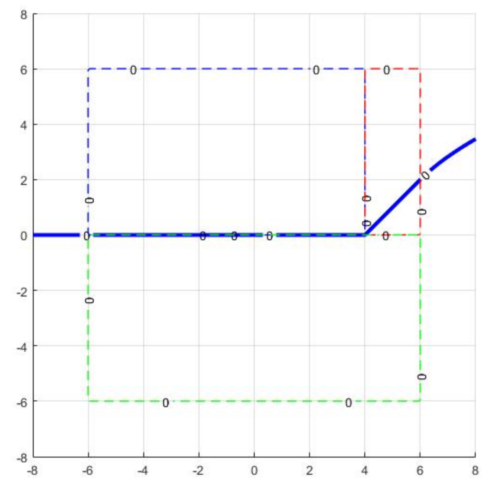
The voronoi-like field deviation allows for the creation of zero contours between SDFs, or in the case of the project, between pairs of grains. These zero contours between certain grains can then be used to interpolate in pairs.

3.2 Voronoi interpolation

With the voronoi-like formation, the first solution that was to avoid interpolating the SDF's of the grains, and rather use the voronoi-like lines to interpolate all the boundaries of a grain and reconstructing the grain after. Figure 11 shows the Voronoi-like SDFs for the top and bottom surface of our test problem.



(a) Voronoi-like contour of two grains on the top surface

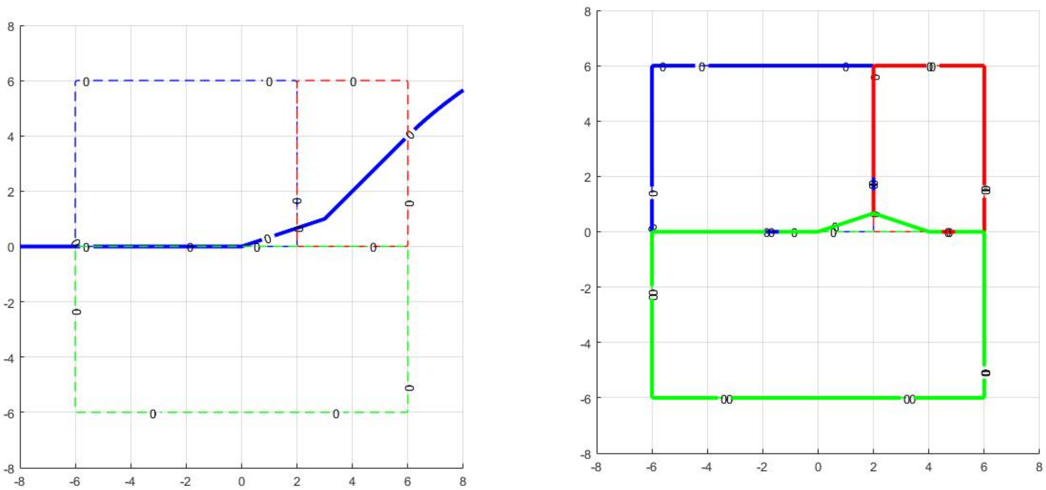


(b) Voronoi-like contour of the bottom surface with a shift in grains

Figure 11: Voronoi-like pair of bottom and top surface

Having established one pair of voronoi-like lines between the two grains, interpolation can be applied. Shown in Figure 12a, the middle layer has difficulty to maintain the bend that exists at the precise location of the triple junction.

Although not perfect, the interpolated result can be combined with further voronoi-like lines to recreate the SDF field. Above only one pair is applied, however since three grains exist, and each grain touches two other grains, a total of six pairs exist to interpolate. The interpolation result can then be combined with other voronoi interpolations to form a grain via the union operator (Equation 1). The combination of all pairs are shown in Figure 12b.



(a) Resulting mid layer voronoi field

(b) Middle layer with grains made of combining voronoi lines

Figure 12: Voronoi-like pair of bottom and top surface

The corner is filled, which is a "solution" to our problem, however depending on how large the shift of a certain grain is, the worse the interpolated result is being projected.

