Shape optimization for temperature regulation in extrusion dies using microstructures

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Plastic profile extrusion – a manufacturing process for continuous profiles with fixed cross section – requires a complex and iterative design process to prevent deformations and residual stresses in the final product. The central task is to ensure a uniform material velocity at the outlet. To this end, not only the geometry of the flow decisively influences the quality of the outflow, but also the temperature profile along the flow channel wall. It is exactly here that this work contributes by presenting a novel design approach for extrusion dies that will allow for optimal temperature profiles. The core of this approach is the composition of the extrusion die through microstructures. The optimal shape and distribution of these microstructures is determined via shape optimization. The corresponding optimization procedure is the main topic of this paper. Special emphasis is placed on the definition of a suitable, low-dimensional shape parameterization. The proposed design-framework is then applied to two numerical test cases with varying complexity.

1 Introduction to the challenges in numerical extrusion die design

In this work, we present a framework that explores passive temperature control through manipulation of the underlying geometry. Although the main focus is on their potential in the context of plastics extrusion, the methods presented in the following can be employed wherever local and flexible temperature regulation is required, whilst keeping weight and material costs to a minimum.

Continuous plastic profiles with a fixed cross section – examples are technical profiles, pipes or skirtings, as well as rubber seals – are generally manufactured via the process of plastics profile extrusion. During this process, a continuous flow of plastics melt is pressed through a shape-giving die and subsequently cooled down and solidified. Unsurprisingly, the geometry and structure of the extrusion die are decisive for the quality of the final product – emphasizing the importance of its design.

The design process of an extrusion die presents the engineer with multifaceted challenges. On the one hand, the list of design objectives is long, containing elements like low pressure loss or a homogeneous outflow-velocity profile. Note however, that the latter is usually considered the most relevant criterion [1]. On the other hand, the highly nonlinear behavior of the plastic melt causes complex effects like die swelling, which are difficult to predict. As a consequence the classic design process often relies on trial and error procedures that are regulated by user-specific domain knowledge. In view of the high time investment and prototyping costs that are associated with this procedure, numerical optimization of the related components has gained much importance in recent years. In the past, these optimization attempts mostly concentrated on the flow channel geometry, either by modifying a distinct set of geometric features [2,4] or by using spline-based approaches [5,6].

In most cases, the flow is considered isothermal [4,5], or constant wall temperatures are assumed [7,8]. The use of such boundary conditions or assumptions is motivated in that the optimization is reduced to the analysis of the melt. Furthermore, simplifications such as isothermal flow can reduce the computational costs significantly. In general, these assumptions are well justified and closely connected to the standard processing conditions, where the extrusion die is homogeneously heated using a heating band. If one can instead locally control the temperature at the flow channel wall, a new optimization opportunity arises. Via local temperature modifications, the melt can be made more or less viscous, which then – next to the flow channel shape – leads to an additional parameter in achieving the desired flow velocity.

From a simulation point of view, this idea translates to modifying the temperature boundary conditions and optimizing the temperature distribution within the flow channel. In [8,9], Lebaal et al. study the effects of varying temperature boundary conditions on the flow. With a similar aim, the present work investigates how predefined temperature profiles can be obtained via microstructured extrusion dies. With the term ”microstructure” we refer to a set-up, where the volume between the extrusion die wall and the flow channel is filled with microtiles, possibly of different geometries or materials, instead of solid material. The microstructures are arranged in such a way that even with homogeneous heating via the heating band, an inhomogeneous temperature distribution can be achieved within the flow channel by passive heat transfer regulation based on the characteristics of the die.

The novel design idea of microstructured extrusion dies profits from modern manufacturing techniques; as the so far standard manufacturing processes for extrusion dies – wire
erosion and milling – do not allow for such a design. However, the recent developments in the area of additive manufacturing open up a completely new design space. In order to make full use of this new design space, the design process can be enhanced with numerical design strategies. State-of-the-art design strategies suitable for microstructures come from the field of topology optimization [10]. Most topology optimization approaches have in common that the geometry representation is voxel based. The clear advantage of this representation is generality. The drawback, however, is that the representation is not compatible with Computer Aided Design (CAD) programs and as such requires extensive post-processing in order to be included into the manufacturing workflow. Instead, within this work, we explicitly emphasize CAD compatibility. We thus restrict the design space to a base geometry that provides a foundation for optimization through appropriate parametrization.

A distinguishing feature of this work is the new paradigm for the design of microstructures using functional composition, presented in [11]. The resulting geometries are watertight and porous by design and not only provide great flexibility, but also CAD compatibility, a feature particularly striking in comparison with classical methods of constructing porous materials [12]. Employing this approach, it is possible to create regular structures, but also bifurcating models and even randomized porous models [13]. Applying such models in shape optimization of extrusion dies has been conceptionally proposed in [14].

