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Subdivision Surfaces for Procedural Design of Imprint Rolls

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Abstract

We discuss the use of subdivision surfaces in the procedural design of imprint rolls for use in the roller imprinting process. Roller imprinting is being developed for the fabrication of microfluidic devices in polymer substrates. Imprint rolls are modeled using Catmull-Clark subdivision surfaces, and are procedurally designed based on feedback from finite-element simulations of the imprinting process. Microfluidic devices exhibit repeating patterns, and can be modeled using a small set of unique entities (or tiles). Imprint rolls are also modeled as a sum of tiles, and rolls are designed by studying the imprinting behavior of clusters of tiles corresponding to the repeating patterns seen in the device. This approach reduces the roll complexity and analysis time. The rolls need to be described in a sufficiently flexible format for the tile-based analysis to be effective. Conventional model representations are too cumbersome for piecewise iterative refinement as they require the manipulation of a large number of variables to modify surface features while preserving continuity. Subdivision surfaces, on the other hand, are naturally continuous and can be modified by manipulating a small number of variables. The ability to apply rule-based, arbitrary refinement on subdivision surfaces makes them especially suitable. The procedural modeling methodology and the subdivision design representation enable the integrated design, analysis, and manufacturing of imprint rolls, and has proven effective in decreasing the design-to-manufacture time of novel microfluidic technology.

Keywords: Subdivision Surfaces, Procedural Design, Roller Imprinting, Finite Element Analysis

1 Introduction

Subdivision surfaces have been widely used for modeling and animation in computer graphics; however, despite this popularity there has not been much use of subdivision surfaces in mechanical design and optimization. In this paper we discuss a novel application of subdivision surfaces in mechanical design. Subdivision surfaces are applied in the design and optimization of imprint rolls used in the roller imprinting process. Mechanical imprinting processes involve the transfer of a design or pattern from a rigid die to a deformable workpiece by applying mechanical loads on the die against the workpiece. In the roller imprinting process, a cylindrical roll with raised features on its surface creates imprints by rolling over a fixed workpiece (please see Figure 1). For a given workpiece material, the precision and accuracy of the imprinted features is dependent on the features of the imprint roll. Precision is measured

by the positional accuracy of the pathways, the form error in the pathway channels, and the profile of the channel surfaces.

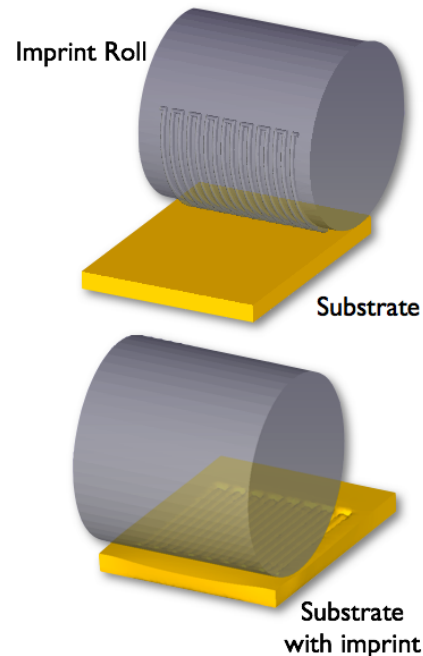


Figure 1: Schematic of the Roller Imprinting process. The imprint roll rotates and moves linearly, while the substrate is fixed.

Roller imprinting is being developed for the fabrication of microfluidic devices in polymer substrates. There has been growing interest in developing methods to rapidly and cheaply fabricate microfluidic devices [Whitesides 2006]. This requires the rapid design of the manufacturing process as well, which in the case of roller imprinting translates to the design and fabrication of the imprint rolls. Imprint roll design depends on not just the design of the microfluidic device being manufactured, but also on the imprinting process parameters and the substrate material properties. As it is difficult to analytically characterize this relationship, imprint rolls need to be designed based on feedback from the imprinting process. Using feedback from imprinting experiments can be resource intensive and time-consuming. Instead, the rolls are designed based on feedback from finite-element (FE) simulations of the imprinting process. Catmull-Clark subdivision surfaces are used in the design representation of the roll and the rolls are procedurally designed based on the microfluidic device design and the substrate material properties. Section 3 describes the procedural methodology and argues the need for flexible model representations. Section 4 discusses the limitations in using conventional representations such as NURBS surfaces. The application of Catmull-Clark subdivision surfaces for modeling the rolls is described in Section 5. In the next section, a brief overview of microfluidic device manufacturing is presented, followed by related work in subdivision surfaces and manufacturing process optimization.

