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Data Assimilation in Fluid Dynamics using Adjoint Optimization

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Abstract

Data assimilation arises in a vast array of different topics: traditionally in meteorological and oceanographic modelling, wind tunnel or water tunnel experiments and recently from biomedical engineering. Data assimilation is a process for combine measured or observed data with a mathematical model, to obtain estimates of the expected data. The measured data usually contains inaccuracies and is given with low spatial and/or temporal resolution.

In this thesis data assimilation for time dependent fluid flow is considered. The flow is assumed to satisfy a given partial differential equation, representing the mathematical model. The problem is to determine the initial state which leads to a flow field which satisfies the flow equation and is close to the given data.

In the first part we consider one-dimensional flow governed by Burgers' equation. We analyze two iterative methods for data assimilation problem for this equation. One of them so called adjoint optimization method, is based on minimization in L^2-norm. We show that this minimization problem is ill-posed but the adjoint optimization iterative method is regularizing, and represents the well-known Landweber method in inverse problems. The second method is based on L^2-minimization of the gradient. We prove that this problem always has a solution. We present numerical comparisons of these two methods.

In the second part three-dimensional inviscid compressible flow represented by the Euler equations is considered. Adjoint technique is used to obtain an explicit formula for the gradient to the optimization problem. The gradient is used in combination with a quasi-Newton method to obtain a solution. The main focus regards the derivation of the adjoint equations with boundary conditions. An existing flow solver EDGE has been modified to solve the adjoint Euler equations and the gradient computations are validated numerically. The proposed iteration method are applied to a test problem where the initial pressure state is reconstructed, for exact data as well as when disturbances in data are present. The numerical convergence and the result are satisfying.

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1 Introduction

Background and Overview

In many application areas there is a growing interest in data assimilation, which is a process for integrating observed or measured data into a physical model. The idea of data assimilation is that measured data is used in combination with the equations, decribing the mathematical model, to derive estimates of the expected data. The measured data usually contains inaccurancies and is given with low spatial and/or temporal resolution. The problem arises in a vast array of different topics: traditionally in meteorological and oceanographic modelling, wind tunnel or water tunnel experiments and recently from biomedical engineering where the ideas to this research project arised. Magnetic resonance imaging technique, which is a non-invasive medical measurement device, is used to measure the velocity field of the blood e.g. in the human heart, see [18]. The measured data is given with low spatial and temporal resolution. The aim of the project was to derive a velocity field with higher resolution and lower inaccuracies, resulting in more sharp and correct images illustrating the blood torrent. This thesis presents a method for solving time dependent flow data assimilation problems parametrized with the initial state using adjoint optimization.

In *Paper I - Iterative methods for data assimilation for Burgers' equation* the adjoint optmimization method is introduced and theory investigated for a one-dimensional problem, Burgers' equation which describes one-dimensional viscous fluid flow.

In *Paper II - Reconstruction of initial state for 3D time dependent Euler flow using adjoint optimization* we consider data assimilation for three-dimensional flow in a tube. Here the focus regards discretization and the derivation of the adjoint equation system with boundary conditions. For computational time reasons we consider inviscid flow instead of viscous flow.

The third appended paper, *Paper III - Reconstruction of velocity data, using optimization*, is a first description of the ideas in this thesis and was presented at the second conference in Computational Fluid and Solid Mechanics at MIT 2003.

The data assimilation problem can be described as follows. Suppose that we have a measured flow field $\mathbf{u}^\delta$ and want to determine a flow field $\mathbf{u}$ which satisfies the flow equation with boundary conditions, and is close to $\mathbf{u}^\delta$. This have been done in various forms; control theory, optimization and probability theory. However, the resulting schemes have many common features and properties. An overview of different data assimilation techniques is given in [5]. The theory of optimal control governed by partial differential equations was initiated by Lions [10].

