Title:
**Topological Modifications through Boolean Compositions on Algebraic Level Sets Constructed from B-rep Models**

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Keywords:
Distance Fields, Algebraic Level Sets, Boolean Compositions, CAE, Isogeometric Analysis

DOI: 10.14733/cadconfP.2019.456-461

Introduction:
Topological changes are common in problems where interfaces evolve with time, such as solidification, void nucleation or shape optimization. If the evolving boundaries are represented explicitly, then modeling topological changes for arbitrary interfaces becomes challenging, requiring contact detection and surface-surface intersection. Thus, implicit representations of the boundary provided by the phase field or level set methods are often used to accommodate large topological changes. Such implicit representations also implicitize physically relevant geometrical parameters such as normals and curvatures and recover the exact interface geometry only in the limit of mesh refinement. In this paper, an explicit boundary tracking method is introduced which allows topological changes such as coalescence without requiring collision detection and intersection computations. The problem of interest is that of void coalescence in a metal line subject to high current density (referred as electromigration). Analysis is performed by capturing the influence of the void interface as an enrichment to the electric field approximation defined over the domain [8]. This influence weakens as we move away from the void. Thus a measure of distance from the void interface is required. Conventionally, such distance estimates are obtained either using iterative techniques such as Newton-Raphson [4], or by generating polytope approximations of the geometry [1]. However, numerical iterations are computationally expensive and often not smooth for analysis purposes, while polytope approximations lose geometric exactness to CAD of the phase interface and are accurate only in the limit of refinement. Here, signed algebraic level sets are generated by implicitizing the void interface using resultant theory [5, 9]. These level sets act as smooth surrogates of distance and are exact in the neighborhood of the geometry. Further for closed geometries the sign of these level sets can be used to classify points as lying inside or outside the geometry [10], thus determining the phase at a point.

In this paper, topological changes in the phases are modeled through algebraic Boolean operations on the level sets. These Boolean operations are performed using R-functions [6, 10] to ensure smoothness and geometric accuracy of the composed level sets and avoid the need for contact detection and computation of intersection of void surfaces during analysis. Prior work using algebraic Boolean operations using R-functions for analysis exist in the literature. In [2, 11], Boolean operations were used during topology optimization to combine free-form geometries with embedded regular-shaped primitives. In general, algebraic Boolean compositions of complex free form parametric geometries do not appear to exist except for that in [10]; they carried out Boolean operations on algebraic level sets constructed on complex parametric CAD geometry. These were then used for static thermal and mechanical analysis.

This extended abstract is divided as follows. First, implicitization of parametric surfaces using the Dixon resultant is discussed. This is followed by the procedure to generate algebraic level sets for parametric geometries. Next, we discuss the electromigration problem and its formulation. Finally a discussion on using Boolean operations on the level sets to effect topological changes such as coalescence is provided.

Implicitization Using the Dixon Resultant:

Curves and surfaces can be expressed with an implicit or parametric representation. Most CAD systems use parametric representations such as Non-Uniform Rational B-Splines (NURBS), which provide a more general as well as intuitive control of the geometry for users. On the other hand, the implicit representation of a surface allows natural generation of level sets that increase monotonically with distance, thereby serving as a surrogate of distance that is necessary for analysis of behavior. It is hence desirable to obtain the equivalent implicit representation for a given parametric curve or surface. This can be done using the Dixon resultant [3] from Elimination theory, as shown in [5]. Resultants are polynomial expressions on the coefficients of a given system of polynomial equations. The given system of equations have a common solution only if their resultant vanishes. A procedure to compute the Dixon resultant shall be discussed presently. While the procedure described is for three-dimensional surfaces, it can be readily adapted for planar curves. Rational parametric representations such as Bézier and NURBS have the general form,

$$x(u,v) = \frac{X(u,v)}{W(u,v)}, y(u,v) = \frac{Y(u,v)}{W(u,v)}, z(u,v) = \frac{Z(u,v)}{W(u,v)} \tag{2.1}$$

