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ON THE ADJOINT EQUATION IN FLUID-STRUCTURE INTERACTION

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Abstract. In this contribution, we revisit adjoint formulations for stationary and nonstationary space-time fluid-structure interaction. The adjoints serve for two purposes: goal-oriented a posteriori error estimation with the dual-weighted residual method and gradient-based numerical optimization. Our developments are substantiated with comments on numerical simulations in some other published studies.

1 Introduction

Fluid-structure interaction (FSI) has been an important topic for at least two decades with numerical applications in applied mathematics, computational science, and engineering [11, 20, 22, 10, 3, 9, 39, 21, 45]. Along to developments for purely solving forward fluid-structure interaction problems, efforts in a posteriori error estimation and numerical optimization have been made. These include goal-oriented techniques employing the dual-weighted residual method [6] with specific findings in fluid-structure interaction, e.g., in [50, 38, 26, 13, 14, 39, 18]. In numerical optimization such as optimal control, optimal design and parameter estimation, we list [37, 27, 31, 16, 15, 30, 40, 48, 17]. For gradient-based techniques, the usual approach is via the formal Lagrange formalism resulting in an optimality system to compute stationary points [32, 1, 28, 44]. We specifically follow the concepts and notation from [5, 36, 41, 33, 8] for space-time modeling of numerical optimization and goal-oriented error estimation. For space-time modeling of fluid-structure interaction, we also refer to [43, 42].

The objective of this contribution is two-fold. First, we derive a space-time fluid-structure interaction model based on arbitrary Lagrangian-Eulerian (ALE) coordinates [12, 29, 19]. A Galerkin space-time discretization is left for future work as it goes beyond the scope of these conference proceedings. The second purpose is on the derivation of the adjoint equation for stationary and nonstationary fluid-structure interaction. This includes both a summary of our previous works and our presentation of space-time ALE fluid-structure interaction.

The outline of this paper is as follows: In Section 2 the notation, abstract problem statements and some simple examples are presented. Next, in Section 3 the ALE concept and fluid-structure interaction are introduced. In Section 4, the adjoint equations are derived. Afterward, in Section 5 short descriptions

of some published numerical simulations are provided. A summary and future directions are outlined in Section 6.

2 Abstract problem statements and first examples

Let $\Omega \subset \mathbb{R}^2$ be a bounded domain with sufficiently smooth boundary $\partial\Omega$. Let $I := (0,T)$ be a time interval with end time value $T > 0$. We adopt the usual Sobolev and Bochner spaces [49]. For $u, v \in L^2(\Omega)$ we define

$$(u,v) := (u,v)_\Omega := \int_\Omega u \cdot v \, dx.$$

For time-dependent functions $u, v \in L^2(I, L^2(\Omega))$, we define

$$((u,v)) := \int_I (u,v)_\Omega := \int_I \int_\Omega u \cdot v \, dx.$$

Of course, these definitions can be extended to other Hilbert spaces.

2.1 Cost and error functionals, PDEs, and the Lagrange formalism

Let X be a function space, e.g., $X := L^2(I, L^2(\Omega))$. We are interested in optimization problems with cost or error functionals $J : X \to \mathbb{R}$ of the abstract form

$$J(u) = \int_I J_1(u) \, dt + J_2(u(T)), \tag{1}$$

where J_1 is a distributed functional over the entire time interval and J_2 is a functional that evaluates the solution at the end time T. In numerical optimization with an additional control variable $q \in Q$ (with Q being the space of controls) the cost functional is defined as $J : Q \times X \to \mathbb{R}$ of the abstract form

$$J(q,u) = \int_I J_1(u) \, dt + J_2(u(T)) + \frac{\alpha}{2} \|q - q_d\|_Q^2,$$

with a typical regularization term involving $\alpha \geq 0$ and some reference control $q_d \in Q$. The state equation is given by: Find $u \in X$ such that

$$A(u)(\psi) = F(\psi) \quad \forall \psi \in X,$$

respectively including $q \in Q$

$$A(q,u)(\psi) = F(\psi) \quad \forall \psi \in X.$$

The corresponding optimization problems read

$$\min_{u \in X} J(u) \quad \text{s.t.} \quad A(u)(\psi) = F(\psi),$$

respectively including $q \in Q$

$$\min_{(q,u) \in Q \times X} J(q,u) \quad \text{s.t.} \quad A(q,u)(\psi) = F(\psi).$$

With the help of the Lagrange formalism, we introduce the Lagrangian $L : Q \times X \times X \to \mathbb{R}$ involving the adjoint variable $z \in X$:

$$L(q,u,z) = J(q,u) - A(q,u)(z) + F(z).$$

The Lagrangian $L(u,z)$ without control q is defined respectively. By taking the directional derivatives of the respective solution variables, the optimality systems read

$$\begin{aligned}
L'_q(q,u,z)(\delta q) &= J'_q(q,u)(\delta q) - A'_q(q,u)(\delta q, z) = 0 \quad \forall \delta q \in Q \quad \text{(Gradient equation)} \\
L'_u(q,u,z)(\delta u) &= J'_u(q,u)(\delta u) - A'_u(q,u)(\delta u, z) = 0 \quad \forall \delta u \in X \quad \text{(Adjoint equation)} \\
L'_z(q,u,z)(\delta z) &= -A'_z(q,u)(\delta z) + F(\delta z) \qquad\quad = 0 \quad \forall \delta z \in X \quad \text{(State equation)}
\end{aligned}$$

respectively

$$\begin{aligned}
L'_u(u,z)(\delta u) &= J'_u(u)(\delta u) - A'_u(u)(\delta u, z) = 0 \quad \forall \delta u \in X \quad \text{(Adjoint equation)} \\
L'_z(u,z)(\delta z) &= -A'_z(u)(\delta z) + F(\delta z) \qquad = 0 \quad \forall \delta z \in X \quad \text{(State equation)}
\end{aligned}$$