A clear challenge while applying linear interpolation to the problem at hand is that any bend or corner makes it difficult to persist through the layers. If a straight line exists, the reliability of interpolating seems to be improved. Another challenge with voronoi lines is the accumulated discrepancy between the lines on the different layers between the top and bottom layer. Due to the calculation of subtracting one field with another, contours that would be equally spaced from each other are no longer spaced correctly (shown in Figure 10). The errors of the voronoi interpolation become visible when transferring the results to the various layers between the top and bottom layer. Only the middle layer is perfectly straight, where as other layers perform differently as a result of the warped contours.

3.3 Conclusion

The voronoi solution provides partial improvements over standard linear interpolation though there are severe limitations to this solution, such as if an extreme shift or angles are found. A clear emphasis to keep the lines as straight as possible allows the corners to be preserved more accurately. However still there is a clear discrepancy to what the triple junction is expecting to appear as.

4 Extrapolating lines

Having experienced the limitations of the voronoi-like field derivation, the ideal solution would be to create true straight lines which extend the boundary. By creating these lines, the region at which the grains would lose information would not occur. Sharp corners can be retained as part of interpolating these infinitely long lines. Starting with the simple test case, only a single straight segment has to be used to describe a grain boundary.

By creating an infinitely long line based on the location and orientation of the single reference segment, a straight line can be created.

4.1 SDF formulation and methodology

As part of this method, a new ”SDF” function had to be created to generate an infinitely long line based on the information available. The SDF function was elegantly optimized through the introduction of a normal vector calculation.

A normal line is created when computing the distance of a each point in the field to the segment. With distance known, assigning one side as negative is important to retain the ability to linearly interpolate. Therefore, by comparing if the point is above or below the vector (Burr 1962), the correct sign can be assigned.

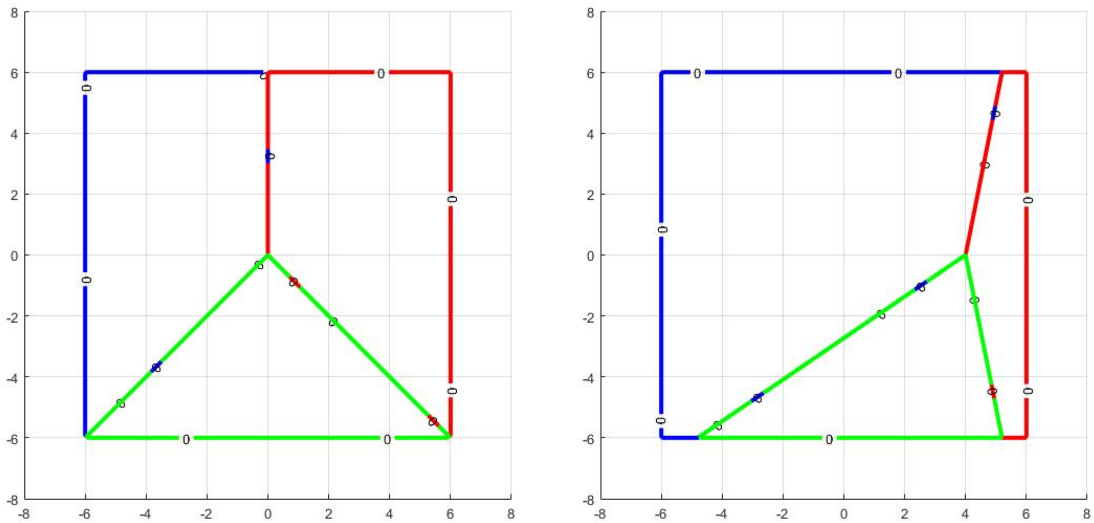
With the negative distances on one side, a check must be done if the negative side is on the correct side. In the case of combining SDF's as done before in Figure 3.1, the negative distance is the side shared with where the grain is located.

In order to create the information required to form this new SDF line, the following step by step process is used.

1. Find the boundaries between two grains at a time.
2. Find the triple junction location by finding the point common in all boundaries.
3. Create an infinitely long line using the points of either end of the boundary, and a known point inside each grain. Make sure that one of the two ends of the boundary ends at the triple junction location.
4. Repeat these steps for the other layer of data.
5. Linearly interpolate the pair of infinitely long lines to obtain infinitely long surfaces.
6. Combine infinite surfaces to grains.

