OPTIMIZATION-BASED METHODS FOR MULTIDISCIPLINARY SIMULATION AND OPTIMIZATION

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ABSTRACT

We discuss algorithms for multidisciplinary simulation and optimization that efficiently couple existing single-discipline codes. The algorithms are based on a strategy in which unknown data at the interfaces is determined through an optimization process. The strategy allows for the user to select the data type at the interfaces for each discipline, so that the method can be tailored to existing codes. We focus on the fluid-structure interaction problem for which we describe the optimization-based methods.

INTRODUCTION

Multidisciplinary simulation and optimization problems arise in a variety of settings in which more than one media, or more than one mathematical model, or more than one dominant effect are present. The direct solution of such problems are a formidable challenge, especially whenever the individual disciplinary problems are themselves complex and whenever their solution are computationally intensive. For this reason, methods which, at the price of requiring an iterative procedure, uncouple the different disciplines are of interest. Here, we discuss uncoupling procedures which are based on using an optimization strategy.

A main virtue of our approach is that it allows for the user to use existing codes for each discipline as black boxes and only requires that the user write a simple code that effects the coupling between the disciplines. One reason we are able to do this is that our methodology allows for complete flexibility with regards to the boundary conditions imposed on each discipline. Another virtue of the optimization-based decoupling is that it allows for the use of efficient iterative strategies, e.g., the fast convergence of the iterative process by which solutions of a sequence of uncoupled problems converge to the solution of the coupled, multidisciplinary problem. Our methodology has other important virtues as well such as allowing for the use of mismatched grids and different discretization methods for each discipline.

Our ultimate goal is to develop robust, efficient, and accurate algorithms for the simulation of multidisciplinary problems, and then apply them to control and optimization problems as well. Here, for the sake of concreteness, we will describe the optimization-based domain decomposition method for fluid-structure interaction problems. The methodologies we describe for fluid-structure interaction problems can also be applied to many other multidisciplinary simulation and optimization problems.

Of course, the subjects of multidisciplinary simulation and optimization have been extensively studied

in the past and continue to be the focus of much attention today. As a result, there is a vast literature on the subject. For example, one may consult the conference proceedings [1]–[6] and the references cited therein.

FLUID-STRUCTURE INTERACTION PROBLEMS

The interactions between fluid flows and solid structures immersed in the flow are of great interest. In practice, fluid-structure interactions are often modeled using elementary fluid models, e.g., involving loading functions, or ordinary differential equations, or linearized models such as panel methods, even when sophisticated models for the solid are used. There is considerable interest in including sophisticated fluid models as well. Although considerable effort has been devoted to such settings, the efficient and robust simulation and control of high-fidelity fluid-structure interactions is still not currently possible.

There are a number of different types of mathematical models for fluid-structure interactions that involve sophisticated fluids, e.g., the Navier-Stokes equations. Each model has a different regime of applicability. We briefly summarize three of the possibilities.

Rigid body motion of solids in a fluid flow. Here, the fluid sees the solids as moving rigid bodies. The motion of the solids is then simply described by a set of ordinary differential equations (6 for each body in three dimensions); the fluid motion is governed by unsteady flow equations, e.g., Navier-Stokes or Euler or potential. Coupling occurs since the region occupied by the fluid changes in time due to the motion of the solids and that motion is affected by the forces exerted by the fluid on the solids. Among the many applications of such fluid-structure interactions are store separation from aircraft, aircraft maneuvers including avoidance and pursuit strategies, response of aircraft to wind gusts and other sudden encounters, electromagnetic or acoustic nondestructive evaluation of pipelines and pipes by remote controlled vehicles swimming in the pipeline or pipe, and medical diagnosis and treatment using microdevices inserted into blood vessels, intestinal track, etc.

Elastic body motions in a fluid flow. Usually, the elastic motions of a solid body immersed in a fluid do not affect the fluid flow because the displacements in the solid are infinitesimal; the solid is affected by the fluid motion through the stress forces exerted by the the fluid on the solid. Such motions are uncoupled in the sense that one may solve for the fluid motion first, and then use that solution to define boundary data for the elastic motion of the solid. However, there is a very important situation for which the fluid and solid motions are fully coupled; this is when the solid is undergoing high frequency vibrations. In this case, although the elastic displacement of the solid may be small, the velocity is large. Then, the adherence (or the no penetration) condition that the fluid motion satisfies at the surface of the solid has the velocity of the solid as data. Among the many applications of such fluid-structure interactions are small amplitude flutter of wings, resonant vibrations of other aircraft components, and structural and other noise producing mechanisms.