2.2 Linear heat equation and a nonlinear PDE

As a simple example for demonstration purposes, we consider the heat equation: Find $u : \Omega \times I \to \mathbb{R}$ such that

$$\begin{aligned}
\partial_t u - \Delta u &= f \quad \text{in } \Omega \times I \\
u &= 0 \quad \text{on } \partial\Omega \times I \\
u(0) &= u_0 \quad \text{in } \partial\Omega \times \{0\}.
\end{aligned}$$

Employing the function space

$$X = \{u |\ u \in L^2(I, H_0^1(\Omega)),\ \partial_t u \in L^2(I, H^{-1}(\Omega))\}$$

we formulate a space-time weak formulation: Find $u \in X$ such that

$$A(u)(\psi) = F(\psi) \quad \forall \psi \in X$$

with

$$\begin{aligned}
A(u)(\psi) &= ((\partial_t u, \psi)) + ((\nabla u, \nabla \psi)) + (u(0), \psi(0)), \\
F(\psi) &= ((f, \psi)) + (u_0, \psi(0)).
\end{aligned}$$

As goal functional let us consider the spatial evaluation of our solution $u \in X$ at the end time:

$$J(u) = \int_\Omega u(T)\, dx.$$

Having at hand the minimization objective and the PDE constraint, the Lagrangian is then given by

$$L(u,z) = \int_\Omega u(T)\, dx - \int_I (\partial_t u, z)\, dt - \int_I (\nabla u, \nabla z)\, dt + \int_I (f, z)\, dt - (u(0) - u_0, z(0)).$$

Then, the optimality system reads: Find $(u,z) \in X \times X$, for all $(\varphi, \psi) \in X \times X$, such that

$$\begin{aligned}
L'_u(u,z)(\varphi) &= \int_\Omega \varphi(T)\, dx - \int_I (\partial_t \varphi, z)\, dt - \int_I (\nabla \varphi, \nabla z)\, dt - (\varphi(0), z(0)) = 0, \\
L'_z(u,z)(\psi) &= -\int_I (\partial_t u, \psi)\, dt - \int_I (\nabla u, \nabla \psi)\, dt + \int_I (f, \psi)\, dt - (u(0) - u_0, \psi(0)) = 0.
\end{aligned}$$

In the adjoint equation, the time derivative acts on the test function φ and we perform integration by parts in time:

$$-\int_I (\partial_t \varphi, z)\, dt = -[(\varphi(t), z(t))]_{t=0}^{t=T} + \int_I (\varphi, \partial_t z)\, dt.$$

With this operation, we obtain as adjoint equation

$$\begin{aligned} L'_u(u,z)(\varphi) &= \int_\Omega \varphi(T)\, dx + \int_I (\varphi, \partial_t z)\, dt - [(\varphi(t), z(t))]_{t=0}^{t=T} - \int_I (\nabla\varphi, \nabla z)\, dt - (\varphi(0), z(0)) \\ &= \int_\Omega \varphi(T)\, dx + \int_I (\varphi, \partial_t z)\, dt - \int_I (\nabla\varphi, \nabla z)\, dt - (\varphi(T), z(T)). \end{aligned}$$

Re-arranging the adjoint equation yields

$$-\int_I (\varphi, \partial_t z)\, dt + \int_I (\nabla\varphi, \nabla z)\, dt + (\varphi(T), z(T)) = \int_\Omega \varphi(T)\, dx$$

with the PDE parts on the left hand side and the functional on the right hand side. Due to the integration by parts, the adjoint problem is running backward in time as we observe that we have initial values for the adjoint at the end time T and due to the minus sign in front of the first term. Moreover, even for nonlinear state equations and nonlinear goal functionals, the adjoint equation is always linear. Let us illustrate this fact by simply extending the state equation to

$$\partial_t u - \Delta u + u^2 = f \quad \text{in } \Omega \times I$$

and the goal functional involving the square of the state solution

$$J(u) = \int_I \int_\Omega u^2\, dx dt.$$

Then, the adjoint equation reads: Given $u \in X$, find $z \in X$ such that

$$-\int_I (\varphi, \partial_t z)\, dt + \int_I (\nabla\varphi, \nabla z)\, dt + 2\int_I (u\varphi, z)\, dt + (\varphi(T), z(T)) = \int_I \int_\Omega u\varphi\, dx dt.$$

We observe that the adjoint variable appears in a linear fashion and moreover, the state variable $u \in X$ enters into the adjoint equation. For time-dependent problems this means that at each time point t_n the state solution must be available; we refer the reader to some further discussions to [5, 8]. In the related work [48] to these conference proceedings, we stored all state solutions on the hard disc. As an example, for the FSI-3 benchmark computed in [48], we had to store 6000 state solutions.