In the present work, we will investigate a series of solutions for controlling the high generality of the chosen design representation. Several low dimensional parameter-sets are discussed that not only help to significantly decrease the computational effort but furthermore allow to restrict deformations and locally impose conditions on the allowed geometry modifications. Additionally, we investigate how the resulting parametrization framework can be included into a shape optimization framework.

In Section 2, we define the optimization problem, detail the solution procedure, and introduce suitable objective functions that help achieve the design goals. In the following Section 3, we state the governing equations and constraints and explain the different steps required to determine their solution. The geometric design-framework, along with different parametrization techniques, is presented in Sections 4. Thereafter, the presented concept is elucidated by means of two numerical examples in Section 5. Finally, Section 6 concludes the topic with a summary and gives a brief outlook on future work.

2  Shape optimization problem and optimization procedure

The proposed optimization problem considers the temperature distribution $T$ along the wall of the flow channel within the extrusion die. Here, the quality of the die is evaluated by means of an objective function based on the unknown temperature field, which itself implicitly depends on the parametrized domain. Hence, this problem fits into the category of PDE-constraint optimization. In the following, we will present the problem and a general solution procedure and various options for the corresponding objective function.

2.1 General solution procedure

We consider the objective function $J$ to be a measure for the quality of our temperature profile on the interior wall $\Gamma_N$. In our optimization problem, the partial differential equation in residual form – here denoted $\epsilon$ – acts as a constraint in our optimization. The complete problem then reads:

\[
\min_{\theta} J(T, \theta),
\]

subject to $\epsilon(T, \theta) = \theta$ on $\Omega_e = \Omega(\theta),

where $\theta$ denotes the design-vector containing all parameters necessary to describe our microstructure in the given framework.

Closed-form solutions of such problems are generally unavailable, hence the need for numerical methods. These approaches vary the parameters iteratively, evaluating the objective function at different points in the parameter space. Building on this idea, a modular shape optimization framework has been built, relying on three major components – a geometry kernel, a PDE-solver, and an optimization driver. The general outline of the optimization framework is depicted in Figure 1.

The geometry kernel is based on the geometric modeling framework itrit [15] which translates the design variables $\theta$ into a corresponding microstructured geometry. This geometry is subsequently sampled and prepared for analysis, which is performed using an in-house finite element solver. Thereafter, the objective function is evaluated based on the results of the temperature problem and returned to the optimization driver. Optionally, an additional step of determining the gradient is performed. The geometry kernel, the analysis tool as well as the optimization driver are modularly connected, which allows to exchange individual parts of the optimization framework. The modules “Geometric Modeling Framework” and “PDE Analysis” will be described in detail in Sections 2.2 and 4.

The updating step is performed by an external optimization driver, building on both gradient-based (e.g., [16]) or gradient-free approaches (e.g., [17]). While gradient-based algorithms generally converge faster, resulting in less objective function evaluations and thus a better performance, they also require knowledge of the gradient, which is in most cases analytically unavailable. In such cases, it can be determined using adjoint methods [18], algorithmic differentiation [19, 20], or by employing finite differences. While adjoint methods are computationally very efficient, they are also characterized by their implementational complexity and can generally not be used, in cases where the design-framework is composed of black-box components. Algorithmic differentiation and finite differences are generally more accessible, however, they also require costs in the...
2.2 Objective function

The choice of a suitable objective function is decisive for the result of an optimization. In this section, we introduce possible choices of objective functions that are suitable for the optimization problem Equation (1). Since extrusion is a steady process, we assume that the heat flux between flow channel wall and plastics melt is constant. Its value can, e.g., be determined using a coupled fluid-structure-interaction simulation. As such, the efforts made here can be regarded as preliminary for a fully surface-coupled simulation between the melt and the extrusion die.

We will further assume that – given a fixed channel geometry – there is an optimal temperature distribution $T_{\text{target}}$ on the inside of the flow channel. As shown by Lebaal et al. [9], this optimum is not necessarily given by a constant temperature distribution, as strongly pronounced edges and detailed features are particularly sensitive and might require a lower viscosity to achieve a uniform material distribution at the outflow. By suitable subdivision of the surface of interest, particularly influential areas can be further highlighted. This can help give even small sub-areas a significant impact on the global objective function. Given these principles, a function that evaluates the quality of a given parametrization looks as follows:

$$J(\theta, T) = \max_i w_i \| T - T_{\text{target}} \|_{L^p(\Gamma_{\text{f}}(\theta))},$$