Large displacement body motions in a fluid flow. When a solid body immersed in a fluid undergoes large displacement, then obviously the motions of the solid and fluid are coupled. Here, the difficulties, e.g., moving boundaries, associated with rigid body motions are present, but are made much more difficult by the fact that the motion of the solid is now governed by a system of partial differential equations. Among the many applications of such fluid-structure interactions are flutter problems involving large amplitude vibrations and the buckling of solid structures under aerodynamic loads.

Of course, the three types of interactions given above may be present in more complex situations. For example, rigid body motions and elastic motions may both be present when a wing is undergoing flutter.

In this paper, we focus on the second case, i.e., *elastic body motions in a fluid flow.*

THE MODEL PROBLEM

Let Ω_f and Ω_s denote the regions occupied by the fluid and solid, respectively. Let Γ denote the interface between the fluid and the solid and let Γ_f and Γ_s denote the boundaries of the fluid and solid regions (other than the interface Γ.)

We assume that the fluid flow is incompressible and viscous so that, in the fluid region, we apply the Navier-Stokes system

$$\begin{cases} \rho_f \dfrac{\partial \mathbf{v}}{\partial t} + \mathbf{v}\cdot\nabla\mathbf{v} - \mu_f \nabla\cdot(\nabla\mathbf{v} + \nabla\mathbf{v}^T) \\ \quad +\nabla p = \mathbf{0} \qquad \text{in } \Omega_f \times (0,T) \\ \nabla\cdot\mathbf{v} = 0 \qquad \text{in } \Omega_f \times (0,T) \\ \mathbf{v} = \mathbf{0} \qquad \text{on } \Gamma_f \times (0,T) \\ \mathbf{v} = \mathbf{v}_0 \qquad \text{in } \Omega_f \text{ at } t = 0\,. \end{cases} \tag{1}$$

Here, ρ_f and μ_f denote the (constant) fluid density and viscosity, $\mathbf{v}$ the fluid velocity, p the fluid pressure, and $\mathbf{v}_0$ the initial velocity. The boundary condition imposed on Γ_f can be replaced with other ones, e.g., outflow conditions, without affecting the sequel in any appreciable way.

In the solid, we apply the equations of linear elasticity

$$\begin{cases} \lambda_s \nabla(\nabla\cdot\mathbf{u}) + \mu_s \nabla\cdot(\nabla\mathbf{u} + \nabla\mathbf{u}^T) \\ \quad -\rho_s \dfrac{\partial^2 \mathbf{u}}{\partial t^2} = \rho_s \mathbf{b} \qquad \text{in } \Omega_s \times (0,T) \\ \mathbf{u} = \mathbf{0} \qquad \text{on } \Gamma_s \times (0,T) \\ \mathbf{u} = \mathbf{u}^0 \qquad \text{in } \Omega_s \text{ at } t = 0 \\ \dfrac{\partial \mathbf{u}}{\partial t} = \mathbf{u}_1 \qquad \text{in } \Omega_s \text{ at } t = 0\,. \end{cases} \tag{2}$$

Here, μ_s and λ_s are the Lame constants and ρ_s the constant density of the solid, $\mathbf{b}$ denotes a given loading force per unit mass, $\mathbf{u}$ the displacement of the solid, and $\mathbf{u}_0$ and $\mathbf{u}_1$ are given initial data.

Along the interface Γ, the velocity of the fluid and solid are equal, as are the stress vector in the fluid and solid. Thus, we have

$$\mathbf{v} = \frac{\partial \mathbf{u}}{\partial t} \qquad \text{on } \Gamma \times (0,T) \tag{3}$$

and

$$\begin{aligned} \lambda_s(\nabla\cdot\mathbf{u})\mathbf{n} + \mu_s(\nabla\mathbf{u} + \nabla\mathbf{u}^T)\cdot\mathbf{n} &= p\mathbf{n} \\ -\mu_f(\nabla\mathbf{v} + \nabla\mathbf{v}^T)\cdot\mathbf{n} \quad &\text{on } \Gamma \times (0,T)\,. \end{aligned} \tag{4}$$

Solving (1)–(4) as a coupled system is a formidable, even impossible, task. Thus, one looks for means to uncouple the computations. There have been proposed numerous ways to effect the uncoupling; here, we present another such method.