3 Fluid-structure interaction modeling

3.1 Notation

In extension to before, we now introduce additional notation. We denote by $\Omega := \Omega(t) \subset \mathbb{R}^d$, $d = 2$, the domain of the FSI problem. The domain consists of two time-dependent subdomains $\Omega_f(t)$ and $\Omega_s(t)$. The FSI-interface between $\Omega_f(t)$ and $\Omega_s(t)$ is denoted by $\Gamma_i(t) = \overline{\partial\Omega_f}(t) \cap \overline{\partial\Omega_s}(t)$. The initial (or later reference) domains are denoted by $\widehat{\Omega}, \widehat{\Omega}_f$ and $\widehat{\Omega}_s$, respectively, with the interface $\widehat{\Gamma}_i = \overline{\partial\widehat{\Omega}_f} \cap \overline{\partial\widehat{\Omega}_s}$. Furthermore, we denote the outer boundary by $\partial\widehat{\Omega} = \widehat{\Gamma} = \widehat{\Gamma}_{\text{in}} \cup \widehat{\Gamma}_D \cup \widehat{\Gamma}_{\text{out}}$ where $\widehat{\Gamma}_D$ and $\widehat{\Gamma}_{\text{in}}$ are Dirichlet boundaries (for the velocities and displacements) and $\widehat{\Gamma}_{\text{out}}$ denotes a fluid outflow Neumann boundary, respectively. The displacements are set to zero on $\widehat{\Gamma}_{\text{out}}$.

3.2 Spaces

For the function spaces in the (fixed) reference domains $\widehat{\Omega}, \widehat{\Omega}_f, \widehat{\Omega}_s$, we define spaces for spatial discretization first. First we define

$$\widehat{V} := H^1(\widehat{\Omega})^d.$$

Next, in the fluid domain, we define further:

$$\begin{aligned}
\widehat{L}_f &:= L^2(\widehat{\Omega}_f),\\
\widehat{L}_f^0 &:= L^2(\widehat{\Omega}_f)/\mathbb{R},\\
\widehat{V}_f^0 &:= \{\widehat{v}_f \in H^1(\widehat{\Omega}_f)^d : \widehat{v}_f = 0 \text{ on } \widehat{\Gamma}_{\text{in}} \cup \widehat{\Gamma}_D\},\\
\widehat{V}_{f,\widehat{u}}^0 &:= \{\widehat{u}_f \in H^1(\widehat{\Omega}_f)^d : \widehat{u}_f = \widehat{u}_s \text{ on } \widehat{\Gamma}_i, \quad \widehat{u}_f = 0 \text{ on } \widehat{\Gamma}_{\text{in}} \cup \widehat{\Gamma}_D \cup \widehat{\Gamma}_{\text{out}}\},\\
\widehat{V}_{f,\widehat{u},\widehat{\Gamma}_i}^0 &:= \{\widehat{\psi}_f \in H^1(\widehat{\Omega}_f)^d : \widehat{\psi}_f = 0 \text{ on } \widehat{\Gamma}_i \cup \widehat{\Gamma}_{\text{in}} \cup \widehat{\Gamma}_D \cup \widehat{\Gamma}_{\text{out}}\}.
\end{aligned}$$

In the solid domain, we use

$$\begin{aligned}
\widehat{L}_s &:= L^2(\widehat{\Omega}_s)^d,\\
\widehat{V}_s^0 &:= \{\widehat{u}_s \in H^1(\widehat{\Omega}_s)^d : \widehat{u}_s = 0 \text{ on } \widehat{\Gamma}_D\}.
\end{aligned}$$

As trial and test spaces for a space-time model, we define

$$\begin{aligned}
\widehat{X} = \{U = (\widehat{v}, \widehat{u}_f, \widehat{u}_s, \widehat{w}, \widehat{p}_f) |\ & \widehat{v} \in L^2(I, \{\widehat{v}^D + \widehat{V}^0\}), \partial_t \widehat{v} \in L^2(I, H^{-1}(\widehat{\Omega})^d), \widehat{u}_f \in L^2(I, \{\widehat{u}_f^D + \widehat{V}_{f,\widehat{u}}^0\}),\\
& \partial_t \widehat{u}_f \in L^2(I, H^{-1}(\widehat{\Omega}_f)^d), \widehat{u}_s \in L^2(I, \{\widehat{u}_s^D + \widehat{V}_s^0\}), \partial_t \widehat{u}_s \in L^2(I, H^{-1}(\widehat{\Omega}_s)^d), \widehat{w} \in L^2(I, \widehat{V}), \widehat{p}_f \in L^2(I, \widehat{L}_f^0)\}
\end{aligned}$$

and

$$\begin{aligned}
\widehat{X}^0 = \{U = (\widehat{v}, \widehat{u}_f, \widehat{u}_s, \widehat{w}, \widehat{p}_f) |\ & \widehat{v} \in L^2(I, \widehat{V}^0), \partial_t \widehat{v} \in L^2(I, H^{-1}(\widehat{\Omega})^d), \widehat{u}_f \in L^2(I, \widehat{V}_{f,\widehat{u},\widehat{\Gamma}_i}^0),\\
& \partial_t \widehat{u}_f \in L^2(I, H^{-1}(\widehat{\Omega}_f)^d), \widehat{u}_s \in L^2(I, \widehat{V}_s^0), \partial_t \widehat{u}_s \in L^2(I, H^{-1}(\widehat{\Omega}_s)^d), \widehat{w} \in L^2(I, \widehat{V}), \widehat{p}_f \in L^2(I, \widehat{L}_f^0)\}
\end{aligned}$$