The main feature of this approach is the use of infinitely long lines. This allows recreating the sharp corners of the grains near the triple junction region.

Before testing this new approach, a custom test case was created. To demonstrate the new method's effectiveness, a shift along with angle changes was evaluated in the test case. The setup of this test case is illustrated in Figure 13.



(a) Bottom layer with symmetric angles

(b) Top layer with large shift and asymmetric angles

Figure 13: Test case setup with shift and angle changes

4.2 Results

The test results of the extrapolating line method with the normal line concept are presented in Figure 14, with the multi-layer plot shown in Figure 15.

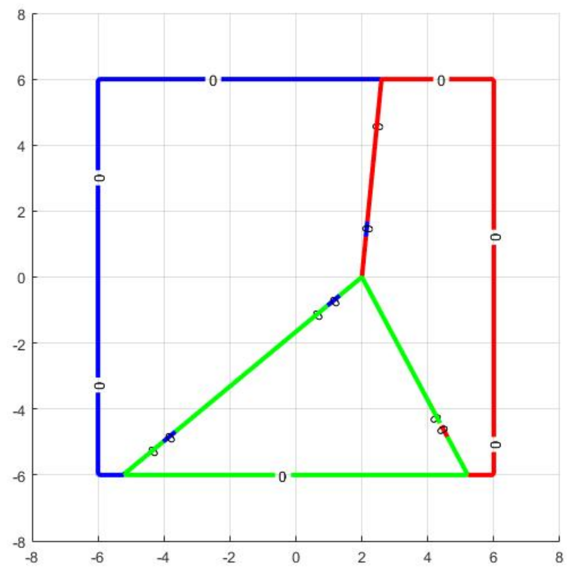


Figure 14: Middle layer interpolated result using extrapolated lines

The normal line interpolation provides accurate results even with large shifts. Additionally, no missing gap is present in the triple junction, along with no disappearing grains in large shifts. Furthermore, on a multi-layer plot, the grain shifts accordingly.

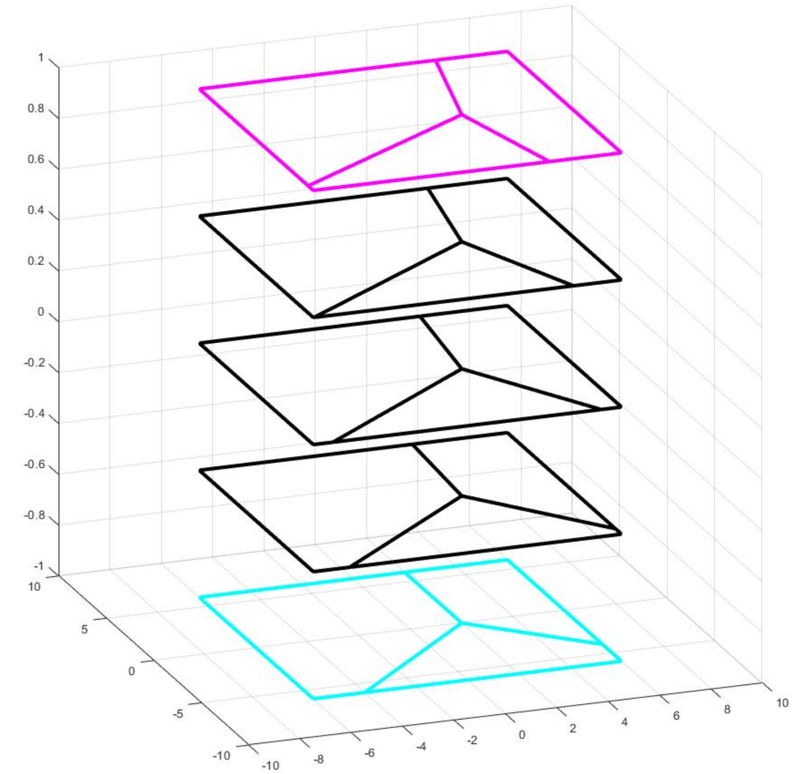
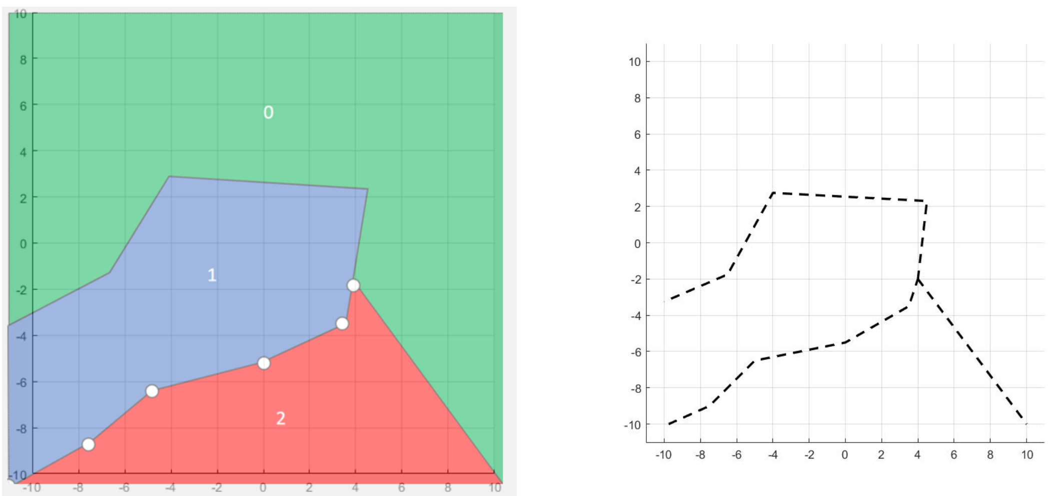