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2 Background and Related Work

2.1 Microfluidic Devices

Microfluidics is the science and technology of systems that manipulate small amounts of fluids (in the pico-liter range) using micro- and nano-scale channels. Microfluidic devices (MFDs) are being increasingly used in a number of applications ranging from bio-defence to molecular biology [Whitesides 2006]. These devices exploit both the small feature sizes as well as the favorable properties of liquids at this scale [Beebe et al. 2002].

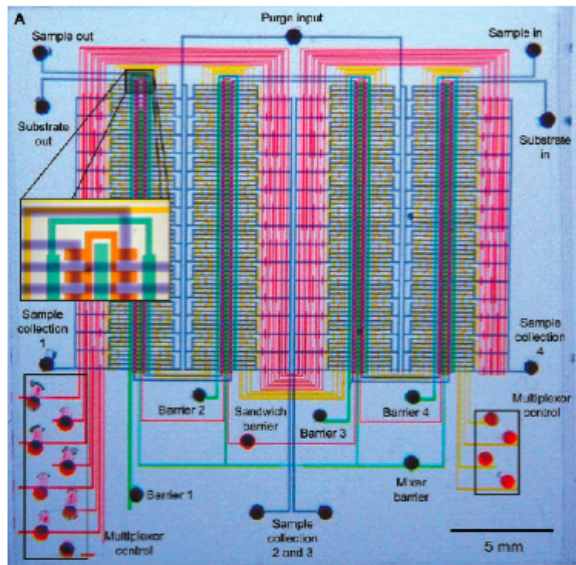


Figure 2: Example of a complex microfluidic device; contains hundreds of independently addressable valves and channels. The channels are 80 μm wide. Source: Thorsen et al. [25]

Microfluidic devices are usually designed as a network of pathway channels of uniform cross-section; chemical and biological analysis is performed as fluid flows down the channels. Hence, it is important that the devices have channels with precisely defined cross-sections and surface features. The channel surfaces may also have patterning and additional features to improve the performance of the devices. Microfluidic devices are usually composed of multiple layers operating in unison to control the in-plane and out-of-plane flow of fluids [Nguyen and Wu 2005]. Hence, the overall spatial configuration of the pathways in each of the layers is very important for the device to perform efficiently. Figure 2 shows a complex multi-layered microfluidic device consisting of thousands of valves and hundreds of independently addressable channels for analysis [Thorsen et al. 2002].

In a recent review [Whitesides 2006] discussed the problems that need to be addressed for the widespread development and adoption of microfluidic technology, highlighting the importance of good design and manufacturing processes for the commercialization of these devices. While there has been considerable research in developing manufacturing technologies for microfluidic devices [Ziaie et al. 2004], there is a paucity of work that addresses ways to control the precision of the manufacturing technologies. There has been even less work in integrating device precision with the manufacturing process design – an approach essential for developing cost-effective microfluidic devices. Our work in this paper is motivated by the need for developing processes with well-defined relationships between process design and device precision.

2.2 Subdivision Surfaces

Subdivision schemes describe smooth curves and surfaces as the limit of a sequence of successive refinements on a given input control mesh [Zorin and Schroder 2000]. [Catmull and Clark 1978] first discussed a method for generating surfaces that approximated cubic B-spline surfaces from meshes of arbitrary topology. For rectangular control meshes Catmull-Clark subdivision at the limit generates a B-spline surface, while for arbitrary meshes a B-spline surface is generated everywhere but at a small number of extraordinary points. Repeatedly applying Catmull-Clark subdivision to an arbitrary mesh results in a mesh with quadrilateral elements everywhere except around extraordinary points.

