# NUMERICAL TOOLS USED IN THE SOFTWARE FOR 2D AND 3D MORPHOLOGICAL ANALYSIS

Consider a scalar order parameter $\phi(\mathbf{r}, t)$ sampled on a cubic lattice. It is represented by a set of $N^3$ variables $\phi_{i,j,k}$ Each variable $\phi_{i,j,k}$ represents the value of the field $\phi(\mathbf{r})$ at the point $\mathbf{r} = (i, j, k)h$, $h$ is the lattice spacing, and $i, j, k = 1, \ldots, N$. In order to get rid of the boundary effects we impose the **periodic boundary conditions** in $x$, $y$, and $z$ directions:

$$\phi_{1,j,k} = \phi_{N,j,k}, \tag{1}$$

$$\phi_{i,1,k} = \phi_{i,N,k}, \tag{2}$$

$$\phi_{i,j,1} = \phi_{i,j,N}, \tag{3}$$

Note that in the periodic box the surface is in fact closed. For example, a plane is topologically equivalent to a tori. Therefore the standard definition of the genus as a number of holes in a closed surface can be used.

The surface separating the domains is given by the following equation

$$\phi\left[\mathbf{r} = (x, y, z)\right] = \phi_0, \tag{4}$$

where $\phi_0$ is an arbitrary threshold value of the field $\phi$. The position of the surface $\phi(\mathbf{r}) = 0$ is determined by interpolation between the neighboring points of different sign. It is highly unlikely, because of numerical accuracy, that a value of the field $\phi(\mathbf{r}) = \phi_{i,j,k}$ at the point $\mathbf{r} = (i, j, k)h$ on the lattice is exactly zero. Therefore the points of the surface have to be localized by interpolation between the neighboring sites of the lattice. If $\phi(\mathbf{r}_1 = (i, j, k)h) = \phi_{i,j,k} < \phi_0$ and $\phi(\mathbf{r}_2 = (i+1, j, k)h) = \phi_{i+1,j,k} > \phi_0$ then the point $\mathbf{r}_0$, for which $\phi(\mathbf{r}_0) = 0$, must lie between the points $\mathbf{r}_1 = (i, j, k)h$ and $\mathbf{r}_2 = (i+1, j, k)h$. Moreover, the location of $\mathbf{r}_0$ depends on the values of the field at the points $\mathbf{r}_1$ and $\mathbf{r}_2$ in the following way

$$\mathbf{r}_0 = \left( i + \frac{|\phi_{i,j,k}|}{|\phi_{i,j,k} - \phi_{i+1,j,k}|}, j, k \right) h. \tag{5}$$

All points of the surface $\phi(\mathbf{r}) = \phi_0$ are found by the interpolation of the points located between the neighboring lattice sites. Due to the discretization the unit cell is divided in $(N-1)^3$ small cubes of the size of the lattice spacing, $h$. The surface $\phi(\mathbf{r}) = \phi_0$ passing through a small cube cuts out of it a polygon. The edges of the polygons are formed by intersection of the surface and the faces of the small cube. The edges can be approximated by straight lines. Unfortunately, the cube lattice decomposition scheme suffers from arbitrary choices i.e. such representation of the surface leads to ambiguous situations. Note that an

alternative way to resolve the ambiguous surface approximations is to divide the original lattice not into cubes, but into more primitive subunits. Each cube can be divided into six 5-vertex pyramids.