3.3 A space-time fluid-structure interaction model

Extending Formulation 3 from [48] to a space-time formulation, we obtain:

Proposition 3.1 (Variational-monolithic space-time ALE FSI in $\widehat{\Omega}$)**.** *Find a global vector-valued velocity, vector-valued displacements, additional displacements (due to the splitting of the biharmonic mesh motion model into two second-order equations) and a scalar-valued fluid pressure, i.e., $\widehat{U} := (\widehat{v}, \widehat{u}_f, \widehat{u}_s, \widehat{w}, \widehat{p}_f) \in \widehat{X}$ such that*

$$\textit{Fluid/solid momentum} \begin{cases} \int_I \Big((\widehat{J}\widehat{\rho}_f \partial_t \widehat{v}, \widehat{\psi}^v)_{\widehat{\Omega}_f} + (\widehat{\rho}_f \widehat{J}(\widehat{F}^{-1}(\widehat{v} - \widehat{w}) \cdot \widehat{\nabla})\widehat{v}), \widehat{\psi}^v)_{\widehat{\Omega}_f} + (\widehat{J}\widehat{\sigma}_f \widehat{F}^{-T}, \widehat{\nabla}\widehat{\psi}^v)_{\widehat{\Omega}_f} \\ + \langle \widehat{\rho}_f \nu_f \widehat{J}(\widehat{F}^{-T}\widehat{\nabla}\widehat{v}^T \widehat{n}_f)\widehat{F}^{-T}, \widehat{\psi}^v \rangle_{\widehat{\Gamma}_{out}} + (\widehat{\rho}_s \partial_t \widehat{v}, \widehat{\psi}^v)_{\widehat{\Omega}_s} + (\widehat{F}\widehat{\Sigma}, \widehat{\nabla}\widehat{\psi}^v)_{\widehat{\Omega}_s} \Big) dt \\ + (\widehat{J}(\widehat{v}(0) - \widehat{v}_0), \widehat{\psi}^v(0))_{\widehat{\Omega}_f} + (\widehat{v}(0) - \widehat{v}_0, \widehat{\psi}^v(0))_{\widehat{\Omega}_s} = 0 \end{cases}$$

$$\textit{Fluid mesh motion (biharmonic/split)} \begin{cases} \int_I \Big((\widehat{\alpha}\widehat{\nabla}\widehat{w}|_{\widehat{\Omega}_f}, \widehat{\nabla}\widehat{\psi}^u)_{\widehat{\Omega}_f} \Big) dt & = 0 \\ \int_I \Big((\widehat{\alpha}\widehat{w}, \widehat{\psi}^w)_{\widehat{\Omega}} - (\widehat{\alpha}\widehat{\nabla}\widehat{u}_{f,s}, \widehat{\nabla}\widehat{\psi}^w)_{\widehat{\Omega}} \Big) dt & = 0 \end{cases}$$

$$\textit{Solid momentum, 2nd eq.} \Big\{ \int_I \Big(\widehat{\rho}_s(\partial_t \widehat{u}_s - \widehat{v}|_{\widehat{\Omega}_s}, \widehat{\psi}_s^u)_{\widehat{\Omega}_s} \Big) dt + (\widehat{u}_s(0) - \widehat{u}_{s,0}, \widehat{\psi}_s^u(0)) \quad = 0$$

$$\textit{Fluid mass conservation} \Big\{ \int_I \Big((\widehat{\text{div}}\,(\widehat{J}\widehat{F}^{-1}\widehat{v}), \widehat{\psi}_f^p)_{\widehat{\Omega}_f} \Big) dt \quad = 0$$

for all $\widehat{\Psi} = (\widehat{\psi}^v, \widehat{\psi}^u_f, \widehat{\psi}^u_s, \widehat{\psi}^w, \widehat{\psi}^p_f) \in \widehat{X}^0$. *In compact form, the above problem reads: Find* $\widehat{U} \in \widehat{X}$ *such that*

$$\widehat{A}(\widehat{U})(\widehat{\Psi}) = 0 \quad \forall \widehat{\Psi} \in \widehat{X}^0$$

where the FSI equations are combined in the semi-linear form $\widehat{A}(\widehat{U})(\widehat{\Psi})$.