where, $X, Y, Z, W$ are functions in the parameters $(u, v)$, with degree $m$ in $u$ and $n$ in $v$. Define,

$$\delta(\mathbf{x}) = \frac{1}{(u-\alpha)(v-\beta)} \begin{vmatrix} xW(u,v) - X(u,v) & yW(u,v) - Y(u,v) & zW(u,v) - Z(u,v) \\ xW(u,\beta) - X(u,\beta) & yW(u,\beta) - Y(u,\beta) & zW(u,\beta) - Z(u,\beta) \\ xW(\alpha,\beta) - X(\alpha,\beta) & yW(\alpha,\beta) - Y(\alpha,\beta) & zW(\alpha,\beta) - Z(\alpha,\beta) \end{vmatrix}$$

Since the determinant is zero whenever $u = \alpha$ or $v = \beta$, $(u - \alpha)$ and $(v - \beta)$ are factors of the determinant and have hence been factored out. For points on the surface, using Eq.(2.1) gives

$$\delta(\mathbf{x}) = 0 \qquad \forall\ \alpha, \beta \in \mathbb{R} \tag{2.2}$$

Now, the quantity $\delta$ depends on $\alpha, \beta, u$ and $v$, and can be expanded to separate these factors as,

$$\delta = \begin{bmatrix} 1 & \alpha & \alpha^2 & \cdots & \alpha^{m-1}\beta^{2n-1} \end{bmatrix} [\mathbf{M_D}(\mathbf{x})] \begin{bmatrix} 1 & u & u^2 & \dots & u^{2m-1}v^{n-1} \end{bmatrix}^{\mathrm{T}} = [\alpha][\mathbf{M_D}(\mathbf{x})][\mathbf{u}] \tag{2.3}$$

For the determinant to vanish for all $\alpha, \beta$, we require,

$$[\mathbf{M_D}(\mathbf{x})][\mathbf{u}] = 0 \tag{2.4}$$

$$|\mathbf{M_D}(\mathbf{x})| = 0 \tag{2.5}$$

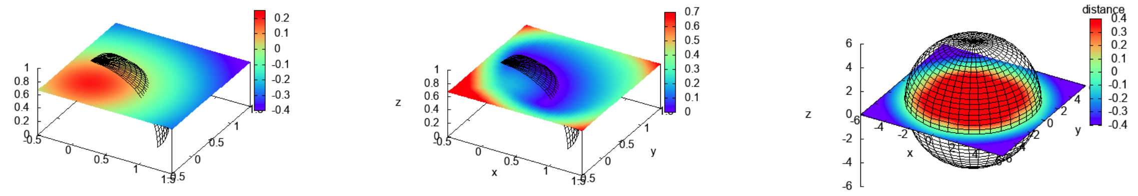
This forms a necessary condition for a point to lie on the parametric surface and can act as its implicit equation. The $2mn \times 2mn$ determinant in Eq. (2.5) is the Dixon resultant [3].

Signed Algebraic Level Sets:

The Dixon resultant derived in Eq. (2.5) allows the generation of the level sets [9],

$$\Gamma(\mathbf{x}) = |\mathbf{M_D}(\mathbf{x})| \tag{2.6}$$

Proceedings of CAD'19, Singapore, June 24-26, 2019, 456-461




(a) (b) (c)

Fig. 1: Algebraic level sets for an octant of a sphere generated from (a) Dixon resultant and (b) after the trimming operation. (c) Signed level sets for a sphere generated using the bounding box procedure.