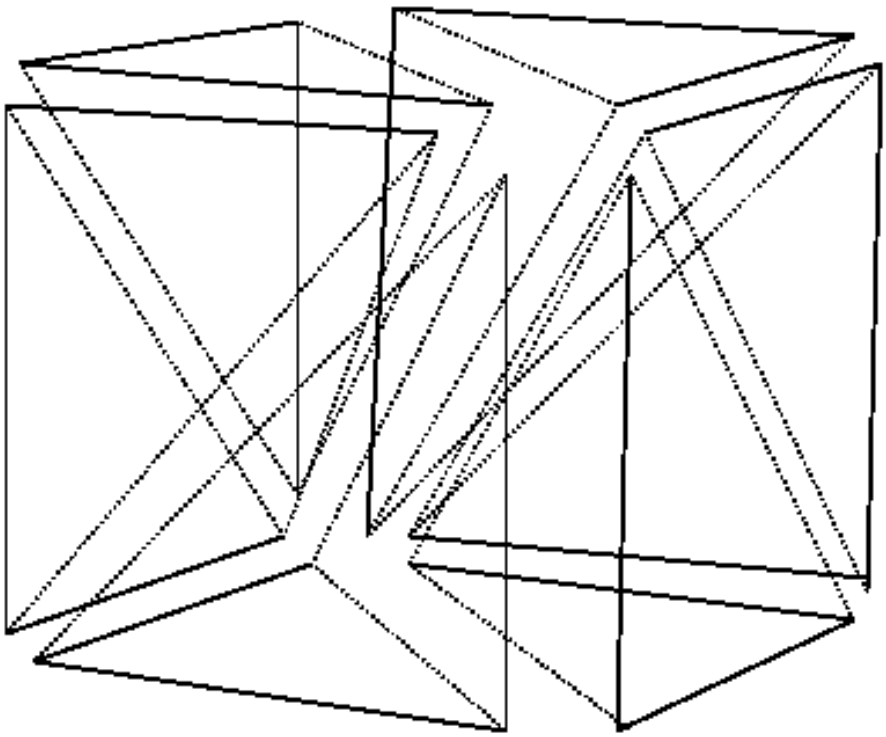

FIG. 1: Decomposition of a cubic lattice cell into six tetrahedrons.

The program `morph3D` uses the simplest method based on the **division of elementary cubes into tetrahedrons** (see Fig. 1). When the tetrahedron decomposition is employed, the surface inside such simplex can be represented by only two cases (polygons): a triangle or a tetragon, as shown in Fig. 2.

From the decomposition described above we can easily get the Euler characteristic, $\chi$. The practical way of computing $\chi$ is related to the coverage of the surface with polygons. Then, the calculation of the Euler characteristic is straightforward when it is based on the Euler

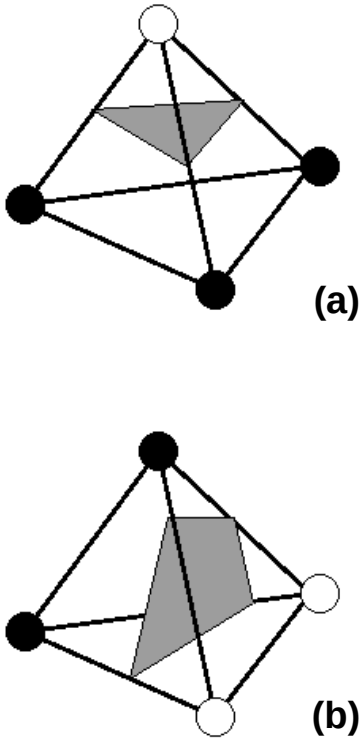


FIG. 2: Two cases of the polygonal surface representation in a single tetrahedron: a triangle (a) and a tetragon (b). The black and the white circles represent the points with the values of $\phi$ higher and lower than the threshold $\phi_0$.

formula:

$$\chi = \#F + \#V - \#E, \tag{6}$$

where $\#F, \#V, \#E$, is the number of faces ($\#F$), vertices ($\#V$), and edges ($\#E$) of all polygons cut by the surface. The surface area is simply the area of all polygons covering the surface. Finally we can use the same polygons to compute the curvatures. Before we do it we present another method which although imprecise is frequently used. From the differential geometry we have the following formulas for the curvatures.

