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主論文の要旨

	Analysis and Numerics of Novel Shape Optimization		
論文題目	Methods for the Bernoulli Problem		
	(ベルヌイ問題に対する新しい形状最適化問題の解析と数値計算)		
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論文内容の要旨

This thesis pays particular attention to state-of-the-art numerical techniques for solving free boundary problems in the framework of shape optimization. Therefore, this work considers the prototype problem of free boundary problems known as the Bernoulli problem (also called as Alt-Caffarelli problem in some literature). In this respect, new shape optimization formulations of the Bernoulli problem are proposed as improvements and/or modifications to existing classical and standard formulations.

The main contribution of this research work is two-fold. On the one hand, we present three reformulations of the Bernoulli problem into shape optimization settings that have not been examined yet in the literature. The main point of departure for the first two formulations is the introduction of a new state problem associated with a classical boundary-data-tracking cost functional minimization approach and a standard energy-like error objective functional minimization problem. The third proposed formulation, on the other hand, consists of a new objective functional which basically tracks the L^2 mismatch at the *free* boundary between the computed Dirichlet boundary data of two auxiliary state problems. As a customary problem, the existence of optimal shape solutions to these shape problems is established through a C^1 -diffeomorphism of a uniform tubular neighborhood of the free boundary under a C^1 -regularity assumption on the unknown free boundary.

On the other hand, we adopt a Lagrangian-like approach based on finite element methods to numerically solve various concrete numerical examples of the proposed shape optimization formulations of the Bernoulli problem. This is in contrast to the fixed-point approach, the level-set method, or the boundary element method which are commonly used numerical techniques in the literature for solving the Bernoulli problem in the context of shape optimization. Towards this end, we design a novel gradient-based optimization procedure exploiting both the gradient and Hessian informations to numerically solve the new shape optimization problems. The novelty of our proposed iterative scheme lies in the practical application of the so-called Sobolev Newton method and in the use of appropriate formula for the step size of the algorithm. We point out that in the standard H^1 Newton method, the exact expression for the (shape) Hessian is used to regularized the descent vector. Here, however, we will only use the Hessian information at the solution of the free boundary problem in preconditioning the said vector. Because the selection of the step size is critical for the efficiency of the algorithm, we will couple our proposed first- and second-order gradient-based methods with a natural choice for the step size formula. We emphasize that the choice for the step size, especially in the case of the second-order method, is new to this work.

The thesis contains three major chapters and an additional chapter for the conclusion. The first chapter gives a brief introduction to shape optimization and reviews the notion of free boundary problems. Essential notations, abbreviations, and necessary function spaces used throughout the thesis are gathered and introduced here. The class of Bernoulli problems is then discussed. Its various shape optimization formulations in the classical setting are recalled and new formulations are presented. In this respect, different methods available to derive the so-called shape derivative of cost functions are reviewed. A short exposition of the theory about optimal shape problems in an abstract setting is also provided. The chapter ends by addressing the existence of optimal shape solutions for the new shape optimization formulations of the (exterior) Bernoulli problem.

Meanwhile, the second chapter provides the essentials and tools for shape optimization problems. An overview of the development of shape calculus through the notion of the velocity (or speed) method and of the perturbation of the identity operator method are discussed. Some properties of the operator of the latter method are also presented. Moreover, several useful identities from tangential calculus are given. Formal definitions of material and shape derivatives of the states, as well as the definition of Eulerian shape derivatives, are also provided, including a fundamental result in shape optimization known as Hadamard-Zolésio structure theorem. The chapter then examines the sensitivity of the cost functionals with respect to domain variations. In this regard, the concept of shape derivatives via minimax differentiability of a Lagrangian due to Delfour and Zolésio is revisited and then applied to derive the first-order Eulerian shape derivative (or *shape gradient*) of the L^2 tracking functional. On the other hand, the chain-rule approach, also known as the material derivative method, is used to calculate the Eulerian shape derivatives (up to the second-order) of an energy-gap-type functional and a new boundary objective functional. The computed shape derivatives of the shape functionals are characterized in accordance with the structure theorem.

The third chapter deals with the numerical treatment of the proposed shape optimization formulations of the Bernoulli problem. It is demonstrated here how the computed first- and second-order shape derivatives of the cost functions can be used to devise an efficient boundary variation algorithm to solve concrete numerical examples of the shape optimization problems. The novel part of the optimization procedure put forward in the chapter is the utilization of the *shape Hessian* (i.e., the second-order Eulerian shape derivative) information at the solution of the Bernoulli free boundary problem, instead of using the exact boundary integral form of the expression, coupled with an original Newton step-size formula. Various numerical experiments are conducted to evaluate the efficiency of the proposed methods. Numerical results are compared with those obtained from classical formulations.

Last but not least, the fourth chapter, which is the last chapter of the thesis, provides the conclusion of the present research. Some recommendations for future works related to the present investigation are also given in this chapter.