4 Adjoint equations

Employing our preliminary considerations from Section 2 for Proposition 3.1, we obtain conveniently the adjoint equation for some given goal/cost functional. Formally, we arrive at

$$\widehat{L}'_U(\widehat{U},\widehat{Z})(\delta\widehat{U}) = \widehat{J}'_U(\widehat{U})(\delta\widehat{U}) - \widehat{A}'_U(\widehat{U})(\delta\widehat{U},\widehat{Z}) = 0$$

where $(\widehat{v},\widehat{u}_f,\widehat{u}_s,\widehat{w},\widehat{p}_f) \in \widehat{X}$ and $(\widehat{z}^v,\widehat{z}^u_f,\widehat{z}^u_s,\widehat{z}^w,\widehat{z}^p_f) \in \widehat{X}^0$ and $(\delta\widehat{v},\delta\widehat{u}_f,\delta\widehat{u}_s,\delta\widehat{w},\delta\widehat{p}_f) \in \widehat{X}^0$. Despite being formally simple, technically, the directional derivatives $\delta\widehat{U}$ of the nonlinear variable $\widehat{U}$ must be computed. This procedure is similar to the tangent problem, required for the nonlinear solution with Newton's method. Details can be found in [46]. By switching test and trial functions in the tangent problem, we obtain immediately the adjoint.

4.1 Time derivatives and their partial integration in time

Let us consider the time derivative terms in more detail. We start with the solid 2nd momentum equation

$$\int_I \widehat{\rho}_s(\partial_t\widehat{u}_s - \widehat{v}|_{\widehat{\Omega}_s}, \widehat{\psi}^u_s)_{\widehat{\Omega}_s}\, dt + (\widehat{u}_s(0) - \widehat{u}_{s,0}, \widehat{\psi}^u_s(0))_{\widehat{\Omega}_s}.$$

The adjoint is obtained by linearizing in $\widehat{u}_s$ and $\widehat{v}$, switching trial and test functions, and employing (1):

$$\int_I \widehat{\rho}_s(\partial_t\widehat{\psi}^u_s - \widehat{\psi}^v_s, \widehat{z}^u_s)_{\widehat{\Omega}_s}\, dt + (\widehat{\psi}^u_s(0), \widehat{z}^u_s(0))_{\widehat{\Omega}_s} = \widehat{J}'_U(\widehat{U})(\widehat{\Psi}).$$

Remark 4.1. *By this procedure, we obtain immediately the adjoint as in [48], Formulation 8, Eq. (16).*

We now perform partial integration in time similar to Section 2.2, yielding

$$-\int_I \widehat{\rho}_s(\widehat{\psi}^u_s, \partial_t\widehat{z}^u_s)_{\widehat{\Omega}_s}\, dt - \int_I \widehat{\rho}_s(\widehat{\psi}^v_s, \widehat{z}^u_s)_{\widehat{\Omega}_s}\, dt + (\widehat{\psi}^u_s(T), \widehat{z}^u_s(T))_{\widehat{\Omega}_s} = \widehat{J}'_U(\widehat{U})(\widehat{\Psi}).$$

For the discretization, we can either apply a space-time Galerkin discretization of the form $cG(s)dG(r)$ or $cG(s)cG(r)$, or (as done in [48]) finite differences in time and Galerkin finite elements in space. For instance, we have used the shifted Crank-Nicolson scheme in [48]. This scheme works in practice, but is not a consistent adjoint-time-stepping scheme; see [5][Remark 3.2] and [23]. As second example, we consider the time derivatives and initial values in the first equation of Proposition 3.1:

$$\int_I (\widehat{J}\widehat{\rho}_f\partial_t\widehat{v}, \widehat{\psi}^v)_{\widehat{\Omega}_f}\, dt + (\widehat{J}(\widehat{v}(0) - \widehat{v}_0), \widehat{\psi}^v(0))_{\widehat{\Omega}_f}.$$

Due to the transformation of the Navier-Stokes equations from the deforming domain $\Omega(t)$ to the reference domain $\widehat{\Omega}$ (for details see [46]) we deal with the transformation determinant $\widehat{J}$. Thus, we transform

first back to $\Omega(t)$, then build the adjoint, afterward integrate by parts, and finally transform back to $\widehat{\Omega}$. This yields

$$
\begin{aligned}
& \int_I (\widehat{J\rho}_f \partial_t \widehat{v}, \widehat{\psi}^v)_{\widehat{\Omega}_f}\, dt + (\widehat{J}(\widehat{v}(0)-\widehat{v}_0), \widehat{\psi}^v(0))_{\widehat{\Omega}_f} \\
\Leftrightarrow \text{ Transformation to } \Omega: \quad & \int_I (\rho_f \partial_t v, \psi^v)_{\Omega_f}\, dt + (v(0)-v_0, \psi^v(0))_{\Omega_f} \\
\Rightarrow \text{ Tangent: } \quad & \int_I (\rho_f \partial_t \delta v, \psi^v)_{\Omega_f}\, dt + (\delta v(0), \psi^v(0))_{\Omega_f} \\
\Rightarrow \text{ Adjoint: } \quad & \int_I (\rho_f \partial_t \psi^v, z^v)_{\Omega_f}\, dt + (\psi^v(0), z^v(0))_{\Omega_f} = J'_U(U)(\Psi)\, dt \\
\Leftrightarrow \text{ Integration by parts: } \quad & -\int_I (\rho_f \psi^v, \partial_t z^v)_{\Omega_f}\, dt + (\psi^v(T), z^v(T))_{\Omega_f} = J'_U(U)(\Psi)\, dt \\
\Leftrightarrow \text{ Transformation to } \widehat{\Omega}: \quad & -\int_I (\widehat{J\rho}_f \widehat{\psi}^v, \partial_t \widehat{z}^v)_{\widehat{\Omega}_f}\, dt + (\widehat{J}\widehat{\psi}^v(T), \widehat{z}^v(T))_{\widehat{\Omega}_f} = \widehat{J}'_U(\widehat{U})(\widehat{\Psi}).
\end{aligned}
$$