(2)

where the temperature distribution is denoted by $T$ and the index $i$ is used to indicate the subsection. Choosing a low value $p$ for the integral norm draws more attention towards the overall deviation from the target profile, whereas a higher degree emphasizes strong local deviations. Here, the $L^2$ provides an analogy to the least squares approach for discrete problems. The extreme would be the choice of $p = \infty$, which corresponds to the supremum of the deviation within the given subdomain $\Gamma_{\text{f}}(\theta)$. If the subsections are of different size, the additional weights $w_i$ can be used to counteract the resulting effects, e.g., setting

$$w_i = \left( \frac{1}{\int_{\Gamma_{\text{f}}(\theta)} \, dS} \right)^{-1/p}.$$  

(3)

This subdivision helps to identify global deviations from the optimal distribution, alongside strong deviations in a smaller area of interest. The choice of the number and distribution of the subsection is to be performed meticulously. Too many subsections, or areas that are too small, can distort the overall picture, as the view might shift too much to individual regions. The right choice thus depends on the complexity of the geometry and must be evaluated on a case by case basis. Another possibility for the objective function is given by

$$J(\theta, T) = \sum_i w_i \| T - T_{\text{target}} \|_{L^p(\Gamma_{\text{f}}(\theta))}.$$  

(4)

Contrary to the first approach in Equation (2), this second objective function always takes all individual subsections into account. This can be advantageous, especially when only one subsection is dominating the overall performance or if differences in size between the subsections negatively impact the result. Further, it can be beneficial with certain optimization methods, as the use of the maximum can reduce the continuity of the objective function. The different objective functions are more thoroughly illustrated in Section 5.1.

3 Model problem

Building on the optimization framework described in Section 2, the following chapter will describe the analysis
stage in more detail. As has already been stated, the objective function, which is based on the temperature field, is constrained by partial differential equations. These underlying equations and assumptions will be discussed in the following.

3.1 Governing equations

The temperature distribution within the extrusion die is governed by the general heat equation for a non-uniform isotropic medium within the domain $\Omega$, which can be written in the form

$$\rho c_p \frac{\partial T}{\partial t} - \nabla \cdot (\lambda \nabla T) = f \quad \text{on} \quad \Omega,$$

(5)

with temperature field $T$, density $\rho$, specific heat capacity $c_p$, and the thermal conductivity $\lambda$. The function $f$ describes volumetric source terms to account for cases, where additional heat is added to the system, e.g., through electric currents. As an approximation, it can in most cases be assumed that the extrusion process remains stationary after an initial settling period. Although it is generally possible to create meta-materials with various interesting thermal properties (e.g., [21]), we will only briefly discuss the integration of such materials into the optimization framework. Further, all heat transfer that might occur within the void of the microstructure will be neglected, hence assuming the internal walls to be adiabatic. One exemplary microstructured extrusion die is depicted in Figure 2.

![Fig. 2: Exemplary microstructured extrusion die with boundary indication](image)

The required boundary conditions are twofold. On the outside of the extrusion die, denoted as $\Gamma_D$, a heating element with temperature $T_0$ is attached. The die is heated to prevent the flow channel from clogging, which can be provoked by a temperature drop and according changes in the melt’s viscosity. Along the interior walls of the flow channel $\Gamma_N$, improper blending of the plastic melt, but also non-uniformity within the temperature profile result in locally varying heat fluxes $q_m$. Accordingly, the boundary conditions are chosen as:

$$T = T_0(x) \quad \text{on} \quad \Gamma_D, \quad \frac{\partial T}{\partial n} = q_m(x) \quad \text{on} \quad \Gamma_N.$$

(6)

Although the geometry of the computational domain $\Omega$ might change, the proposed optimization framework considers the imposed boundary conditions as constant and given. Further, the outer geometry, i.e., the contour of the domain, remains unchanged, including the geometry of the flow channel within the extrusion die.

3.2 Discretization of the governing equations

The result of the geometry parametrization is given by a spline-based representation of the extrusion die using volumetric trivariate splines [22]. Subsequently, this representation is then regularly sampled and prepared for analysis, resulting in a mesh representation of the computational domain. The set of underlying equations as presented in Section 3.1 is then solved using a finite element approach. The resulting mesh is provided to an in-house solver, which is based on a highly templatized C++ library, aiming to maximize compiler optimization extensively and using a-priori knowledge at compile time where possible.

4 Geometric modeling

The underlying geometrical model is constructed using a composition of microstructures as introduced by Elber in [11]. In this section we will recall the main features of this approach alongside the necessary adaptations to the optimization process, therefore reintroducing and extending the notation employed in [11].