$$H = -\frac{1}{2}\nabla \mathbf{n} = -\frac{1}{2}\nabla \left( \frac{\nabla \phi}{|\nabla \phi|} \right) \tag{7}$$

and

$$K = \frac{1}{2}\left[ (\nabla \mathbf{n})^2 - (\partial_i n_j)^2 \right] \tag{8}$$

where $\mathbf{n}$ is the vector normal to the surface at point $\mathbf{r}$, where we calculate the curvatures and $n_j$ is its $j$-th component. Thus using the whole distribution of $\phi$ we can compute the

distributions of curvatures. The errors produced by the use of the approximate formulas for the derivatives of $\phi$ are especially big if the spatial derivatives of the field $\phi$ have sharp peaks at the phase interface. This is a common situation in the late-stage kinetics of the phase ordering process, when the order parameter is saturated and the domains are separated by thin walls. There is however a simpler method which involves the previously defined polygons. It comes from integral geometry and does not suffer from the before-mentioned problems.

Consider a polyhedron which is a discrete representation of the phase interface $\phi(\mathbf{r}) = \phi_0$ obtained in the triangulation procedure. For each vertex of the polyhedron we can define the angle deficit by:

$$T_i = 2\pi - \sum_{j=1}^{m} \alpha_i^j \tag{9}$$

where $m$ is the number of triangles which meet at $i$-th vertex and $\alpha_i^j$ is the angle between the two edges of $j$-th triangle at this vertex (see Fig. 3). The Gaussian curvature at $i$-th vertex is given by:

$$K_i \approx T_i / S_i \tag{10}$$

where $S_i$ is one third of the area of the triangles. To prove this formula, let us first show that the integral of the Gaussian curvature over the surface region $\Sigma_i$ (over triangles sharing the same vertex) is

$$\int_{\Sigma_i} K(S) dS = T_i. \tag{11}$$

The total angle deficit of the polyhedron, $T = \sum_{\{v_i\}} T_i$ is related to the number of its vertices $\#V$, faces $\#F$, and edges $\#E$ (Cartesian theorem) as

$$T = 2\pi(\#V + \#F - \#E). \tag{12}$$

On the other hand, the total integral from the Gaussian curvature can be expressed by using the Gauss theorem:

$$2\pi(\#V + \#F - \#E) = \int_{\Sigma} K(S) dS. \tag{13}$$

By using the fact that

$$\int_{\Sigma} K(S) dS = \sum_{\{v_i\}} \int_{\Sigma_i} K(S) dS \tag{14}$$

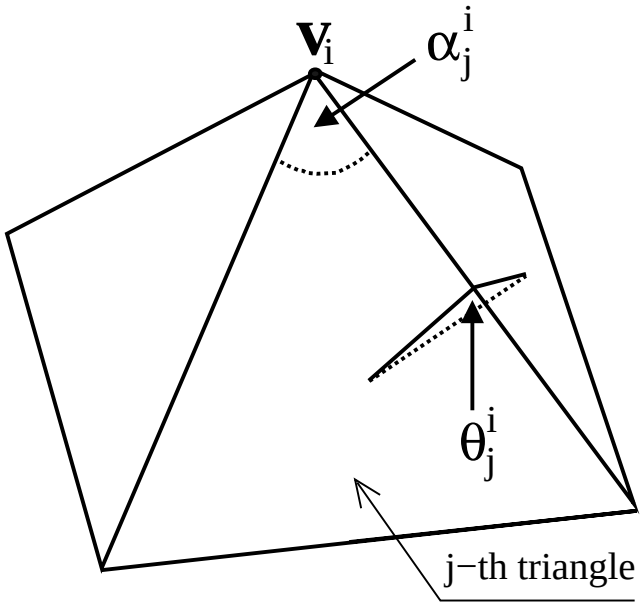


FIG. 3: A piece of polyhedron's surface composed of triangles meeting at the vertex $v_i$: $\alpha_i^j$ is the angle between two edges of the $j$-th triangle shearing the vertex $v_i$, $\theta_i^j$ is the angle between the faces of two adjacent triangles.

and comparing (12) to (13), Eq. (11) is deducted. Now, by assuming that the Gaussian curvature is constant within the region $\Sigma_i$, the formula (10) is obtained from (11).