We use the Catmull-Clark subdivision scheme in modeling the imprint rolls as it is very suitable for mechanical part representation. B-spline and NURBS surfaces, which are commonly used in engineering design and analysis, can easily be represented using Catmull-Clark subdivision and vice-versa [Peters 2000]. Quad-meshes are also more suitable for mechanical parts due to the rectangular symmetry seen in the parts. Adaptive subdivision methods have also been developed based on Catmull-Clark subdivision [Pakdel and Samavati 2005], and help in reducing the mesh complexity.

There has been very limited work in applying subdivision surfaces for modeling mechanical parts. [Gonsor and Neamtu 2001] investigated the usefulness of subdivision surfaces in modeling for engineering applications and concluded that more work is required before they can be effectively used. They highlighted some of the advantages and disadvantages subdivision surfaces hold over the traditional NURBS-based surfaces used in engineering applications. In Section 5 we argue why subdivision surfaces are suitable in our application despite some of these disadvantages.

While prior researchers have demonstrated the advantages of integrated modeling and analysis with subdivision surfaces [Green et al. 2002] [Cirak et al. 2002], these methods require the development of custom, subdivision-based numerical solvers. There has not been much work done in using subdivision surface representations with commercial numerical solvers.

2.3 Manufacturing Design Optimization

Finite element analysis and other numerical methods have been used extensively to study the effect of tooling design in forming and forging processes [Hartley and Pillinger 2006]. The capability of numerical methods for tooling design are limited by the design representations of the parts analyzed. Using B-spline surfaces places a topological limitation on the part features. NURBS-surfaces somewhat relax this limitation, but the optimization problem is more complex due to the increase in the degrees of freedom. Moreover, 3D simulations require the optimization of shapes described using multiple NURBS and B-spline patches, and it is very difficult to optimize the surface shapes while obeying continuity requirements at the interface of the patches. [Gonsor and Neamtu 2001] identify this as a major limitation in using NURBS surfaces for engineering analysis.

3 Procedural Modeling

The feature complexity seen in microfluidic devices makes it tedious to manually design imprint rolls. Moreover, the effect of the substrate material properties and imprinting process parameters on the imprint geometry should be accounted for in the roll design, and this makes manual design even more challenging. We know from 2D imprinting simulations that the imprint precision (for a given

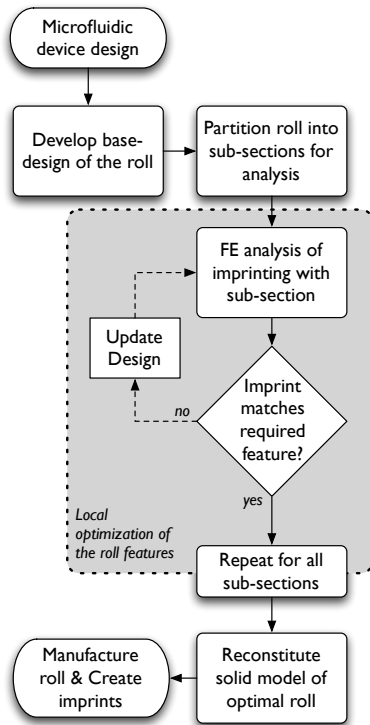


Figure 3: Procedural modeling methodology

set of process parameters and material properties) is a function of only local features [Vijayaraghavan et al. 2008]. The 2D imprinting analysis also showed that the spacing (or linear pitch) of the roll features had a very strong influence on the shape of the imprints created. Hence imprint shape is not a function of all the features in the roll, but only of the features nearest to the imprint. Classic results from metal plasticity and deformation behavior also confirm the local nature of material deformation [Hosford and Caddell 2007].

Hence, imprint rolls are designed procedurally based on the microfluidic device design, the imprinting process parameters, and the substrate material properties. The local deformation behavior of the substrate during imprinting is used in modeling the roll. Since it is difficult to analytically model the substrate deformation, finite-element simulations are used and the roll is designed piecewise locally. Piecewise design and analysis has the additional benefit of decreasing computational time.