Figure 15: Resulting multi layer plot interpolation using extrapolated lines

5 Adapting extrapolated line structures to complex curvatures

In the previous chapter, an ideal solution has been developed that works with major shifts and orientation changes in the previous test cases. The next step is to apply and validate the extrapolating line method on complex geometry.

As illustrated in the EBSD maps in Figure 1 and Figure 2, typically grain structures can have simple straight boundaries, but are more likely to have a few curves in the geometry. Before creating a new method that can be applied to any complex geometry, a reference grain boundary focused at a triple junction is used.



(a) Reference image used

(b) Three grain boundaries created

Figure 16: Reference geometry creation

Before applying the existing extrapolated lines method, several changes in the approach have to be applied.

5.1 Adjusted methodology using polygon selection

To create a complete ”SDF” for a given complex geometry, each of the separate parts must be combined. The first major change is including several segments. The curved boundaries are discretized by multiple straight line segments. By using equation Equation 1, multiple segment signed distance fields can be connected.

The step by step process that starts with the provided array and ends with the correct ”SDF” is shown below:

1. From the provided array of points, create separate distances fields of all segments.
2. Combine all the segments using union (Equation 1) in a for loop.

3. Take the first two and last two points of the provided array, and use these to create infinitely long lines on the ends. Do not assign any negative distances at this point.

   Remove any data of the infinitely long lines that coincides with the other segments. Only the ends should be calculated

4. Combine the segments and partial infinitely long lines via union (Equation 1).
5. Create points via linear extrapolation that extend beyond the ends of the group of segments.
6. Create a polygon using the provided array of points along with extrapolated points and a point far away from the group of segments (see Figure 18a, bottom right corner).
7. Using a query algorithm, use the created polygon to identify and adapt the values found inside of the polygon to a negative distance.
8. Repeat for all other grain boundary array lists.
9. Interpolate the appropriate pair on the other layer.
10. Make an alternate distance field for all distance fields by flipping the sign.
11. Strategically combine the various distances fields to recreate the grain on the layer of interest.

The combined segments along with the ends being combined are shown in Figure 17. At this stage, the flipping process using a large polygon has not been applied.