A DECOMPOSITION INTO SINGLE DISCIPLINES

Suppose, for some function $\mathbf{g}$, we add to the system (1) the boundary condition

$$p\mathbf{n} - \mu_f(\nabla\mathbf{v} + \nabla\mathbf{v}^T)\cdot\mathbf{n} = \mathbf{g} \quad \text{on } \Gamma \times (0,T)\,. \tag{5}$$

Then, (1) and (5) form a closed system, i.e.,we may solve for $\mathbf{v}$ and p. Likewise, if we add to the system (2) the boundary condition

$$\begin{aligned} \lambda_s(\nabla\cdot\mathbf{u})\mathbf{n} + \mu_s(\nabla\mathbf{u} + \nabla\mathbf{u}^T)\cdot\mathbf{n} \\ = \mathbf{g} \quad \text{on } \Gamma \times (0,T)\,, \end{aligned} \tag{6}$$

then we may solve (2) and (6) for $\mathbf{u}$. For any choice of $\mathbf{g}$, we thus have that (1), (2), and (4) are satisfied. However, for an arbitrary choice for $\mathbf{g}$, the interface condition (3) will not be satisfied. On the other hand, we know that there exists a $\mathbf{g}$ such that the solution of (1), (5) and (2), 6) coincides with the solution of the coupled system (1)–(4); one merely has to let

$$\begin{aligned} \mathbf{g} = \widehat{\mathbf{g}} &= \widehat{p}\mathbf{n} - \mu_f(\nabla\widehat{\mathbf{v}} + \nabla\widehat{\mathbf{v}}^T)\cdot\mathbf{n} \\ &= \lambda_s(\nabla\cdot\widehat{\mathbf{u}})\mathbf{n} + \mu_s(\nabla\widehat{\mathbf{u}} + \nabla\widehat{\mathbf{u}}^T)\cdot\mathbf{n}\,, \end{aligned} \tag{7}$$

where $(\widehat{\mathbf{v}}, \widehat{p}, \widehat{\mathbf{u}})$ denotes the exact solution of (1)–(4).

The question then remains: how does one determine the correct $\widehat{\mathbf{g}}$? Since we wish for the interface condition (3) to hold, we attempt to find the correct $\mathbf{g}$

by solving the problem

$$\min_{\mathbf{g}} \mathcal{J}(\mathbf{g}), \tag{8}$$

where

$$\mathcal{J}(\mathbf{g}) = \frac{1}{2}\int_0^T \int_{\Gamma_0} (\frac{\partial \mathbf{u}}{\partial t} - \mathbf{v})^2 \, d\Gamma dt, \tag{9}$$

where $\mathbf{u}$ and $\mathbf{v}$ are related to $\mathbf{g}$ through (1), (5) and (2), (6), respectively. Clearly, if the coupled system (1)–(4) has a solution, this constrained minimization problem has a solution and, in fact, the two solutions are the same. Thus, we propose to solve the coupled fluid-structure interaction problem by solving a constrained optimization problem in which uncoupled fluid and solid systems act as constraints and in which the functional to be minimized measures the discrepancy in one of the interface conditions.

Adjoint equations and the gradient of the functional

In order to solve the optimization problem, we could employ a method which uses the gradient of the functional (9) with respect to the unknown interface function $\mathbf{g}$. That gradient may be determined via sensitivities or adjoint variables. Since an accurate discretization of $\mathbf{g}$ would involve many variables, e.g., nodal values, there results in the need to calculate many sensitivities. Therefore, it is more efficient to use adjoint variables, and that is the approach we follow here.

Consider the *adjoint system*

$$\begin{cases} -\rho_f \dfrac{\partial \xi}{\partial t} - \mu_f \nabla \cdot (\nabla \xi + \nabla \xi^T) + \nabla \eta \\ \qquad = \mathbf{0} \qquad \text{in } \Omega_f \times (0,T) \\ \nabla \cdot \xi = 0 \qquad \text{in } \Omega_f \times (0,T) \\ \xi = \mathbf{0} \qquad \text{on } \Gamma_f \times (0,T) \\ \xi = \mathbf{0} \qquad \text{in } \Omega_f \text{ at } t = T \\ -\eta \mathbf{n} + \mu_f (\nabla \xi + \nabla \xi^T) \cdot \mathbf{n} \\ \qquad = \left(\dfrac{\partial \mathbf{u}}{\partial t} - \mathbf{v} \right) \qquad \text{on } \Gamma \times (0,T) \end{cases} \tag{10}$$