The procedural design methodology is as follows (please see Figure 3). The input for the design process is the microfluidic device design, the device material properties, and the imprinting process parameters. Based on the microfluidic device design, a base-design (or zeroth iteration) of the imprint roll is modeled. The model is then partitioned into sub-sections for analysis. Following this, finite-element analysis (FEA) of the imprinting process is used to iteratively design regions of the roll corresponding to the sub-sections. The roll features are then modified based on analyzing the conformance (or fitness) of the imprinted feature from the finite-element analysis to the required feature. This process is iterated until the imprinted features match the required device features within a specified tolerance. The features modification is carefully controlled to ensure that the iterations converge. All the sub-sections are analyzed this way, and a final imprint roll is composited from these results. Micro-machining processes are then used to manu-

facture the roll, with which imprints are created.

For the procedural methodology to be effective, we require the following:

- Accurate FE-analysis of material deformation
- Optimization loop converging to a valid solution
- Minimal error during roll partition and re-constitution

3.1 Tile-Based Modeling

The effectiveness of procedurally modeling the rolls depends largely on the ease in which the roll model can be partitioned into sub-sections for analysis. Procedurally implementing the partitioning can be challenging due to the complexity of the devices. Hence, the roll model should be described in a way that allows for easy partitioning. This can be achieved by exploiting the pattern redundancy commonly seen in microfluidic devices. We describe microfluidic devices using a set of repetitive entities, or tiles. Due to the regularity of features in the device designs, devices can be fully described using a small set of unique tiles. For example, the most common types of fluidic pathways designs have regularly spaced, orthogonally intersecting straight channels. Devices with this pathway design can be described using a unique set of five tiles (please see Figure 4). Each of these tiles can be oriented in four different ways by in-plane rotation, and thus there are a total of 15 possible tiles that can be used (discounting the symmetry cases). Figure 5 shows an example of a pattern being represented with this set of tiles. We have addressed some of the advantages of this tile-based approach in an earlier work [Vijayaraghavan and Dornfeld 2007].



Figure 4: Set of tiles for modeling microfluidic devices with regularly spaced, orthogonally intersecting straight channels. Dark regions denote the fluid pathways. The tiles are shown in top-view.

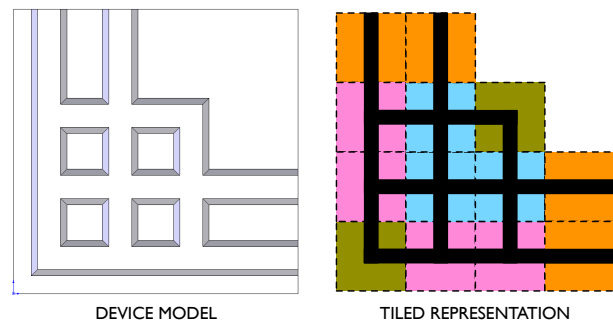


Figure 5: Example of a device model represented as a set of tiles.

Imprint rolls for a microfluidic device design are modeled with the same tiles as the device. The tile-based model provides a flexible way to partition the roll into sub-sections for analysis. The sub-sections can be as small as one tile, or can be a group of tiles that represent some specific, repeating pattern. The next section discusses finite-element analysis (FEA) using the tile-based representation.

3.2 Finite Element Analysis with Tiling

With this tile-based description, it is easy to study the imprinting behavior of specific, repeating patterns seen in the imprint roll. Figure 6 shows FEA results from imprinting a pattern compared to imprinting sub-sections of the same pattern. The sub-sections are chosen to represent a repeating feature seen in the pattern (in this case, a serpentine feature and a cross-hatch feature). The imprints from the latter case were compared to the former case, and both the stress fields as well as the surface features matched within a 1% error. The reduced analysis also showed a marked decrease in the computational time when compared to the full analysis as analysis time scales linearly with the number of tiles in the model. The reduced analysis took approximately 25% of the time as the full analysis (16 tiles, vs. 64 tiles). Microfluidic devices are usually modeled with hundreds of tiles, and given that the repeating patterns are usually modeled with tens of tiles, the tiling analysis can potentially decrease the computational time by an order of magnitude.