The generated level sets for an octant of a sphere are shown in Fig. 1a. It can be seen that while the parametric surface is restricted to just an octant, the resultant generates level sets over the entire parametric range, i.e., for the entire sphere. It is hence required that the implicitization is restricted to the required parametric domain. This is achieved using a trimming procedure based on R-functions [1, 6]. The convex hull of the parametric surface, defined by the field $\Phi(\mathbf{x}) \geq 0$, is used as the trimming region. The resultant is first normalized to allow composition with the hull distance field. The normalized resultant is defined as,

$$f(\mathbf{x}) = \frac{\Gamma(\mathbf{x})}{\|\nabla\Gamma(\mathbf{x})\|} \tag{2.7}$$

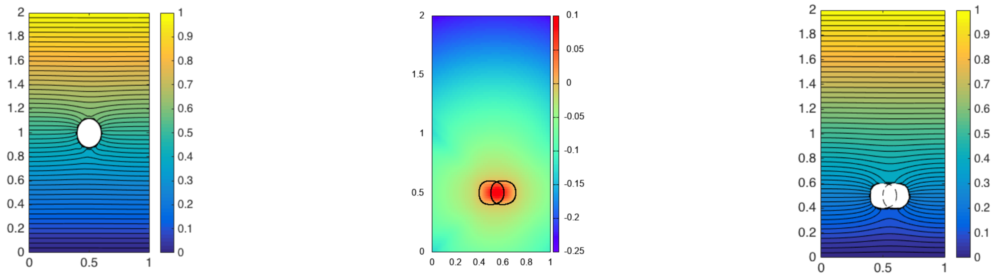
The trimmed distance field, $g(\mathbf{x})$, is now given by the R-function [7],

$$g(\mathbf{x}) = \sqrt{f^2 + \frac{(|\Phi| - \Phi)^2}{4}} = \begin{cases} |f(\mathbf{x})| & \Phi(\mathbf{x}) \geq 0 \\ \sqrt{f^2 + \Phi^2} & \Phi(\mathbf{x}) < 0 \end{cases} \tag{2.8}$$

Within the trimming region, the original implicitization is recovered, while outside the region a composite field is obtained. Usage of the R-function ensures that the subsequent distance field is smooth. Trimmed level sets generated for the sphere octant are shown in Fig. 1b; it can be seen that the level sets are globally monotonically increasing.

For parametric splines such as NURBS, Eq. (2.1), and therefore the resultant, change with each knot span. Such splines are decomposed into their Bézier segments, trimmed distance fields are obtained for each Bézier segment and R-disjunction [6] of these distance fields is used to generate a smooth distance field for the parametric spline.

Closed geometries divide the space into inside and outside regions, thereby allowing definition of signed algebraic level sets. As a convention, distances in the inside region are assumed positive and those outside, negative. Signed level sets can be used to resolve point containment queries, required in multi-body contact and interference detection. A bounding box procedure is used to handle containment queries in a point-by-point basis [10]. A close-fitted bounding polygon is constructed for the closed spline geometry, from the convex hulls of individual Bézier components. For each Bézier component, the sign of the Dixon resultant $\Gamma$ is set such that the resultant is negative for control points that lie on the bounding polygon (and hence outside the geometry). This is a one-time process for a given geometry. During sign determination, the point of interest is first classified with respect to the bounding box. If the point is outside the bounding box, then it is also outside the given geometry and its distance can be taken to be negative. Query points that lie inside the bounding box are then classified with respect to the convex hulls of the Bézier components. If the point lies inside any of the hulls, then the sign of the distance is the same as the sign of the Dixon resultant of the corresponding Bézier component, evaluated at the



(a) (b) (c)

Fig. 2: Contours of the electric potential solution for a system with (a) single void (c) two overlapping voids. (b) Algebraic level sets for a multiple void system generated using R-Function Boolean operations

point of interest. If the query point does not lie inside any of the individual convex hulls, but lies inside the bounding box, then it lies inside the closed geometry and its distance can be taken to be positive. Signed algebraic level sets for a sphere are given in Fig. 1c as an example.