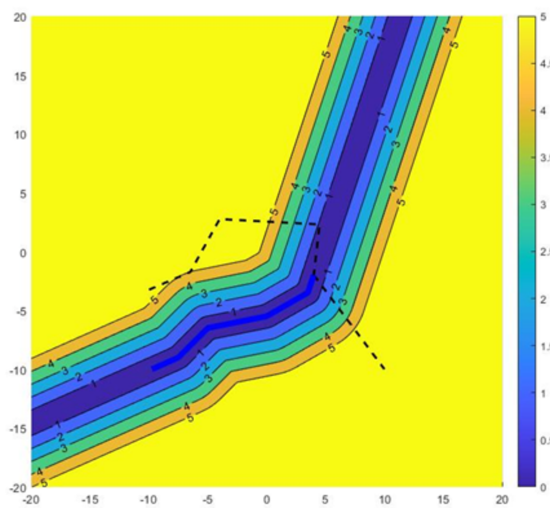
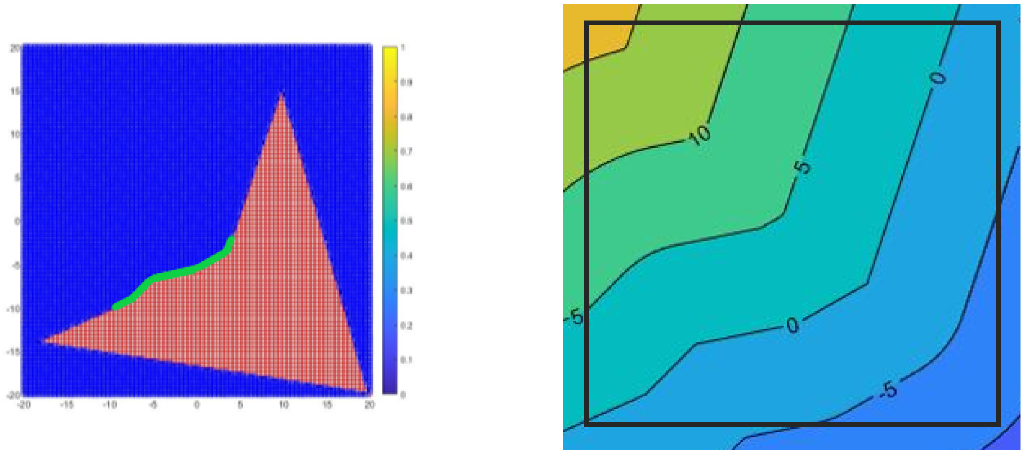


Figure 17: Infinitely long lines and segment distance fields applied on the bottom left grain boundary

The process of using a larger polygon to determine the sign of the SDF is visualized Figure 18a. The points found inside of the polygon must be negative, shown in red. Note that additional points are taken far away enough to be able to complete the geometry.



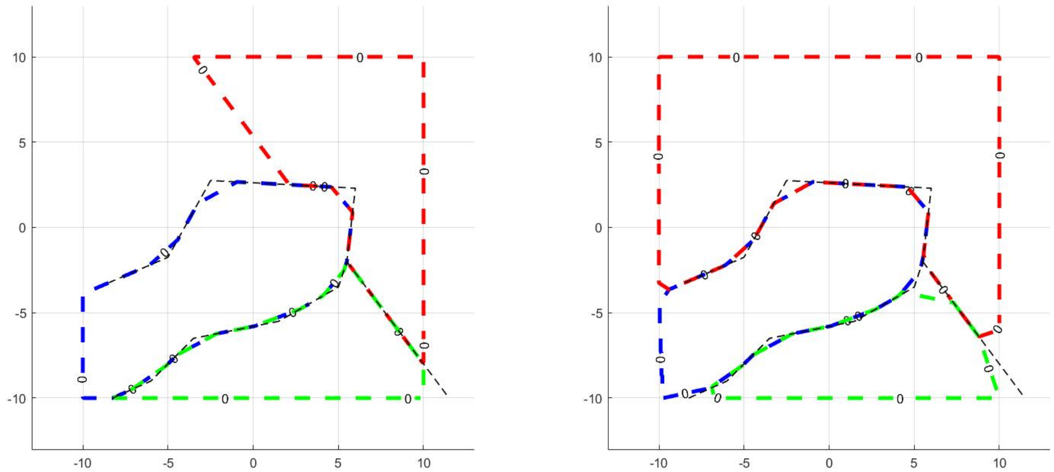
(a) Large polygon created using additional points, the red region values are made negative