The integral of the mean curvature $H$ over the surface region $\Sigma_i$ can be written as

$$\int_{\Sigma_i} H(S)dS = \tilde{H}_i, \tag{15}$$

where

$$\tilde{H}_i = \frac{1}{4}\sum_{j=1}^{m} l_i^j \theta_i^j; \tag{16}$$

$l_i^j$ is the length of the edge of $j$-th triangle and $\theta_i^j$ is the angle between two adjacent triangles $j$ and $j+1$ (see Fig. 3). Assuming again the constancy of the mean curvature within the region $\Sigma_i$, its value can be evaluated as

$$H_i \approx \tilde{H}_i / S_i. \tag{17}$$

Note that in Eq. (16) the angles $\theta_i^j$ can have either sign, depending on the orientation of the surface of the polyhedron.

The curvature $k$ of the interface in two dimensions can be calculated in a similar way. Namely, consider a polygon consisting of vertices $v_i$ connected by edges $l_i$. Let us denote by $l_i$ the length of the edge between $(i-1)$-th and $i$-th vertex. The curvature $k_i$ at the $i$-th vertex can be then approximated as follows: $k_i \approx 2\theta_i/(l_i + l_{i+1})$, where $\theta_i$ denotes the angle between two edges which meet at the vertex $v_i$. Note also that the two-dimensional version of the Gauss-Bonnet theorem implies that the sum $\sum_i \theta_i$ taken over all vertices gives $\pm 2\pi$, where the sign depends on the orientation of the polygon boundary. In the program `morph2D` more procise method to calculate the curvature $k$ is applied. We use the fact that the curvate at a givent point $\mathbf{x_i}$ of the contour can be approxiamted as a second derivative of a parabole tangent to the contour at $\mathbf{x_i}$ (see Fig. 4). In order to calculate the curvature $k_i$ at the $i$-th vertex a parabole $y = ax^2 + bx + c$ going through three subsequent vertices $i-1$, $i$, and $i+$ is determined. The curvature is then calculated as the second derivative of $y$ at $v_i$,

$$k_i \approx \frac{d^2y}{dx^2}, x = \mathbf{x_i} \tag{18}$$

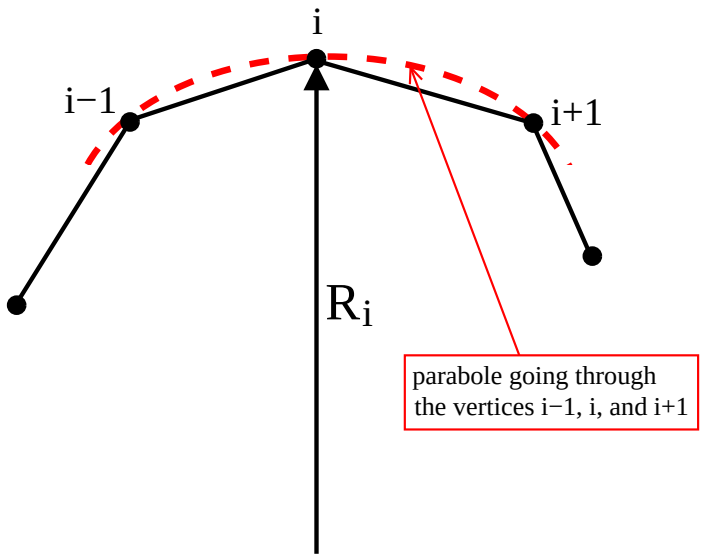


FIG. 4: A piece of polygon's border composed of vertices connected by a break line. In order to calculate the curvature $k_i$ at the $i$-th vertex a parabole $y = ax^2 + bx + c$ going through three subsequent vertices $i-1$, $i$, and $i+$ is determined. The curvature is then calculated as the second derivative of $y$ at the vertex $v_i$.

## REFERENCES


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