Mathematically one should minimize the difference $\mathbf{u}-\mathbf{u}^\delta$ in a suitable norm over the solution set for the flow equation. A well-known and widely used method for this purpose is the so called adjoint optimization method, which uses adjoint technique to calculate the gradient for the minimization problem and thereafter an iterative gradient method is applied. The use of adjoint technique is common in shape optimization, pioneered by Pironenneau [14, 16], especially aerodynamic design, see for example [7, 8]. In shape optimization one search for the shape or boundary of a region, which gives for example an airplane wing lowest possible drag. Various method for shape optmization is given and discussed in [13]. Adjoint methods have also been used in data assimilation problems, see for example [2, 17].

Method and Theory for Burgers' equation

We start by introduce the ideas of adjoint optimization, this is done for our model problem, Burgers' equation

$$
\begin{aligned}
\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \mu\frac{\partial^2 u}{\partial x^2} &= 0, \quad (x,t) \in Q_T, && (1)\\
u(0,t) = u(1,t) &= 0, \quad t \in (0,T) && (2)\\
u(0,x) &= v(x), \quad x \in (0,1) && (3)
\end{aligned}
$$

where $Q_T = (0,1) \times (0,T)$.

The aim is to use a iteration method for finding the optimal initial state, i.e. the initial state $v(x)$ such that $u(x,t)$ satisfies (1)-(3) and minimizes the functional

$$I = \int_{Q_T} \frac{1}{2}(u-u^\delta)^2 dxdt, \tag{4}$$

where $u^\delta \in L^2(Q_T)$ is a given function. The iteration process is written

$$v_{k+1} = v_k + \delta v_k, \quad k = 0, 1, \ldots, \tag{5}$$

where the update δv_k is choosed by adjoint technique in each step such that $\{I(v_k)\}$ becomes a decreasing sequence. We denote the solution to (1)-(3) with $v = v_k$ by u_k.

One way to determine δv_k is the following. We define the Lagrangian $\mathcal{L}$ to the minimization problem as

$$\mathcal{L} = \frac{1}{2}\int_{Q_T}(u-u^\delta)^2 dxdt + \int_{Q_T}\psi\left(\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} - \mu\frac{\partial^2 u}{\partial x^2}\right)dxdt,$$

where $\psi(x,t)$ is a Lagrange multiplier. By formal calculations we obtain for the first variation

$$\delta\mathcal{L} = \int_{Q_T}(u-u^\delta)\delta u dxdt + \int_{Q_T}\psi\left(\frac{\partial \delta u}{\partial t} + \frac{\partial (u\delta u)}{\partial x} - \mu\frac{\partial^2 \delta u}{\partial x^2}\right)dxdt,$$

and further by Greens formula

$$\begin{aligned}\delta\mathcal{L} = &\int_{Q_T}\left(u - u^\delta - \frac{\partial\psi}{\partial t} - u\frac{\partial\psi}{\partial x} - \mu\frac{\partial^2\psi}{\partial x^2}\right)\delta u dxdt \\ &+ \int_0^1\Big(\psi(\cdot,T)\delta u(\cdot,T) - \psi(\cdot,0)\delta u(\cdot,0)\Big)dx.\end{aligned} \tag{6}$$

In order to get a decreasing sequence of iterates we demand $\delta\mathcal{L} < 0$, thus we set $\psi(\cdot,T) = 0$ and integrate

$$-\frac{\partial}{\partial t}\psi - u\frac{\partial}{\partial x}\psi - \frac{\partial}{\partial x^2}\psi = u - u^\delta, \tag{7}$$

backwards in time with $\psi(0,t) = \psi(1,t) = 0$. Then we choose

$$\delta v_k = \alpha_k\psi_k(\cdot,0), \tag{8}$$

where $\alpha_k > 0$ and ψ_k is the solution to (7) with $u = u_k$.