Again, this is a linear equation in the adjoint variable $\widehat{z}^v$ and running backward in time. As before, we can discretize in time by (non-consistant) finite differences or a full space-time Galerkin method.

4.2 Example from [48] with One-Step-θ time stepping

In [48], including an optimal control q, we deal with the problem: Given $\widehat{U}^0 \in \widehat{X}$, find $\widehat{U} = (\widehat{U}_h^n)_{n=1}^N \in \widehat{X}_h^N$ such that

$$
\begin{aligned}
\sum_{n=1}^{N} \Bigg(& \widehat{A}_{T,k}(\widehat{U}_h^n, \widehat{U}_h^{n-1})(\widehat{\Psi}_h^n) + \theta k \widehat{A}_E(\widehat{U}_h^n)(\widehat{\Psi}_h^n) \\
& + k\widehat{A}_P(\widehat{U}_h^n)(\widehat{\Psi}_h^n) + k\widehat{A}_I(\widehat{U}_h^n)(\widehat{\Psi}_h^n) + (1-\theta) k \widehat{A}_E(\widehat{U}_h^{n-1})(\widehat{\Psi}_h^n) \Bigg) = 0 \qquad \forall\, (\widehat{\Psi}_h^n)_{n=1}^N \in \widehat{X}_h^N.
\end{aligned}
\tag{2}
$$

Based on this form, we obtain the adjoint by linearizing in $\widehat{U}_h^n$ and $\widehat{U}_h^{n-1}$: Find $\widehat{Z} \in \widehat{X}_h^N$ such that

$$
\begin{aligned}
\sum_{n=1}^{N} \Bigg(& \partial_{\widehat{U}^n} \widehat{A}_{T,k}(\widehat{U}_h^n, \widehat{U}_h^{n-1})(\widehat{\Psi}_h^n, \widehat{Z}_h^n) + \partial_{\widehat{U}^{n-1}} \widehat{A}_{T,k}(\widehat{U}_h^n, \widehat{U}_h^{n-1})(\widehat{\Psi}_h^{n-1}, \widehat{Z}_h^n) \\
& + \theta k\, \partial_{\widehat{U}^n} \widehat{A}_E(q, \widehat{U}_h^n)(\widehat{\Psi}_h^n, \widehat{Z}_h^n) + k\, \partial_{\widehat{U}^n} \widehat{A}_P(\widehat{U}_h^n)(\widehat{\Psi}_h^n, \widehat{Z}_h^n) + k\, \partial_{\widehat{U}^n} \widehat{A}_I(\widehat{U}_h^n)(\widehat{\Psi}_h^n, \widehat{Z}_h^n) \\
& + (1-\theta) k \partial_{\widehat{U}^{n-1}} \widehat{A}_E(q, \widehat{U}_h^{n-1})(\widehat{\Psi}_h^{n-1}, \widehat{Z}_h^n) \Bigg) = \widehat{J}'(q, \widehat{U})(\widehat{\Psi}) \qquad \forall\, (\widehat{\Psi}_h^n)_{n=1}^N \in \widehat{X}_h^N.
\end{aligned}
\tag{3}
$$

Here $\partial_{\widehat{U}^n} \widehat{A}$ denotes the directional derivative of the form $\widehat{A}$ with respect to its $\widehat{U}^n$ argument, and the first argument of the second parentheses denotes the respective direction. As before, we integrate by parts in time, but now using a finite difference quotient and switching the meaning of θ to keep the property (implicit/explicit) of the time-stepping scheme. An example is provided in the next subsection.

4.3 Example with the help of the heat equation

The One-Step-θ time discretization of the heat equation from Section 2.2 for the weak form