4.1 Recalling the microstructure construction

As illustrated in Figure 3, the full structure consists of a microtile $M$, which is repeatedly set into a macro-spline, also called deformation function, via functional composition. Each microtile in itself is a combination of curves, surfaces and/or trivariates. The $n_p$ geometrical parameters of an individual microtile are collected in a parameter vector $P_{ij}^M$. The macro-spline, instead, is specified by a trivariate Bézier or B-spline function $T : D \subset \mathbb{R}^3 \rightarrow \mathbb{R}^3$, which maps from the parametric domain of the deformation function into the physical space. During the composition, resulting in the microstructure $T(M_{ijk}) \forall i, j, k$, the microtiles are (typically periodically) placed into the parametric domain $D$ along a grid $(n_s, n_r, n_c)$. In case of B-spline deformation functions, this microtile grid is aligned with the non-zero knot spans. This ensures an undisturbed composition, remembering that the continuity at knots is finite.

As described in the previous paragraph, the resulting microstructure can be fully characterized by the parametrized microtile $M$ with parameters $P^M$, the grid dimensions $(n_s, n_r, n_c)$, and the deformation function $T$. Here, the distribution of the individual building blocks is predetermined by the choice of the deformation function. However, the tile’s distribution within the microstructure has a significant influence on the quality of the composed geometry. Therefore, we introduce a new set of parameters $P^{T}$, which aim to modify the deformation function’s parametrization. This parametrization is constraint by (1) the contour of the macro-spline, which should remain unaltered and (2) the alignment...
4.2 Parametrization of the deformation function

The deformation functions $\mathcal{T}$ are defined using trivariate B-spline representations. This geometry representation is not necessarily unique in a broader sense, meaning that there can be more than one spline representation resulting in the same outer geometry, which differ in their internal parametrization. As the microtiles are set into the parametric domain of the individual elements of the deformation function resulting in the microstructure by composition.

of the grid dimensions within the non-zero knot spans. The appropriate choice of said parametrization is based on the non-exclusivity of the B-splines, i.e. the existence of different representations for the same contour. Recalling the algorithm originally presented in [14], we extend it to include a possible optimization of the deformation function as well as a possible abstraction of the microtile parameter set $\mathcal{P}^M$, as presented in Section 4.3. The resulting procedure is depicted in Algorithm 1.

The optimization-specific parametrizations of both the outer as well as the inner geometry will be described in more detail in Sections 4.2 and 4.3 respectively.

Algorithm 1: Microstructure synthesis during optimization adapted from Antolin et al. [14], extending it by parametrization of the deformation function as well as local parameter retrieval.

**Input:**
- $\mathcal{M}$: a parametric microtile parametrized with respect to $\mathcal{P}^M_{ijk}$
- $\mathcal{T}$: a deformation function parametrized with respect to $\mathcal{P}^T$
- $(n_x, n_y, n_z)$: the grid dimensions
- $\mathcal{O}$: an optimization routine
- $\mathcal{P}^M(\xi, \mathcal{P}^M)$: microtile parameter abstraction and global parameters $\mathcal{P}^M$

**Output:**
- $\mathcal{M}$: microstructure
- $\mathcal{P}: \{\mathcal{P}^T, \mathcal{P}^M\}$: optimized set of parameters

**Algorithm:**

1. $\mathcal{P} \leftarrow$ Initialize parameter set;
2. **while** not optimized **do**
   1. $\mathcal{M} \leftarrow \emptyset$;
   2. $\tilde{\mathcal{T}} \leftarrow \mathcal{T}(\mathcal{P}^T)$;
   3. **for** $(i, j, k) \in (n_x,n_y,n_z)$ **do**
      1. $\mathcal{P}^M_{ijk} \leftarrow \mathcal{P}^M(\xi, \mathcal{P}^M)$;
      2. // retrieve microtile parameters from location in parametric space
      3. $\mathcal{M}_{ijk} \leftarrow \mathcal{M}(P^M_{ijk})$;
      4. // redefine microtile
      5. $\tilde{\mathcal{M}}_{ijk} \leftarrow \tilde{\mathcal{T}}(\mathcal{M}_{ijk})$;
      6. // functional composition
      7. $\mathcal{M} \leftarrow \mathcal{M} \cup \tilde{\mathcal{M}}_{ijk}$;
      8. // add to microstructure
   4. $\mathcal{P} \leftarrow \mathcal{O}(\mathcal{M})$; // update parameter set
**end**

Points, i.e. $i_k \neq \{0, m_k - 1\}$ do not contribute to the trivariate contour. As a consequence, they can be used to modify the tile density within certain areas. This approach is very limited in its scope, but still deserves to be mentioned as it might be sufficient in certain scenarios to distort the internal geometry of the microstructure.