and

$$\begin{cases} \lambda_s \nabla (\nabla \cdot \phi) + \mu_s \nabla \cdot (\nabla \phi + \nabla \phi^T) \\ \qquad -\rho_s \dfrac{\partial^2 \phi}{\partial t^2} = \mathbf{0} \qquad \text{in } \Omega_s \times (0,T) \\ \phi = \mathbf{0} \qquad \text{on } \Gamma_s \times (0,T) \\ \lambda_s (\nabla \cdot \phi)\mathbf{n} + \mu_s (\nabla \phi + \nabla \phi^T) \cdot \mathbf{n} \\ \qquad = \dfrac{\partial^2 \mathbf{u}}{\partial t^2} - \dfrac{\partial \mathbf{v}}{\partial t} \qquad \text{on } \Gamma \times (0,T) \\ \phi = \dfrac{\partial \phi}{\partial t} = \mathbf{0} \qquad \text{in } \Omega_s \text{ at } t = T. \end{cases} \tag{11}$$

We refer to ξ, η, and ϕ as the adjoint fluid velocity, fluid pressure, and solid displacement, respectively. Note that the left-hand side is merely the adjoint of the linearized state equations (1), (5) and (2), (6) and the right-hand side involves the derivative of the functional (9) with respect to the state variables $\mathbf{v}$ and $\mathbf{u}$. Note that that the adjoint system (10) and (11) is posed with terminal conditions at $t = T$ in contrast to the state system (1) and (2) which is posed with initial conditions at $t = 0$. Also, the adjoint system is *linear* in the adjoint variables.

It can be shown that the gradient of the functional (9) with respect to the unknown interface function $\mathbf{g}$ can be expressed in terms of the state and adjoint variables in the form

$$\frac{d\mathcal{J}}{d\mathbf{g}} = -\int_0^T \int_{\Gamma} (\xi + \phi) \, d\Gamma dt \tag{12}$$

A gradient method for the optimization problem

A simple gradient method for the solution of the optimization problem (8) and thus of the fluid-structure interaction problem (1)–(4) is given as follows.

- Choose an initial guess $\mathbf{g}^{(0)}$;
- for $n = 0, 1, 2, \ldots$ until satisfactory convergence is obtained,

  1a. solve (1) and (5) to obtain $\mathbf{v}^{(n)}$ and $p^{(n)}$;

1b. solve(2) and (6) for $\mathbf{u}^{(n)}$;

2a. solve (10) to obtain $\xi^{(n)}$ and $\eta^{(n)}$;

2b. solve (11) to obtain $\phi^{(n)}$

3. choose a step size α_n and then determine a new guess for $\mathbf{g}$ from

$$\mathbf{g}^{(n+1)} = \mathbf{g}^{(n)} + \alpha_n \int_0^T \int_\Gamma (\xi^{(n)} + \phi^{(n)})\, d\Gamma dt\,.$$

Of course, in practice, this algorithm is implemented on discretized versions of the various partial differential equations. It can be shown that, with appropriate choices of the step sizes α_n (which can be determined in practice, e.g., by monitoring the value of the functional $\mathcal{J}(\cdot)$ or by a line search algorithm), the gradient method converges to an optimal solution. The gradient of the functional (12) can also be used in more sophisticated optimization algorithms, e.g., nonlinear conjugate gradient and quasi-Newton methods.

Note that Step 1a of the above algorithm is simply a single discipline fluid flow calculation and is totally uncoupled from the single discipline elasticity calculation of Step 1b. Thus, two single-discipline codes can be used without modification to effect the calculations of Steps 1a and 1b. Likewise, the adjoint fluid calculation of Step 2a is uncoupled from the adjoint elasticity calculation of Step 2b. The adjoint fluid calculation of Step 2b involves a *linear* system (as does, of course, Step 2b) so that these may be effected at much less cost than that of the nonlinear calculation of Step 1a. Also note that Steps 1a and 1b may be done in parallel as can Steps 2a and 2b.

Other boundary conditions

The single discipline problems solved in the above algorithm involve the boundary conditions (5) and (6) which were created as part of the optimization-based algorithm. It is possible that these boundary conditions are not convenient, e.g., available single-discipline codes may not be able to handle them. One would like to tailor the optimization-based method so that the boundary conditions created are the most convenient with regard to available single discipline codes. This is entirely possible.

