P 3 Shape optimization for fluid-structure interaction (W. Ring, M. Ulbrich, E. Ullmann) $\rightarrow$ AO, NS, IS

This project contributes to the advancement of the theory and the numerical solution of shape optimization problems for fluid structure interaction (FSI) based on monolithic approaches. The mathematical study of this practically important field offers many research opportunities. The first project investigates ALE in combination with the method of mappings. The second project addresses a fully Eulerian approach combined with the level set method.

State of the art. Optimal shape design problems for elastic structures in flows arise frequently in applications. Often, the solid deforms under the flow forces and this requires to employ FSI models, which form a particularly important subclass of multi-physics problems. For FSI simulations, partitioned as well as monolithic approaches have been proposed. Partitioned methods use a Lagrangian (material) framework for the solid and an Eulerian (spatial) framework for the fluid. They typically apply fixed point iterations to the coupling interface equations, which can be accelerated by Quasi-Newton or other techniques [18, 34].
Monolithic approaches [20, 22, 27, 31, 55], such as arbitrary Lagrangian-Eulerian (ALE) and fully Eulerian methods, use the same reference frame for fluid and solid. They often employ joint test spaces, thus enforcing the stress coupling condition weakly. The ALE framework [20, 22, 31] uses a reference domain $\hat{\Omega} = \hat{\Omega}_s \cup \hat{\Omega}_f \cup \hat{\Gamma}_i$ with the Lagrangian frame $\hat{\Omega}_s$ for the solid, an ALE reference frame $\hat{\Omega}_f$ for the fluid and the interface $\hat{\Gamma}_i$. Fluid reference points $\hat{x} \in \hat{\Omega}_f$ correspond to spatial points $x \in \Omega_f(t)$ via homemorphisms $\hat{T}_f(t) : \hat{x} \mapsto x$. Usually, $\hat{T}_f(t)$ is defined by $\hat{T}_f(\hat{x}, t) = \hat{x} + \hat{u}_f(\hat{x}, t)$, where $\hat{u}_f$ is a suitable (e.g., harmonic) extension of the solid displacement $\hat{u}_s$ to $\hat{\Omega}_f$. Fully Eulerian approaches [22, 55] use the spatial reference frame and transform the elasticity equations accordingly. The Eulerian domain $\Omega = \Omega_s(t) \cup \Omega_f(t) \cup \Gamma_i(t)$ is fixed, while its subdomains are moving in time.

So far, shape optimization for FSI has mainly been tackled by applied, engineering approaches [32, 33, 40, 41, 42], with some more weight on partitioned methods, which can use specialized single-physics solvers and tend to be less intrusive than monolithic approaches. Mathematical analyses of FSI problems [3, 6, 15, 16, 21, 36, 49] mostly rely on monolithic formulations, which also provide a well suited setting for PDE constrained optimization techniques in function spaces as well as for duality-based adaptivity. For (very) strong couplings, e.g., in hemodynamics, monolithic solvers tend to be more robust than partitioned methods [31].

Shape optimization problems can be analyzed and solved with different, yet closely related, techniques. On one hand, shape calculus [19, 29, 30, 43, 47, 48, 53] can be used to investigate functionals $J(\Omega)$ that depend on a domain Ω. The Eulerian derivative $dJ(\Omega; V)$ admits a representation by the Hadamard-Zolésio shape gradient, a distribution that is supported on the design boundary and only acts on the normal boundary variation $V \cdot n$. If a state equation is involved, then the Eulerian derivative either contains the shape derivative of the state (sensitivity approach) or an adjoint state. The (preconditioned) shape gradient can be used to drive a level set method [2, 9, 10, 46]. An alternative approach is the method of mappings (or perturbation of identity) [4, 28, 35, 39, 44, 52] which parameterizes the shape by a bi-Lipschitz homeomorphism $\tau : \mathbb{R}^d \to \mathbb{R}^d$ via $\Omega = \tau(\tilde{\Omega})$, where $\tilde{\Omega} \subset \mathbb{R}^d$ is a nominal (or reference) domain. Optimization can be performed based on the function $\tilde{J} : \tau \mapsto J(\tau(\tilde{\Omega}))$. An underlying state equation is then transformed to $\tilde{\Omega}$ and derivatives of $\tilde{J}$ can be obtained via sensitivities or adjoints. Both calculi can be deduced from each other. The method of mappings directly yields an optimal control setting in Banach spaces and it can provide exact discrete derivatives.

In realistic shape optimization problems initial conditions, loadings, or material parameters are often not known precisely and should be modeled as random functions. In addition, the geometry of the object can be uncertain. Shape optimization under uncertainty has been investigated only recently. See e.g. approaches based on level sets [11, 12, 13, 14, 17, 23], or other related works [1, 37, 38, 51].

