# An optimal shape matters

## Developing Scalable Shape Optimization Algorithms for Fluid Dynamics and Structural Mechanics

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### In Short

- In many design process of highly efficient devices, the shapes or the contour of material distribution determine the overall performace.
- In fluid dynamics the drag is a measurement of a design's efficiency; therefore it is necessary to invest high computational efforts into simulation and optimization.
- These are addressed within the field of PDE Constrained Shape Optimization
- We develop and investigate optimization algorithms which both exhibit scalability in extreme scales and are capable of handling complex shape contours involving geometric singularities.

Since many years now, computer simulations have become a state of the art substitute for expensive experiments in industry grade applications. In many situations, the underlying processes are modelled by partial differential equations (PDEs). The next level is then the optimal control or parameter identification in order to obtain a desired behavior of the system. A particular question is the one for an optimal shape of a specimen within the experiment leading to the field of PDE constrained shape optimization, which we are going to address here. With a tremendous number of applications, the field of shape optimization constrained to partial differential equations is one of the most active in the field of numerical optimization (cf. [1]).

In a natural way the description of shapes in three dimensional space leads to a large number of degrees of freedom. Especially when the application demands high resolutions of complex contours, there is no way around investigating, developing, and using efficient optimization algorithms. Thus, not only methods for the simulation of the PDE system have to show algorithmic scalability, but also the optimization build around these solvers has to exhibit mesh independent convergence.

While possible applications are many, we address two fields within this project. On the one hand, we investigate algorithms for a well-known benchmark example from fluid dynamics [3]. Within a flow tunnel the shape of an obstacle is to be optimized with respect to the minimal drag while the volume and the barycenter are fixed as Figure 1 shows. This experiment is of particular interest since it involves three methodological challenges. First, the shape of the initial geometry is non-smooth, whereas in the optimal configuration singularities in different locations have to be formed. The choice of geometrically simple reference configurations is motivated by the application of geometric multigrid strategies for the PDE solutions. A geometry like the depicted box can be precisely resolved on a hierarchy of refined computational meshes.

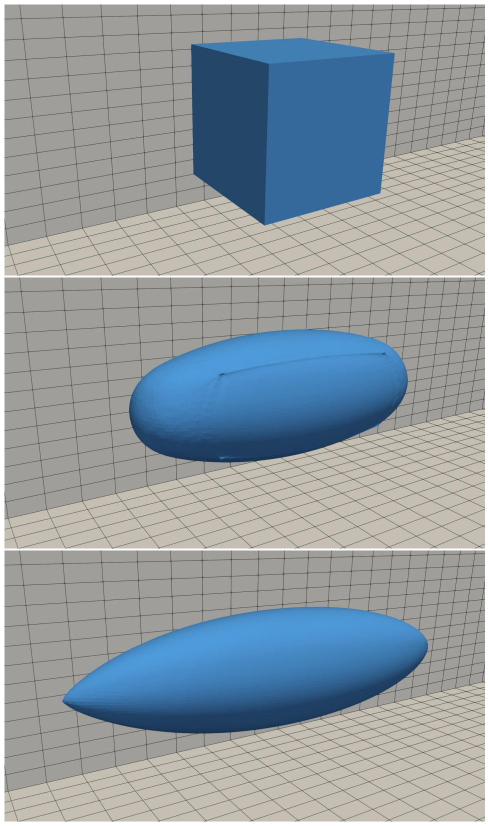

***Figure 1:** Optimization of an obstacle in a stationary, incompressible Navier-Stokes flow. Initial configuration in the top figure and optimal shape in the bottom. The optimization is constrained to a fixed volume and barycenter of the shape within a flow tunnel.*

These issues can be addressed by a proper choice of the space of admissible shapes. A well-established method is to define a reference configuration and then parameterize the set of admissible shapes via transformations in a suitable function space. In recent studies (cf. [2]) the approximations of Lipschitz continuous deformations via a p-Laplacian relaxation have shown to be advantageous compared to Hilbert space approaches. The challenge arising here is to develop scalable and efficient algorithms to compute shape updates in these particular function spaces.

One further crucial aspect is the treatment of geometric constraints, for instance the aforementioned constant volume and barycenter. This is usually achieved by penalty based algorithms, like the augmented Lagrange method. However, such approaches typically involve a significant number of highly problem dependent parameters that have to be heuristically determined. Within this project we investigate a more robust approach to incorporate geometric constraints by adding them as additional conditions to search for the steepest descent direction in the shape space.

The third challenge, exhibited by the second benchmark problem addressed within this project, is the robustness of the applied method with respect to large geometric deformations. Figure 2 shows an optimization example in structural mechanics. A composite of a bulk material with inclusions of different elastic properties is to be optimized in order to withstand forces applied on top of the domain [4,5]. Additionally, the geometric condition of having minimal surface with maximum space filling is set on the inclusions. For this experiment the shape optimization method has to be able to handle large deformations. In principle, the computational mesh is only relevant for the solution process of the PDE. It is however computational attractive not to generate a new mesh after a shape update, but to iteratively apply the deformation to the discretization nodes of the reference domain. Especially in the methods investigated here, where the shape deformation is computed via operators acting on the entire domain and not on the surface only, the descent step can be utilized in order to deform the computational mesh. In this situation it is of particular interest that the mesh quality is maintained, which can be realized via properties encoded in the functions space of the transformations.

The overall goal of our project is thus the development and investigation of an algorithmic framework using multigrid solvers for the simulation as well as (Quasi-)-Newton optimization techniques. Developing efficient parallel implementations for optimization schemes in more general Banach spaces will be a key part of the realization of our project. The novel algorithms will be designed to show scalability to a very large number of degrees of freedom.

## WWW

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## More Information

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[2] P. M. Müller et al. “A novel p-harmonic descent approach applied to fluid dynamic shape optimization”. *Struct. Multidisc. Optim.* (2021). doi: 10.1007/s00158-021-03030-x

[3] B. Mohammadi and O. Pironneau. “Shape Optimization in Fluid Mechanics”. *Annual Review of Fluid Mechanics* 36 (2004), pp. 255-279. doi: 10.1146/annurev.fluid.36.050802.121926

[4] M. Siebenborn and A. Vogel. “A shape optimization algorithm for cellular composites”. (2021), doi:10.51375/IJCVSE.2021.1.5

[5] J. Pinzon, M. Siebenborn, and A. Vogel. “Parallel 3d shape optimization for cellular composites on large distributed-memory clusters”. *Journal of Advanced Simulation in Science and Engineering* 7.1 (2020), pp. 117-135, doi: 10.15748/jasse.7.117

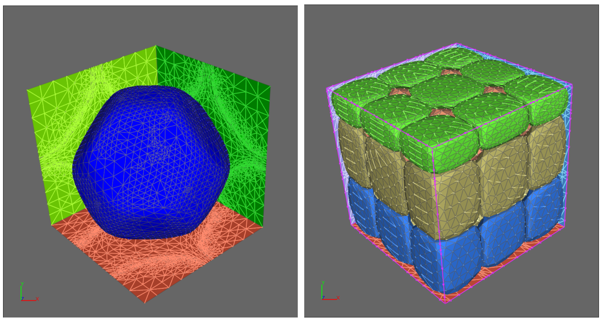

***Figure 2:*** *Shape optimization of elastic composite materials. The left figure shows a purely geometric benchmark test case where a space filling design with minimal surface is searched leading to a so called tetrakaidecahedron element. In the right hand side figure, the optimization of a composite material with several inclusions is shown. Here the elastic compliances are minimized while the specimen undergoes forces applied on the top surface.*

## Project Partners

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