The derivation above of the iteration method is not rigorous, but widely used in applications. In order to apply known theory and convergence results we rewrite the minimization problem as an inverse problem. For this purpose we introduce the non-linear operator F as

$$u = F(v),$$

i.e. F maps an initial state $v(x)$ to the corresponding solution $u(x,t)$. The operator F is well-defined since it can be shown that for $v \in L^2(0,1)$ problem (1)-(3) has a unique solution $u \in C(0,T;L^2(0,1))$. Using the operator F, the minimization of I is reformulated as

$$\inf_{v\in L^2(0,1)}\|F(v) - u^\delta\|_{L^2(Q_T)}, \tag{9}$$

where u^δ is a given function. This is the corresponding least square problem for the equation $F(v) = u^\delta$. It is shown that the operator $F : L^2(0,1) \to$

$F(L^2(0,1)) \subset L^2(Q_T)$, does not have a continuous inverse, hence the inverse problem (9) is ill-posed.

Ill-posed inverse problems are treated by regularization methods, and examples of such methods are Tikhonov and Landweber, see for instance [3], [4] or [9] for a survey of regularization methods. In *Paper I* it is shown that the adjoint optimization method (5),(8) with constant α_k coincides with the Landweber iteration method. In proving that the iteration method is regularizing, the fundamental role plays the inequality

$$\|F(v) - F(\tilde{v}) - F'(v)(v - \tilde{v})\|_{L^2(Q_T)} \leq \eta \|F(v) - F(\tilde{v})\|_{L^2(Q_T)}, \qquad (10)$$

which is proven in *Paper I* for v sufficiently close to $\tilde{v}$. This inequality allow us to apply known results on iteration methods for nonlinear ill-posed problems, which guarantees that the method is convergent if it is supplied by a suitable stopping rule, see [6]. These convergence results are valid if the operator F satisfies inequality (10) with $\eta < 1/2$, for v and $\tilde{v}$ sufficiently close to start iteration v_0. If u^δ does not belong to the range of F the iteration method cannot converges to exact solution, but still yield a stable approximation of the solution to the inverse problem with exact data, provided the iteration is stopped according to a discrepancy principle [3, 6].

In *Paper I* we also consider the minimization problem

$$\min \int_{Q_T} \left(\partial_x (u - u^\delta)\right)^2 dxdt,$$

i.e. we minimize the difference in gradients instead of function values. We show that this problem always has a minimum, whereas the problem (9) does not have a solution in general. Moreover we prove that the inverse operator which is defined on the closed set $F(L^2(0,1))$ is locally Lipschitz continuous.

Numerically, the convergence of the two methods is compared in three cases: the given data u^δ is exact; and for small and large discrepancy levels in u^δ. The start iteration or initial approximation is chosen as $v_0 = 0$. First, when the given data is exact the convergence for L^2-minimization is satisfactory, at least for the initial steps. For minimization in the stronger norm, it turns out that the choice of initial approximation is important. The convergence is very slow if the initial approximation is not properly chosen, but with a good initial approximation the convergence is superior. Thus one can perform a few initial iterations with the L^2-method and then switch to the stronger method. Therafter the case when the given data u^δ contains noise is considered. For small disturbance levels, if the initial approximation is suitable, the convergence for gradient norm minimization is much faster than for L^2-minimization. If the disturbance level is more significant the L^2-norm method handles the data reconstruction well, but the gradient norm minimization method interrupts in a local minima. This is not surprising, since the data approximation contains significant noise and derivatives need to be numerically estimated, thus the already uncertain data becomes even worse.

Application to 3D flow

Let us apply the method described in the previous section to a more realistic problem, which is more numerically complicated.