Current Through a Line with a Void:

As an application, the electrostatic problem of a line with a void is considered. This is of relevance in studying void growth due to electromigration, a failure concern in the semiconductor industry. A rectangular domain $\Omega$ with an arbitrarily shaped void is considered. To allow irregular shapes, voids are represented using NURBS. The electric potential $\phi$ is solved for from the Laplace equation, $\Delta\phi = 0$ in $\Omega$. Dirichlet boundary conditions are applied at the top and bottom surfaces, and no electric flux is assumed to flow through the walls. Additionally, there is no flux entering or exiting the surface of the void $\Gamma$,

$$\frac{\partial \phi}{\partial n} = 0 \quad \text{on } \Gamma \tag{2.9}$$

Here, an enriched isogeometric approach is used [8], where the potential is expressed as a weighted blending of a continuous approximation $\phi_c$, and an enrichment $\phi_e$ representing the influence of the void,

$$\phi(\mathbf{x}) = (1 - w(\mathbf{x}))\, \phi_c(\mathbf{x}) + w(\mathbf{x})\phi_e(\mathcal{P}(\mathbf{x})) \tag{2.10}$$

Here, $\mathcal{P}(\mathbf{x})$ is the projection of $\mathbf{x}$ on to the void interface. Thus, the potential solution $\phi_c$ at $\mathbf{x}$ is blended with the interface solution $\phi_e$ at the projection of $\mathbf{x}$ on the void interface. The weight function $w(\mathbf{x})$ is defined such that it is 1 on the void surface and falls monotonically with distance away from the surface,

$$w(\mathbf{x}) = \exp\left(-(d/d_0)^2\right) \tag{2.11}$$

where $d_0$ is a scaling parameter for the distance field $d(\mathbf{x})$. Since the void is represented as a NURBS curve, a signed distance field can be obtained using the algebraic level sets described in this work. This form of the electric potential automatically satisfies the void boundary condition Eq. (2.9). The system is solved using isogeometric analysis for an elliptical void, and the resulting potential solution is shown in Fig. 2a. The potential lines are distorted around the void to satisfy Eq. (2.9), but unaffected far away.

Boolean Operations for Multiple Void Systems:

Complications in electromigration problems usually arise when multiple voids interact. These voids can merge and separate, and this poses a challenge for explicit interface representations. Such representations usually require detection of overlap between multiple voids and computation of their intersections, which are challenging problems for arbitrarily shaped voids. In this work, this problem is circumvented by using Boolean operations on the algebraic level sets. A Boolean union operation is used to generate level sets of a coalesced void from the algebraic level sets of individual voids. Since the analysis procedure depends only on the algebraic level sets, interacting voids can be easily accommodated without requiring collision detection and intersection computations. The union operation is carried out using the R-disjunction operation [6]. If $g_1(\mathbf{x})$ and $g_2(\mathbf{x})$ are the signed distance fields of two coalescing voids, then the union of these fields is given by,

$$g(\mathbf{x}) = g_1 \vee g_2 = g_1(\mathbf{x}) + g_2(\mathbf{x}) + \sqrt{g_1^2 + g_2^2} \tag{2.12}$$

By nature of R-disjunction, the resultant field is positive when either field is positive; this ensures that the region inside the coalesced void is positive. This is depicted in Fig. 2b. The usage of R-functions ensures that the composed field is smooth, allowing analysis. The solution for the electric potential for two merged elliptical voids is provided in Fig. 2c.

Conclusions:

The Dixon resultant was used to generate algebraic level sets for parametric geometries. These level sets provided a measure of distance from the geometry, and were signed allowing point containment queries. An enriched isogeometric analysis method for the current in a line with a void was discussed, where the void was modeled as an enrichment whose influence weakened with distance. It was shown that topological changes such as coalescence could be handled through Boolean operations on the algebraic level sets, without having to resort to overlap detection and intersection computations. The developed procedure provides the benefits of using explicit interface representations without requiring intersection computation to model topological changes.

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