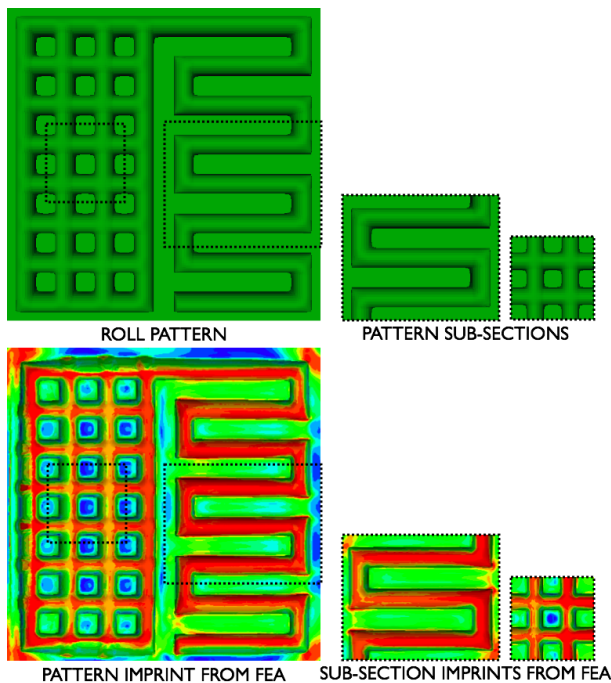


Figure 6: Comparison of substrate features from imprinting with entire roll and imprinting with sub-section patterns of the roll. The colors in the imprints correspond to stress-fields.

4 Limitations of Conventional Model Representations

Using conventional solid model representations in the procedural modeling of the imprint rolls poses two main problems: in the creation and optimization of parametrically modeled tiles, and in discretization for numerical analysis. It is necessary to model the tiles parametrically to allow for open-ended design optimization. But with conventional model representations such as B-Spline and NURBS surfaces, the topology of the tile is fixed, limiting the feature optimization possible. NURBS surfaces also limit the use of local refinement. This drawback of NURBS surfaces in design refinement was highlighted by [DeRose et al. 1998]. They argued that refining NURBS surfaces required the addition of entire rows or columns (or both) of control-points. They also pointed out the dif-

ficulty in creating smooth surfaces due to the seams of intersecting NURBS patches. It is also much more complex to optimize surfaces made of multiple patches, especially if requirements of continuity have to met at the patch interfaces.

NURBS surfaces also have to be discretized when they are used in numerical analysis of the imprinting process. Due to the multiple, local parameterizations in NURBS surfaces, surface discretization is usually a complicated process and it is difficult to realize error-free discretization, leading to further errors when meshing the models for finite-element analysis. Additional errors are also seen at the interface of tiles when individually modeled tiles are joined using boolean operations. Figure 7 shown an implementation of tile-based modeling in the ACIS solid modeler. Gaps and seams are seen in the intersection of some of the tiles, which led to errors during meshing for finite-element analysis.

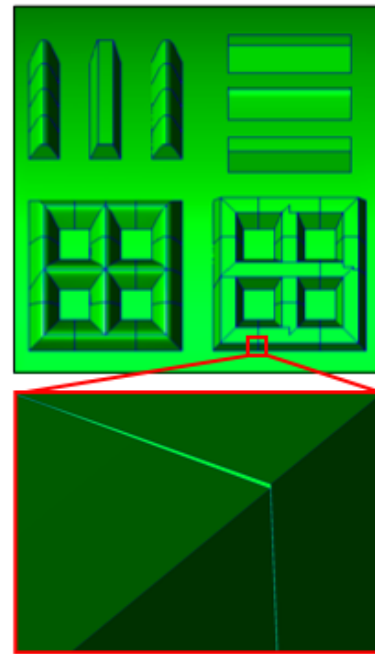


Figure 7: Boolean error at tile interface in ACIS model of Roll.

4.1 Requirements for Procedural Modeling

Based on the procedural methodology and based on the limitations seen in conventional representations, the following requirements are identified for modeling imprint rolls:

- Ability to create parametrized surfaces which can be joined easily
- Capacity of local feature refinement for model optimization
- Ease of discretization for application in numerical methods.