$$
\int_I (\partial_t u, \psi)\, dt + \int_I (\nabla u, \nabla \psi)\, dt = 0
$$

reads

$$
\begin{aligned}
&\Rightarrow \frac{(u^n - u^{n-1}, \psi)}{k} + \theta(\nabla u^n, \nabla\psi) + (1-\theta)(\nabla u^{n-1}, \nabla\psi) \\
\Rightarrow \text{Tangent:} \quad &\frac{(\delta u^n, \psi)}{k} - \frac{(\delta u^{n-1}, \psi)}{k} + \theta(\nabla \delta u^n, \nabla\psi) + (1-\theta)(\nabla \delta u^{n-1}, \nabla\psi) \\
\Rightarrow \text{Adjoint:} \quad &\frac{(\psi^n, z)}{k} - \frac{(\psi^{n-1}, z)}{k} + \theta(\nabla \psi^n, \nabla z^n) + (1-\theta)(\nabla \psi^{n-1}, \nabla z^n) = J'(u^n, u^{n-1})(\psi) \\
\Rightarrow \text{Integration by parts:} \quad &-\frac{(\psi^n, z^n - z^{n-1})}{k} + (1-\theta)(\nabla \psi^n, \nabla z^n) + \theta(\nabla \psi^n, \nabla z^{n-1}) = J'(u^n, u^{n-1})(\psi) \\
\Rightarrow \text{Re-arranging terms:} \quad &\frac{(\psi^n, z^{n-1} - z^n)}{k} + \theta(\nabla \psi^n, \nabla z^{n-1}) + (1-\theta)(\nabla \psi^n, \nabla z^n) = J'(u^n, u^{n-1})(\psi).
\end{aligned}
$$

for $n = N, N-1, \ldots, 1, 0$. By the (discrete) integration by parts in time, we switch also θ to maintain an implicit time-stepping scheme $\theta \in [0.5, 1]$.

4.4 Adjoint of stationary optimization with fluid-structure interaction

We finally recall from [46][Chapter 4] the adjoint to stationary optimization with fluid-structure interaction. Find $(\widehat{q}, \widehat{U}, \widehat{Z}) \in \widehat{Q} \times \widehat{X} \times \widehat{X}$ with the primal solution $\widehat{U} = \{\widehat{v}_f, \widehat{v}_s, \widehat{u}_f, \widehat{u}_s, \widehat{p}_f\}$ and the adjoint solution $\widehat{U} = \{\widehat{z}^v_f, \widehat{z}^v_s, \widehat{z}^u_f, \widehat{z}^u_s, \widehat{z}^p_f\}$, such that

State equation

$$
\begin{aligned}
\widehat{A}(\widehat{q}, \widehat{U})(\widehat{\Psi}) = &(\widehat{\rho}_f \widehat{J}(\widehat{F}^{-1}\widehat{v}_f \cdot \widehat{\nabla})\widehat{v}_f), \widehat{\psi}^v_f)_{\widehat{\Omega}_f} + (\widehat{J\sigma}_f \widehat{F}^{-T}, \widehat{\nabla}\widehat{\psi}^v_f)_{\widehat{\Omega}_f} + (\widehat{F\Sigma}, \widehat{\nabla}\widehat{\psi}^v_s)_{\widehat{\Omega}_s} \\
&- \langle \widehat{g}_f, \widehat{\psi}^v_f \rangle_{\widehat{\Gamma}_N} - (\widehat{v}_s, \widehat{\psi}^u_s)_{\widehat{\Omega}_s} + (\alpha_u \widehat{\nabla}\widehat{u}_f, \widehat{\nabla}\widehat{\psi}^u_f)_{\widehat{\Omega}_f} \\
&+ (\widehat{\mathrm{div}}(\hat{J}\hat{F}^{-1}\widehat{v}_f), \widehat{\psi}^p_f)_{\widehat{\Omega}_f} - \langle \widehat{q}, \widehat{n}_f \cdot \widehat{\psi}^v_f \rangle_{\widehat{\Gamma}_Q} \\
= &\, 0 \quad \forall \widehat{\Psi} \in \widehat{X},
\end{aligned}
$$

with $\widehat{\Psi} \in \widehat{X}$ as previously defined.