First thesis project: *Shape optimization for fluid structure interaction using ALE and the method of mappings* to be supervised by Michael Ulbrich. This subproject uses an ALE approach to obtain a monolithic variational formulation of the FSI problem and combines it with the method of mappings for shape optimization. These two concepts fit each other very well since both employ the idea of domain transformations. For a given material shape $\hat{\Omega}_s$ of the solid, the ALE formulation provides a reference frame $\hat{\Omega}$ for solid and fluid. The method of mappings is now used to express shape changes of $\hat{\Omega}_s$ by a bi-Lipschitz homeomorphism $\tau : \mathbb{R}^d \to \mathbb{R}^d$ that maps a fixed nominal shape frame $\tilde{\Omega} = \tilde{\Omega}_s \cup \tilde{\Omega}_f \cup \tilde{\Gamma}_i$ to the current shape's reference frame $\hat{\Omega}$ and satisfies $\tau(\tilde{A}) = \hat{A}$ for $A \in \{\Omega_s, \Omega_f, \Gamma_i\}$. The ALE-FSI formulation can thus be transformed to the nominal shape frame. We expect that τ is explicitly needed only on $\tilde{\Omega}_s$. In practice, τ will be obtained via extension of design boundary deformations, where we can use different approaches and parameterizations from our earlier work [7, 8, 39]. An adjoint-based approach combined with derivative-based optimization methods will be developed. For the stationary setting, a formal adjoint-based method and its implementation were recently discussed in [50]. This can serve as a starting point, but our main target are unsteady FSI problems, for which a formal sensitivity approach is considered in [24].

For developing a theoretical foundation, the project will, in exchange with the partner subproject, study the continuity and differentiability of the state and the reduced objective function w.r.t. domain variations. The planned work builds on the available existence and regularity theory for FSI [3, 6, 15, 16, 21, 36, 49] and takes into account the (quite scarce) available literature [45, 56] (both address the steady case) on the differentiability of FSI problems w.r.t. parameters. First-order optimality systems will be derived and analyzed. Especially, the adjoint equation and derivative-based optimization approaches that build on it will be investigated in detail. For FSI, adjoint equations have so far been derived and applied formally in a stationary setting [50, 54], but a detailed analysis of their properties, especially in the unsteady case, still remains to be carried out. Whereas steady FSI shape optimization problems can most likely be analyzed based on variants of the implicit function theorem, this is questionable for non-stationary problems. In fact, our previous work on Fréchet material derivatives for the unsteady Navier-Stokes equations [8, 39] and on the identification of material parameters in the elastic wave equation [5] required advanced, direct estimation techniques and can provide guidance for the investigation of non-stationary FSI shape optimization problems.

In previous work on shape optimization for Navier-Stokes flow [7, 8, 39] we used that it is possible to do essentially all calculations, including adjoints, on the current shape domain. Similarly, we expect that in the ALE-FSI case the calculations can mainly be done on the reference domain $\hat{\Omega}$ (rather than $\tilde{\Omega}$) if desired. With a suitable discretization of the method of mappings, we can achieve that the obtained discrete material derivatives are exact, whereas discretizing the Hadamard-Zolésio shape gradient directly would ignore the dependency on the structure of the interior discretization. As a platform for numerical implementations, we can take advantage of our previous experience and existing software developments in the Trilinos/Sundance framework. Test cases shall be derived from the DFG FSI benchmark collection in coordination with the partner project.

Since shape optimization with FSI is a theoretically and numerically challenging problem class, we will use that there are hierarchies of increasing difficulty, ranging from steady to unsteady, from fixed to moving fluid-solid interfaces, and from linear to nonlinear models.

Second thesis project: *Shape optimization for fluid structure interaction using fully Eulerian and level set methods* to be supervised by Wolfgang Ring. A recently developed alternative to ALE formulations for FSI are fully Eulerian monolithic approaches [22, 25, 55] where both, fluid and solid domains are treated as time-variable with an undeformed (reference) configuration given by $\hat{\Omega}_s$ and $\hat{\Omega}_f$ (often $\hat{\Omega}_s = \Omega_s(0)$, $\hat{\Omega}_f = \Omega_f(0)$). The respective physical models are set up in Eulerian coordinates. The advantage in comparison to ALE is that large deformations are treatable and that the occurrence of topological singularities such as self-contact of the solid domain is — in principle — possible. This advantage is bought at the cost of a necessary local front-tracking procedure, usually done employing localized transformations. We propose to combine the fully Eulerian approach with a level-set based description of the undeformed geometry in order to solve shape optimization problems in the FSI framework. This is especially advantageous if the optimal configuration is considerably different from the startup configuration and the problem of large deformations occurs also in this respect. The front tracking of the undeformed geometry (the design variable) and the moving boundaries $\Omega_s(t)$ and $\Omega_f(t)$ shall be described in a uniform, level-set based, way. The solution of shape optimization problems in this setting will need sensitivity information of the state on the moving geometry at time t with respect to perturbations of the undeformed geometry, thus rendering the development of an appropriate chain rule in shape sensitivity analysis necessary.

Further topics. In close cooperation with the two proposed PhD projects, E. Ullmann will carry out initial studies on the effect of random data in shape optimization. The goal is to determine an optimal shape which is *robust* with respect to random inputs. This requires minimization of the expected value of a stochastic cost functional. Shape optimization under uncertainties is a challenging problem class and therefore this subproject will not consider the full FSI problem. We restrict the study to steady and/or unsteady Navier-Stokes flows with random viscosity or random inflow conditions. The method of mappings will be employed, see, e.g., the PhD thesis [39] for theoretical and numerical results with deterministic data. It has been supervised by M. Ulbrich and can serve as a starting point. Shape optimization with random loading is studied e.g. in [13, 14, 17, 26]. In these works the PDE and the shape gradient of the cost functional depend linearly on the stochastic parameters which simplifies the calculations. The study proposed here goes beyond these problems since in Navier-Stokes flows the state and hence the cost functionals will depend nonlinearly on the underlying random parameters.

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