5 Modeling with Subdivision Surfaces

Subdivision surfaces satisfy these requirements for procedural modeling. Subdivision surfaces are piecewise polynomial patches which can be arbitrarily sectioned for analysis. They preserve continuity properties everywhere in the mesh (for example, Catmull-Clark surfaces are C_2 everywhere except at extraordinary vertices, where they are C_1). They also have a global parameterization based

on the limit surface they converge to [Gonsor and Neamtu 2001]. Moreover, since subdivision can be used to represent surfaces both smoothly and as a discretized mesh, they can be easily applied in numerical analysis. In this section we examine the advantages subdivision surfaces offer over conventional representations in the procedural design of imprint rolls, and discuss the use of subdivision surfaces in creating models using the tiling approach.

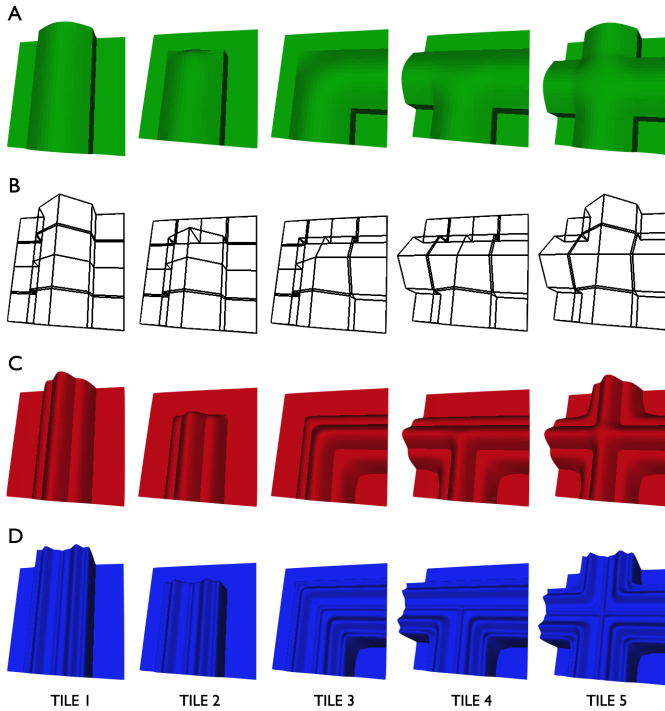


Figure 8: Tiles from Figure 4 are modeled with subdivision surfaces. A: With a simple curved cross-section. B: Control mesh for tiles in A. C: With a ridged cross-section. D: With a serrated cross-section.

With subdivision surfaces, tiles are created as a mesh of control points. The number of control points in the initial tile-mesh is chosen depending on the complexity of the features in the tile. Figure 8 shows examples of tiles (corresponding to those shown in Figure 4) created with different cross-sections. Note that the tiles do not need to have a rectangular control mesh, and that their parameterization is not limited to the uv parameterization seen in NURBS surfaces.

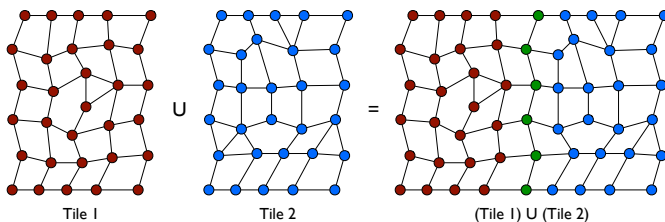


Figure 9: Joining tiles by updating mesh connectivity. The green nodes denote the common vertices.

Using subdivision surfaces for tiles also makes it easy to union them into a full model of an imprint roll. Since tiles are designed to be regular and repeating, their control meshes are designed such that they have common edges along which they can be joined. It has to be noted here that the tiles are created and joined into the full roll

before refinement and optimization - hence the union operations can exploit the common edges in the tiles. After a full model of the roll is created, mesh refinement and modification is done to ensure that refinement can happen smoothly across the interfaces of the tiles. To join two tiles along an edge, vertices of the tiles are first combined by overlapping the common row of vertices along the edge. Following this, the connectivity of this new tile is set by combining the connectivity information of the original tiles. With this method the seams between the tiles are water-tight and have no redundant vertices, leading to smooth interfaces when the tiles are subdivided. Figure 9 illustrates this method. Figure 10 shows examples of rolls created using multiple tiles.