If a more complex deformation approach is required, we propose to take advantage of the way microtiles are inserted into the non-zero knot spans individually. If we assume that the microstructures are generally much smaller than the outer geometry, then there is more than one microtile within each knot span. Using knot insertion, it is possible to take active control of the positioning of the microtiles by subdividing existing elements and simultaneously reducing the number of microtiles therein. The newly inserted knots can then serve
as parameters for the optimization and thus contribute to $P^T$. Similarly, if the deformation function is composed of a series of surface splines, this reparametrization approach can be applied to only a subset of the overall geometry representation, as is done in Section 3.2. Knot insertion is a standard operation that is very cheap to perform and thus does not meaningfully contribute to the cost of the optimization. This procedure is illustrated in Figure 4.

![Image of knot insertion](Image)

**Fig. 4: Refinement of existing elements via knot insertion to influence distribution of microtiles.** The upper image consists of a cubic B-spline with an open knot vector from 0 to 1 and no internal knots. Additional knots were inserted into the lower microstructures at $\xi = 0.3$ and $\xi = 0.7$ respectively. The colors indicate the respective knot spans, the dashed lines show the control grid.

In certain situations, the methods mentioned so far might be insufficient, because they do not allow to adjust the geometric position of knots. As the tiles are set into the individual knot spans, each knot restricts the placement of the tiles. This can potentially become a problem, especially when the macro-spline has a complex outline and thus requires a high number of knots. Although it might, in some cases, be possible to remove some of these knots without affecting the precision much [24], this is generally not the case. More complex approaches can take advantage of manufacturing precision, manipulating the geometry representation to a certain extent, where the final product is not affected. For instance, methods like spline fitting can be used to approximate the macro geometry with simpler representations. Although the exact outline of the deformation function is generally not preserved, this approach can reduce the complexity significantly. By presetting the knot vector, it is further possible to influence the distribution of the microtiles already in the approximation step.

The manipulation of the macro-spline influences the distribution of the microtiles within the microstructure. However, as the tiles are distorted by the deformation function, they also become smaller in denser areas and thicker in sparse areas (see Figure 4). In the case of heat conduction, this is an important disadvantage, because the average cross-sectional area within a region decisively influences the transmitted heat flux. Any benefits from an increased number of microtiles can be significantly reduced by the associated contraction. In order to counteract these effects, we will discuss ways to additionally modify the microtiles via appropriate parametrization in the following section.

### 4.3 Parametrization of the microtiles

The individual tiles can be adapted to the specific application both in terms of their geometry, but also with respect to more general aspects, such as their material parameters. This way, the individual microtiles $M_{ijk} = M(P_{ijk})$ can be adapted to local requirements before being inserted into the parametric domain of the deformation function. One possible adaptation is the modification of the material properties. Note, however, that even though such a modification might be very appealing from a simulation point of view, a subsequent realization of the resulting microstructured component poses significant demands on the manufacturing process; requiring either a vast range of different materials or the creation of meta-materials. As this is not widely available, we propose to resort to purely geometrical modifications.

Such a geometrical modification can be realized, for example, by parameterizing the thickness of a microtile. If we consider, e.g., a simple cross tile, as depicted in Figure 4, the individual widths of the branches towards neighboring elements, could serve as optimization parameters $P^M$. In order to ensure continuity between two neighboring microtiles, the thickness of two connected branches must be equivalent, while the center cuboid dimensions can be adjusted accordingly. More complex parametrization models are equally attainable, involving bifurcation techniques and microtile specific manipulations – e.g., with regard to angles, radii etc..

### 4.4 Parameter abstraction

As described in Section 4.3, several parameters may be necessary for each individual microtile, in order to realize the full potential of localized parametrization. If one now further considers the large number of microtiles involved in certain applications, such an optimization can quickly surpass 100,000 design variables. Such a high number of optimization parameters is infeasible in practice, especially if the optimization is performed by external blackbox drivers. Each evaluation of the objective function requires solving the underlying partial differential equation, which is the cost-defining operation for most applications. Hence, this motivates regrouping the parameter set using a small subset of super-ordinate parameters $P^M$, reducing the number of degrees of freedom accordingly. This reduced set of design variables then serves as a basis for optimization. The reclassification stage can further be used to show local correlations, e.g., affecting tiles in a specific region, providing some intuition for the resulting microstructured geometry.
Cubic scalar B-spline to be composed with the deformation function along with the geometry of the tile affecting the thicknesses of the tiles

One intuitive way of regrouping the parameter set is by defining functions within the parametric domain. These functions need to meet certain criteria. These include:

- at least \( C^0 \) continuity within the parametric domain \( D \),
- extendability,
- intuitive representation and local control.