(b) Resulting "signed" distance field, within window of interest which bounds -10 till 10

Figure 18: "SDF" algorithm steps

5.2 Interpolation results

With the new method created, the test case is applied. The reference geometry shown in Figure 16b is taken as a bottom layer, with the bottom being shifted to the right by 3 units. The result of the interpolation is shown in Figure 19a, alongside the original method of interpolating the SDF's of the grains themselves.



(a) Resulting complex curvature interpolation

(b) Original interpolation method

Figure 19: Comparison of solutions

The figures are placed side by side for clear comparison. The first item to note is that the old method (shown Figure 19b) clearly has missing regions in the inside of the triple junction and on outer corners of the SDFs. The proposed solution of this paper fixes this entirely, as shown in Figure 19a. The corner that is present in the triple junction location is kept sharp as it was on both the top and bottom layer.

Two major discrepancies exist in the example. In both methods, any corners in the grain boundaries not at the triple junction are still rounded off. Although there are no gaps on the grain boundaries, there are still minor deviations observed. The accuracy of the interpolation is therefore limited with respect to these regions of the curvature.

The second discrepancy is the missing region of the top grain (shown in red). This discrepancy is present due to the fact that the infinitely extended line of the bottom right grain boundary is cutting through the grain structure (see Figure 20). Due to relying on the intersect operator to connect the separate extended boundary lines, not the whole area is captured. Using the union operator would allow for the whole region to be captured, but detail would be lost in the small region above the triple junction, which deviates from the actual geometry. Due to this, the use of any method proposed in this paper is not compatible with extremely curved boundaries. The left grain is too drastic in curvature changes for the proposed method to work correctly.

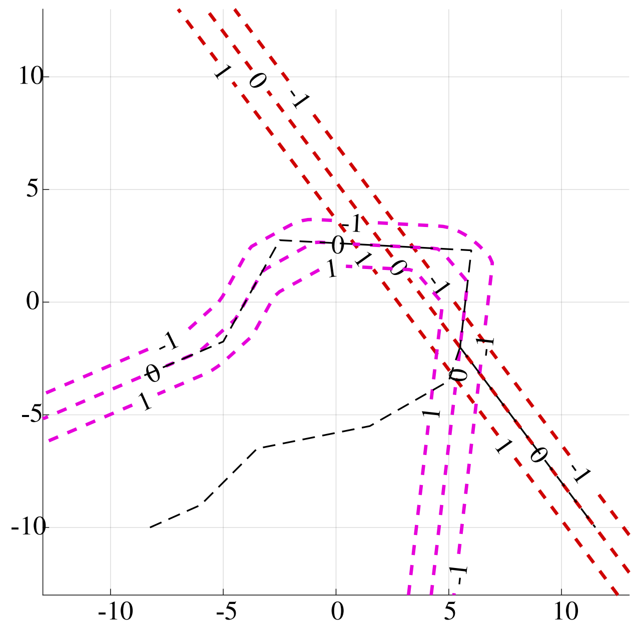
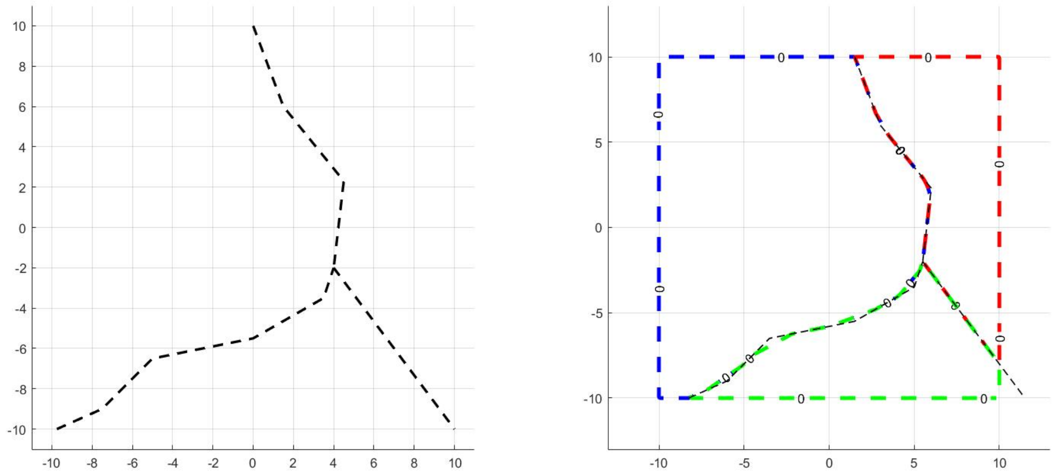