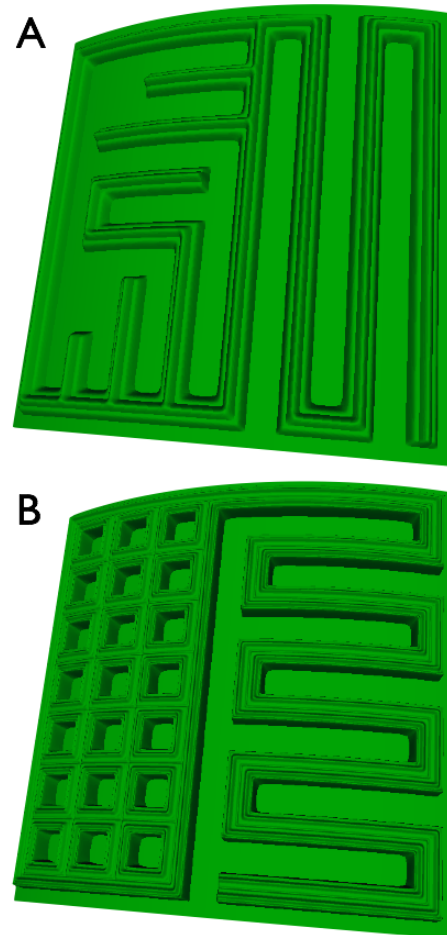


Figure 10: Rolls modeled with multiple tiles. A: Roll with ridged cross-section features. B: Roll with serrated cross-section features.

A similar strategy may also be adopted with NURBS patches when only rectangular meshes are needed for the tiles. A problem however, is that we do not a priori know the parameterization required when defining the patches. Creating tiles with a very sparse parameterization may restrict the features that are possible during optimization, while creating with a very fine parameterization may unnecessarily increase the degrees of freedom in the model. For non-rectangular meshes multiple NURBS patches will be needed, making optimization even more difficult.

The use of subdivision surfaces in modeling the imprint rolls enables local refinement and optimization of the roll features. The tile-based representation makes it easy to study small sections of the roll (as illustrated in Section 3), and features can be controlled

and modified locally by manipulating the subdivision control mesh. The extent of control over the local features can be tweaked by operating on the control mesh at different levels of subdivision. We are currently developing algorithms to optimize the roll design based on iterative local subdivision mesh manipulation.

6 Implementation

Catmull-Clark subdivision meshes for the roll models were implemented using a half-edge data structure [Botsch et al. 2002]. The semi-sharp scheme from [DeRose et al. 1998] was applied to model feature edges and corners. Semi-sharp schemes are very important when modeling mechanical parts because perfectly sharp corners and edges cannot be manufactured. This is especially the case for the rolls as they are manufactured using end-milling, and the smallest radius achievable at an edge with end-milling is limited by the radius of the tooling used. Details of the finite-element analysis implementation, including meshing, boundary conditions, and workpiece material properties are discussed in more detail in [Vijayaraghavan et al. 2008].

7 Conclusions

Subdivision surfaces are more appropriate for application in the procedural design of optimal imprint rolls than conventional NURBS-based representations. The flexibility of subdivision surfaces in simultaneously providing both a discretized and a smooth representation is exploited in the design methodology. It is also convenient to change the features of the roll on an ad hoc basis while preserving properties of continuity in the mesh. Rule-based, arbitrary refinement is also easy to apply to subdivision surfaces, making it very suitable for procedural modeling. However, more research is needed before subdivision surfaces can be used for general-purpose mechanical modeling. Describing analytical features can be difficult, and much of the benefit of local part refinement is lost when the model does not require any embellishment. It is also difficult to perform “true” boolean operations with subdivision surfaces, which limits its applicability in general purpose modeling.

Our procedural modeling methodology and the subdivision design representation contribute towards developing a specialized framework for the integrated design, analysis, and manufacture of imprint rolls. The framework provides a flexible representation for modeling the rolls, and a functionally driven procedural methodology for designing them – both of these components work seamlessly together to enable true integrated design and analysis of the imprint rolls. This approach has proven effective in decreasing the design-to-manufacture time for novel microfluidic technology.

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