The continuity of the resulting microstructure can only be attained if two adjacent tiles are continuous in the parametric domain. The mapping into the physical domain by means of composition can preserve this continuity. Further, it is generally favorable to have an extendable framework of equations, such that one can reuse previous results as a starting point for subsequent optimizations. Using some arbitrary set of \( n_{PP} \) basis functions \( \phi \) and super-parameters as coefficients \( \tilde{p}_i^M \), the parameters at the tile position \( \xi \) in the parametric domain \( D \) can be described using:

\[
\tilde{p}^M(\xi) = \sum_{i} \phi_i(\xi) \tilde{p}_i^M
\]

For sake of simplicity, hat functions would be a suitable choice, as they are easily extendable by adding more anchor points. These anchor points can be regularly spaced within the domain, but also be adapted to the locally required level of refinement. The choice of these basis functions can be arbitrarily complex and should be selected specifically for the problem. This allows to put special emphasis on certain properties of the geometry. Here, it is also beneficial to have non-negative functions to simplify compliance with the allowable range, e.g., to ensure positive values if the thickness of the building blocks is prescribed.

Based on the idea of basis function interpolation and the associated requirements, it comes natural to integrate spline basis functions into the framework, by introducing a separate spline that is evaluated to determine the individual microtile parameters. This approach is similar to the basic idea of isogeometric analysis [25], however, the spline that is used to determine the microtile parameters does not require the same representation as the geometry. As a consequence, any trivariate spline can be employed in this context. This concept is schematically presented in Figure 5. Both splines need to share the parametric domain \( D \), if this should not be the case, linear reparametrization must first be employed [23]. Also note that in some cases, additional constraints may apply, especially when two sides of the spline are conjoined. In this case, the parameters on these sides of the parametric spline must also be matched to ensure continuity of the parameters. Using the aforementioned spline techniques like knot insertion and order elevation, splines provide a versatile basis with modifiable continuity and complexity. Their non-negative basis functions further have the advantage that they facilitate setting constraints on the individual parameters only by their coefficients.

5 Numerical examples

We present two examples, where the previously introduced methods are applied to problems with varying complexity and different intentions. The first example serves to illustrate some of the above concepts in a more intuitive and schematic way, the second example shows their applicability to more complex geometries.

5.1 Cuboid microstructure

The first test case consists of a simple cross tile, which is placed into a \( 10 \times 5 \times 1 \) tile grid within a cuboid deformation function with dimensions \( 4 \text{ m} \times 2 \text{ m} \times 0.4 \text{ m} \). The tile’s thickness, i.e., the width of its branches, is parametrized. Further, the structure is geometrically closed on the top and bottom surface, to facilitate the imposition of boundary conditions. The cuboid is represented by a single linear Bézier spline, see Figure 6. The material is set to be homogeneous and isotropic. Due to its high geometrical complexity, the resulting finite element mesh consists of 353 280 trilinear hexahedron elements. Choosing an appropriate discretization ultimately determines the quality of the geometry approximation. In this numerical example, we sampled each splines regularly with 9 nodes in every parametric dimension, which led to a total of approximately 8500 degrees of freedom per tile. This rather fine discretization was only possible due to the small number of microtiles and has shown to be an appropriate compromise between computational effort and geometric exactness.

This first numerical example is separated into two parts. First, we will examine the objective functions mentioned above and investigate their influence on finding an optimum. Secondly, we will use our findings and introduce more parameters into our optimization.

We consider the following boundary conditions. On the bottom part of the cuboid, the temperature is fixed at \( T = 0 \text{ °C} \), whereas a heat flux is imposed on the top surface, pointing into the geometry, i.e., heating up the microstructure. The flux is irregular along the \( x \)-direction, described by...
the following equation:

\[
q_m(x) = \frac{27(4-x)x^2}{256} + 1, \quad \text{in} \quad \left[ \frac{K}{m^2} \right]. \quad (8)
\]

The target temperature profile is defined along the x-axis as a linear progression from 25°C on the left end to 30°C on the right end.

In this first example, we aim to evaluate the objective functions presented in Section 4.2. To this end, we subdivide the top surface into four distinct, equally spaced subsections. The thickness parameters of the individual tiles are interpolated using a linear function solely depending on the horizontal position x, as demonstrated in Section 4.3. Setting this function to a preset value of 0.13 at x = 0 m, we simplify the system to a single parameter, namely the thickness t_{x=4} at the right side of the depicted cuboid. By sampling the structure at various points, we will evaluate the different objective functions and discuss their influence on the result. The evolution of the different objective functions with varying thickness are displayed in Figure 7. The figure shows the course of the two objective functions presented in Equations (2) and (4). As the individual subsections are all of the same size (see Figure 6), all weights are chosen as w_i = 1. The third function was added in order to illustrate the effect of the subdivision. It is equivalent to Equation (4), but computed over the entire domain \( \Gamma_{\text{total}} \). Note in addition that with only one subsection, there is no difference in the resulting objective function. In this particular example, all objective functions show convex behavior for the given parametrization, which is beneficial considering optimization. In all cases, a distinct minimum can be determined, however, these optima are most pronounced for the sum-based objective function and the objective function that only considers a single section – note, that the graph is plotted logarithmically.