One obvious modification of the optimization-based algorithm is to switch the roles of the Dirichlet and Neumann boundary conditions. Thus, if the single discipline codes are better suited to Dirichlet boundary conditions, we replace (5), (6), and (9) with the boundary conditions

$$\begin{aligned} &\frac{\partial \mathbf{u}}{\partial t} = \mathbf{q} \quad \text{or} \\ &\qquad \mathbf{u} = \mathbf{u}_0 + \int_0^t \mathbf{q}\, dt \qquad \text{on } \Gamma \times (0,T) \end{aligned} \tag{13}$$

and

$$\mathbf{v} = \mathbf{q} \qquad \text{on } \Gamma \times (0,T) \tag{14}$$

and the functional

$$\mathcal{K}(\mathbf{q}) = \frac{1}{2} \int_0^T \int_\Gamma |\tau_f - \tau_s|^2\, d\Gamma dt\,, \tag{15}$$

where $\tau_f = -p\mathbf{n} + \mu_f(\nabla \mathbf{v} + \nabla \mathbf{v}^T)\cdot \mathbf{n}$ and $\tau_s = \lambda_s(\nabla \cdot \mathbf{u})\mathbf{n} + \mu_s(\nabla \mathbf{u} + \nabla \mathbf{u}^T)\cdot \mathbf{n}$ denote the stress vectors in the fluid and solid, respectively. Then, uncoupling between disciplines is effected by minimizing $\mathcal{K}(\mathbf{q})$ over suitable $\mathbf{q}$, where $\mathbf{v}$, p, and $\mathbf{u}$ are related to $\mathbf{q}$ through (1), (14) and (2), (13), respectively.

One does not need to use the same type of boundary condition along the interface for the fluid and solid. For example, one may one to use (14) for the fluid and (6) for the solid. In this case, one would minimize the functional

$$\mathcal{L}(\mathbf{g}, \mathbf{q}) = \frac{1}{2} \int_0^T \int_\Gamma \left(\left| \frac{\partial \mathbf{u}}{\partial t} - \mathbf{q} \right|^2 + |\tau_f - \mathbf{g}|^2 \right) d\Gamma dt$$

over suitable $\mathbf{g}$ and $\mathbf{q}$, where $\mathbf{v}$ and p are related to $\mathbf{q}$ through (1), (14) and $\mathbf{u}$ is related to $\mathbf{g}$ through (2), (6).

Other functionals

The functionals we have explored in this paper provide for relatively easy implementations. However,

they may not provide for the fastest convergence of optimizer iterations or the best accuracy of discretizations. For example, instead of (9), one can employ the functional

$$\frac{1}{2}\int_0^T \int_\Gamma \left| \mathbf{u} - \mathbf{u}_0 - \int_0^t \mathbf{v}\, d\xi \right|^2 d\Gamma dt$$

which leads to more regular solutions of the optimization problem. Using this functional instead of (9) yields the same adjoint equations, e.g., (10) and (11), except that the boundary conditions along the interface Γ are now given by

$$-\eta \mathbf{n} + \mu_f(\nabla\xi + \nabla\xi^T)\cdot\mathbf{n} = \int_t^T \Big(\mathbf{u} - \mathbf{u}_0 - \int_0^s \mathbf{v}(\mathbf{x},\tau)\, d\tau\Big)\, ds \qquad \text{on } \Gamma \times (0,T)$$

for the fluid and

$$\lambda_s(\nabla\cdot\phi)\mathbf{n} + \mu_s(\nabla\phi + \nabla\phi^T)\cdot\mathbf{n} = \mathbf{u} - \mathbf{u}_0 - \int_0^t \mathbf{v}(\mathbf{x},\tau)\, d\tau \qquad \text{on } \Gamma \times (0,T)$$

for the solid.

MULTIDISCIPLINARY OPTIMIZATION

We close with a few words about the use of the methods we have described in the setting of multidisciplinary optimization. In this a setting, we are *given* a functional that is to minimized (or maximized, depending on the application) and some parameters that can be varied in order to effect the optimization. Thus, in general we have a problem of the type

$$\min_\alpha \mathcal{F}(\mathbf{v},\mathbf{u},p,\alpha) \tag{16}$$

subject to (1)–(4). We again want to solve this problem by a decomposition algorithm which uses already developed single discipline codes. As in the multidisciplinary simulation case, we introduce the functional (9) and the optimization problem (8), where now we have the constraints (1), (2), (5), and (6). As a result, we are let to a multiobjective optimization problem involving the given functional (16) and the functional (9) which is artificially introduced in order to effect the decomposition into separate disciplines.

The multiobjective minimization problem may be solved by a variety of means, the simplest of which is to form the single functional

$$\mathcal{F}(\mathbf{v},\mathbf{u},p,\alpha) + \delta\mathcal{J}(\mathbf{g})$$

which is minimized with respect to both $\mathbf{g}$ and α, where δ is a penalty parameter. Optimization methods can again be defined that utilize single discipline codes as black boxes. See [7] for an analytical and computational study of this approach in a simplified setting.

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