Adjoint equation

$$
\begin{aligned}
&\widehat{A}'_{\widehat{U}}(\widehat{q}, \widehat{U})(\widehat{\Psi}, \widehat{Z}) = \widehat{\rho}_f \left(\widehat{\nabla}\widehat{\psi}^v \widehat{J\widehat{F}^{-1}} \widehat{v}_f + \widehat{\nabla}\widehat{v}_f \widehat{J\widehat{F}^{-1}} \widehat{\psi}^v, \widehat{z}^v_f \right)_{\widehat{\Omega}_f} + \widehat{\rho}_f \left(\widehat{\nabla}\widehat{v}_f [\widehat{J\widehat{F}^{-1}}]'(\widehat{\psi}^u)\widehat{v}_f, \widehat{z}^v_f \right)_{\widehat{\Omega}_f} \\
&+ \left(\widehat{\rho}_f \nu_f (\widehat{\nabla}\widehat{\psi}^v \widehat{F}^{-1} + \widehat{F}^{-T}(\widehat{\nabla}\widehat{\psi}^v)^T) \widehat{J\widehat{F}^{-T}}, \widehat{\nabla}\widehat{z}^v_f \right)_{\widehat{\Omega}_f} + \left(\widehat{\rho}_f \nu_f (\widehat{\nabla}\widehat{v}_f [\widehat{F}^{-1}]'(\widehat{\psi}^u) + [\widehat{F}^{-T}]'(\widehat{\psi}^u)\widehat{\nabla}\widehat{v}^T_f) \widehat{J\widehat{F}^{-T}}, \widehat{\nabla}\widehat{z}^v_f \right)_{\widehat{\Omega}_f} \\
&+ \left(\widehat{\rho}_f \nu_f (\widehat{\nabla}\widehat{v}_f \widehat{F}^{-1} + \widehat{F}^{-T}\widehat{\nabla}\widehat{v}^T_f) [\widehat{J\widehat{F}^{-T}}]'(\widehat{\psi}^u), \widehat{\nabla}\widehat{z}^v_f \right)_{\widehat{\Omega}_f} - \left(\widehat{p}_f [\widehat{J\widehat{F}^{-T}}]'(\widehat{\psi}^u), \widehat{\nabla}\widehat{z}^v_f \right)_{\widehat{\Omega}_f} - \left(\widehat{\psi}^p \widehat{J\widehat{F}^{-T}}, \widehat{\nabla}\widehat{z}^v_f \right)_{\widehat{\Omega}_f} \\
&+ \left(\lambda_s (\mathrm{tr}\widehat{E}'(\widehat{\psi}^u)\widehat{F} + \mathrm{tr}\widehat{E}\widehat{F}'(\widehat{\psi}^u)) + 2\mu_s (\widehat{F}'(\widehat{\psi}^u)\widehat{E} + \widehat{F}\widehat{E}'(\widehat{\psi}^u)), \widehat{\nabla}\widehat{z}^v_s \right)_{\widehat{\Omega}_s} \\
&- (\widehat{\psi}^v, \widehat{z}^u_s)_{\widehat{\Omega}_s} + (\alpha_u \widehat{\nabla}\widehat{\psi}^u, \widehat{\nabla}\widehat{z}^u_f)_{\widehat{\Omega}_f} + \left(\hat{\partial}_1 \widehat{\psi}^{v_1} + \hat{\partial}_2 \widehat{\psi}^{v_2}, \widehat{z}^p_f \right)_{\widehat{\Omega}_f} \\
&+ \left(\hat{\partial}_2 \widehat{\psi}^{u_1} \hat{\partial}_1 \widehat{v}_{f,1} - \hat{\partial}_2 \widehat{\psi}^{u_2} \hat{\partial}_1 \widehat{v}_{f,2} - \hat{\partial}_1 \widehat{\psi}^{u_2} \hat{\partial}_2 \widehat{v}_{f,1} + \hat{\partial}_1 \widehat{\psi}^{u_1} \hat{\partial}_{f,2} \widehat{v}_2, \widehat{z}^p_f \right)_{\widehat{\Omega}_f} \\
&= J'_{\widehat{U}}(\widehat{q}, \widehat{U})(\widehat{\Psi}) \quad \forall \widehat{\Psi} \in \widehat{X},
\end{aligned}
$$

with $\widehat{\Psi} \in \widehat{X}$ as previously defined. The gradient equation is omitted here.

5 Numerical examples from some other published studies

The algorithmic developments of the previous sections were realized in different collaborations and programming codes. These are revisited in the following.

5.1 Optimal control and optimal design for stationary fluid-structure interaction

In [40] stationary fluid-structure interaction was considered by us for optimal control and optimal design problems. Therein a specific emphasis was on monolithic formulations and the influence of the adjoint equation (Section 4.4) within the optimization loop. Parts of these developments go further back to the author's PhD thesis [46]. The numerical examples were computed with the help of DOpElib [24] (based on deal.II [2]).

5.2 Differentiability of solution operator for stationary fluid-structure interaction

In [47] well-posedness results (existence results first established in [25]) on the existence of stationary fluid-structure interaction were extended to uniqueness under small problem data assumptions and to differentiability of the solution map. The latter result is useful for numerical optimization in which often sufficient regularity of the state solution is assumed, but not proven.

5.3 Temporal error estimation and adaptivity of nonstationary fluid-structure interaction

In [18], a monolithic space-time formulation of nonstationary fluid-structure interaction was considered. Within [4] (see also the PhD thesis [15]) adjoint-based goal-oriented error control and temporal adaptivity was developed. For several benchmark problems, excellent error reduction and effectivity indices could be measured. Similar to Section 4, the adjoint equation was derived from a space-time formulation and discretized with the help of a Galerkin representation of the Fractional-Step-θ scheme [34, 35].

5.4 Optimal control and optimal design for nonstationary fluid-structure interaction

In [48] using again DOpElib [24], numerical optimization for nonstationary fluid-structure interaction was considered. This numerical example formed the basis of the WCCM oral presentation. Therein, the adjoint equation was formally derived with the Lagrange formalism, but temporal discretization was carried out with One-Step-θ schemes; see Section 4.2. The numerical optimization approach was based on a reduced approach while eliminating the state variable. As final solution algorithm, we employed gradient descent and a (inverse) BFGS (Broyden-Fletcher-Goldfarb-Shanno) algorithm.

6 Conclusions

In this work, we considered the adjoint equation for fluid-structure interaction. Specific emphasis was on space-time modeling and the partial integration in time yielding the backward-in-time running problem. By realizing the space-time discretization in terms of $cG(s)dG(r)$ or $cG(s)cG(r)$ discretizations, formally, we can proceed further as shown in [8, 7]. Apart from such consistent time-stepping schemes derived by rigorous arguments, a computational alternative are classical One-Step-θ time discretizations in which locally at each time point the adjoint is derived. The latter approach was employed in [48], which forms the basis of the corresponding WCCM oral presentation. The full space-time Galerkin approach is however appealing and will be further addressed in upcoming studies.

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