Figure 20: The two boundary SDF contours meant to be combined for the upper red grain in (Figure 19a)

5.3 Less extreme curvature test case

The original complex curvature test case (illustrated in Figure 16) has been adjusted to be less complex in curvature. The new test case and the result of it being shifted and interpolated is presented in Figure 21b.



(a) New test case

(b) Resulting plot of same shift conditions as applied before

Figure 21: Final test case and result

5.4 Discussion

The method of extrapolating line structures proved to be a successful concept to model a 3D structure of a complex case of a single phase poly crystalline structure. The clear limitation of the proposed solution is having extreme curvature. If the shapes are too complex in it's changes of geometry, the solution will not be able to generate the appropriate SDF. That said, in this project the triple junction problem is fixed to the largest subset of possible grain situations in a single phase poly crystalline structure, which was the goal of this project.

6 Conclusion

Throughout this paper several methods have been tested and evaluated to model the 3D structures of single phase poly crystalline structures. The original interpolation method does not create the appropriate geometry around the triple junction. In the process of finding a solution, the voronoi-like fields clearly indicated that preserving corners requires interpolating straight lines. The initial implementation of infinitely-long SDF lines worked effectively on both original test cases, even in large shifts and angle changes. The last area to extend the method of infinitely long SDF lines was with complex geometry, where it remains functional provided that the material sample is a single phase poly crystalline structure consisting of shapes are not too drastically complex.

7 Recommendations

Many different methods are still viable to further improve the 3D reconstruction of single phase polycrystalline grain structures. Throughout the process of exploring, developing and applying different solutions, multiple alternatives were established. However, due to time limitation, not all these options could be explored. These alternative methods could further improve the accuracy of the interpolation, and allow for more compatibility with complex shapes and multi-phase materials. The following section will discuss these alternatives.

7.1 Aligning interpolation

Halfway through this project, one approach was briefly considered, but not explored. This involved realizing the limitations of normal interpolation. In exploring linear interpolation, one key issue related to major shifts causing no mid-layer SDF to form. Taking the SDF's of two fields, and moving them such that they are directly above each other. Via verifying that one shape is larger than the other, normal interpolation is expected to function correctly.

7.2 Shape morphing via hierarchical interpolation

One clear shortcoming of linear interpolation is the retention of sharp corners especially when large shifts are applied. [Yang and Feng 2009]'s article on shape morphing via feature marching and hierarchical interpolation is a clear different approach that is worthwhile investigating, instead of relying on normal linear interpolation.

7.3 Commercial software and other scientific fields

As part of multiple 3D modelling software, variants of shape morphing are available. For 2D sketches between two different heights or to path based surface modelling, a plethora of methods exist that could be a better solution to linear interpolation. Examples of this are Siemens^{TM} NX's "Through curves" and Autodesk^{TM} Fusion 360's "lofting", with other names used to describe the process of "[inbe-]tweening". Each software has their own algorithms, with multiple settings. Utilizing and expanding on the approaches used in these software packages hold potential to solving the current problems of interpolation.

With a focus on computational mechanics, several solutions from the medical field are also seen as promising.

Examples such as Computed Tomography (CT) scans and Functional Magnetic Resonance Imagining (fMRI) use morphing operations and several filters that could provide alternative solution pathways to optimizing the interpolation of grain structures in crystalline structures.

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