It is further interesting to discuss the influence of the subdivision of the surface into smaller subsections. For this purpose, Figure 8 shows the respective norm in the individual areas. From this representation, it is clear, that the mean deviation from the target temperature is smaller when no subdivision is considered. However, this global performance increase comes at the cost of more significant outliers, which is why the the maximum consideration is favorable, when even small areas can influence the overall result, as is often the case for plastic extrusion. Here, these small areas can already induce residual stresses, as the material flow can be influenced significantly.

In order to choose the best objective function, there are further aspects to consider. The maximum norm can also affect the convergence of the optimization algorithms. At points where there is a change of the dominant subdomain – i.e. where the "worst" subsection changes – kinks are introduced and consequently the objective function is only \( C^0 \) at these points. In particular, many gradient based methods, which require a certain continuity, can be impaired.

In the second part of this example we will perform an optimization whilst increasing the total number of parameters. The thickness distribution will now be represented by a B-spline trivariate, which is quadratic along the x-axis and linear in the remaining directions consisting of \( 4 \times 2 \times 1 \) control points (parameters). The thickness does not change along the z-axis, which results in 8 total design variables. The quality of the solution is assessed using the objective function from Equation (2), on the same subsections as presented in Figure 6. With the aforementioned considerations regarding the continuity and in order to avoid the costly calculation of the gradients via finite differences, the optimization utilizes the gradient free COBYLA (constrained optimization by linear approximation) algorithm [17]. Initially, all control points of the parameter spline were set to a constant value of 0.14, thus resulting in uniform microtiles. The comparison between the initial and the optimized geometry is illustrated in Figure 9. Further, the temperature distribu-
5.1 Subsections

The $\mathcal{L}^1$ norm of the error in each subdomain is plotted along the $x$-axis in Figure 8. The subdomains are numbered from 1 to 4, with each bar representing the $\mathcal{L}^2$ norm of the error in that subdomain. The mean $\mathcal{L}^2$ norm across all subdomains is shown at the rightmost bar labeled "Mean." The norms for subdomains 4 are $t_{x=4} = 0.156$ and $t_{x=4} = 0.152$.

![Fig. 8: $\mathcal{L}^2$ norms evaluated on the different subdomains.](image)

As was to be expected, uniform tiling leads to a temperature profile that strongly resembles the progression of the applied heat flux, with a pronounced peak in the area of maximum heat flux. Note that the ripples in the temperature profile are due to the increased heat transport in the center of the microtiles. Even though the differences between the two geometries are only subtle at first glance, the temperature distribution clearly shows an improvement with respect to the deviation from the target temperature. Indeed, already with such a simple configuration, the objective function value was reduced by about 72%.

5.2 Slit profile geometry

Building on these first results, we will reuse the cross tile in our second example to create a slit-profile extrusion die. As in the first test case, the outer geometry of the extrusion die is fixed. This follows from the specifications on the required plastic profile and assumes an optimized flow channel geometry. The desired cross section is a slit profile with circular edges. Here, all circular arcs are approximated by a fourth order B-splines to ensure the required polynomial representation. The geometry of the outflow is depicted in Figure 11.

![Fig. 9: Comparison between the initial and optimized geometry and the resulting temperature distribution](image)

![Fig. 10: Temperature distribution before and after the optimization. Graph expansion represents temperature distribution along the y-axis, with mean temperature shown with dashed line.](image)

In order to increase the efficiency of our calculations, we benefit from the die’s symmetry and only consider a quarter die in our simulations. The slit has a width of $w_s$ of 0.1 m, with an edge radius of 0.004 m, which corresponds to half the slit height, the radius of the circumference of the extrusion die $R_{ext}$ is 0.1 m. The inflow radius and extrusion screw connection (see Figure 12) has a radius of 0.025 m and the die has a total length of 0.1 m.

![Fig. 11: Definition of the outer geometry of the slit profile extrusion die for $\theta = 0.5$](image)

Compared to the previous example, the geometry parametrization is extended to also consider the deformation function in order to modify the microtile distribution within the microstructure. The extrusion die volume representation is formed through linear interpolation between two surface splines. Initially, the outer cylindrical wall is approximated by a fourth order B-spline consisting of a single element. In order to influence the distribution of the tiles within the optimization procedure, two additional knots are inserted at positions $\theta$ (matching the multiplicity of the corresponding flow channel surface) and $1 + \theta/2$, where $\theta$ acts as an optimization parameter. The additional knot at position $\theta$ is illustrated in Figure 12. At the flow channel surface, the element bound-
ary at knot $\theta$ lies at the intersection between the circular radius and the upper contour. The straight upper line is consequently divided in half by the second additional knot. The control points of the deformation function as well as the element boundaries are represented in Figure 11. It is entirely described by a single B-spline with degrees $3 \times 1 \times 2$ in angular, radial and axial direction, respectively. The resulting microstructure consists of a total of $12 \times 7 \times 9$ microtiles.

The thickness is described by a B-spline trivariate with quadratic polynomials along the angular direction and linear polynomials along the other directions. The parametric spline is defined using a grid of $4 \times 2 \times 2$ control parameters. Together with knot position $\theta$, this leads to a total of 17 design variables. The resulting microstructure is then discretized into trilinear hexahedral finite elements. Contrary to the first example, the individual tiles are sampled with a much coarser grid in order to save computational costs, resulting from the large number of microtiles. In this example, a single tile is discretized using approximately 350 elements, resulting in a total number of 466,832 degrees of freedom. To determine the gradient. Particularly, a quasi-Newton algorithm was employed, using relative finite differences to determine the gradient. The initial guess shows rather poor correspondence with the target temperature profile. The initial knot position $\theta$ was chosen at 0.3. The initial geometry along with the respective temperature field is shown in Figure 14a. The convergence tolerance was chosen to be $1 \times 10^{-5}$.

Contrary to the first example, the gradient based optimization algorithm was employed, using relative finite differences to determine the gradient. Particularly, a quasi-Newton algorithm was used [20]. This choice was motivated by the vast number of optimization parameters, where a faster convergence can ultimately reduce the number of total necessary evaluations, even considering the additional steps to determine the gradient. These expectations were confirmed by preliminary testing on a small scale example. As initial conditions, a regular thickness was described and the initial knot position $\theta$ was chosen at 0.3. The initial geometry along with the respective temperature field is shown in Figure 14a. The convergence tolerance was chosen to be $1 \times 10^{-5}$.

The initial guess shows rather poor correspondence with the target temperature profile. The average absolute temperature deviation from $T_{\text{target}}$ is approximately 71.3 K. This is also reflected in the objective function, which initially evaluates to 5.09. After 12 optimization steps, the objective function is reduced by factor 9.7. After 213 optimization steps (and 132 gradient calculations), the optimization
finished with an objective function value of 0.0506, reducing the objective function by more than 99%. The resulting microstructure is shown in Figure 14b. Further, Figure 13 shows the temperature profile as well as the deviation from the target temperature along the flow channel wall.

![Initial and optimized microstructure](image)

Fig. 14: Initial and optimized microstructure of the slit profile extrusion die. The knot position in the optimized configuration is at θ ≈ 0.163 which is reflected in the compression of microtiles on the right hand side.

Even after the optimization has been carried out, deviations from the desired temperature profile can still be observed at points along the flow channel. As in the first experiment, these are due to the docking sites of the individual microtiles. They can potentially be reduced by increasing the tile density and by broadening the wall surface. By inserting knots into the parameter spline and consequently augmenting the number of control points, the number of design parameters can be increased starting from the obtained solution, which shows the extendability of this approach.

6 Conclusion

A framework for the parameterization of microstructured geometries based on functional composition was presented and applied to the optimization of extrusion dies. The approach pursues two contradictory objectives, namely:

- Maximum geometric flexibility
- Minimum number of design parameters

In order to achieve these goals, methods were presented to independently influence the distribution of the tiles in the domain and to locally modify geometric and material-specific parameters thereof. The reduction of the potential degrees of freedom is performed via spline techniques and parametric basis functions. Special emphasis is directed to locality and intuitiveness. The quality of the resulting geometry is then improved using numerical optimization algorithms. Here, the influence of the choice of the quality function is discussed.

Two test cases illustrate the capabilities of the methods presented. The first use case exemplifies the idea based on an abstract academic example, focusing on the basic applicability of the above methods and the appropriate choice of the objective function. In a second step, the previously presented methods were brought to a realistic extrusion die geometry to demonstrate the applicability in an industrial context.

In future work, further attention will be given to the analysis part within the optimization cycle. Particularly, the potential of isogeometric analysis will be addressed. Recently, new methods, tailored specifically towards microstructures were presented by Hirschler et al. [27], to significantly reduce assembly costs. Furthermore, the possible use of adjoint methods will be explored, allowing to determine the gradient of the objective function in a cost-effective manner. The available gradient-based optimization methods have already shown great potential in initial tests, but were not suitable for practical use due to the high costs associated with finite differences. Lastly, an effort is made to couple the presented design-framework with melt-flow simulations through the extrusion die. This fluid-structure-interaction simulation will replace the currently still rather rigid Neumann boundary condition for the heat flux.

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References