We consider 3-dimensional time dependent inviscid compressible fluid flow in a tube, see figure 1. The boundary has an inlet and an outlet where

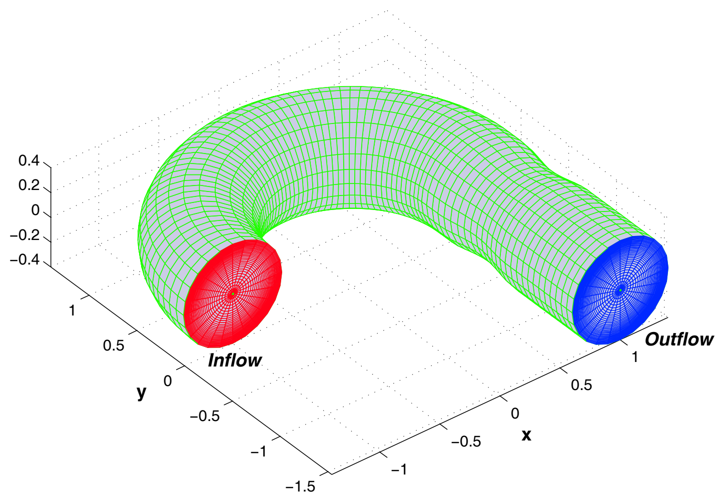

Figure 1: The flow domain Ω.

the flow is known to be streaming into and out of the tube respectively. The remaing part of the boundary is solid wall, where no fluid passes through. The flow is governed by the Euler equations

$$\frac{\partial \rho}{\partial t} + \operatorname{div}(\rho \mathbf{u}) = 0, \tag{11}$$

$$\frac{\partial(\rho u_i)}{\partial t} + \operatorname{div}(\rho u_i \mathbf{u}) + \frac{\partial p}{\partial x_i} = 0, \quad i = 1, 2, 3, \tag{12}$$

$$\frac{\partial(\rho E)}{\partial t} + \operatorname{div}(\rho \mathbf{u} H) = 0, \tag{13}$$

where

$$E = \frac{p}{(\gamma - 1)\rho} + \frac{|\mathbf{u}|^2}{2}$$

is the total energy and

$$H = E + \frac{p}{\rho} = \frac{\gamma p}{(\gamma - 1)\rho} + \frac{|\mathbf{u}|^2}{2}$$

is the entalphy.

If all five dependent variables $(\rho, \mathbf{u}, p)$ are prescribed at the boundary the hyperbolic problem becomes overdetermined and not well-posed. From the theory of characteristics one should specify 4 boundary conditions at the inlet and one at the outlet. The wall boundary condition is $\mathbf{u} \cdot \mathbf{n} = 0$. At the inlet the boundary condition is a total states condition, and at the outlet the pressure is given.

We shall now consider the inverse problem to determine the initial states $(\rho_0, \mathbf{u}_0, p_0)$ when a measured approximation $\mathbf{u}^\delta$ to the exact flow field $\mathbf{u}^*$ is given. In *Paper II* the adjoint equations with corresponding gradient expressions are derived for this problem. The test problem for which the numerical examples are carried out, deals with reconstruction of the initial pressure, and assumes that the initial density and velocity field are known. This restriction is not necassary for the method, however it is a way to reduce the degrees of freedom and obtain a test problem that can be solved in reasonable time with limited computer resources. Here we study a time history of a pressure pulse applied to a steady state solution. To do this, the corresponding steady state problem is solved and we denote the solution by $(\rho_s, \mathbf{u}_s, p_s)$, and the initial conditions for the time dependent problem (11)-(13) is set to

$$\begin{aligned} \rho_0 &= \rho_s \\ \mathbf{u}_0 &= \mathbf{u}_s \\ p_0 &= p_s + \Phi, \end{aligned}$$

where Φ is the applied pressure pulse. The pulse Φ is parametrized

$$\Phi = \sum_{n=1}^{N} c_n \phi_n,$$

where $\{\phi_n\}$ is any set of base functions which does not violate the boundary conditions.

The adjoint equations have been implemented in an existing flow solver EDGE, see [1]. The adjoint and Euler solutions are posted and the gradient and optimization iterations computations are carried out in Matlab. The derivation and implementation have been validated numerically, the computed gradients are compared to finite differences. Here effects by convergence of the flow solutions are studied. The test shows that the gradient approximated with a finite central difference method and the adjoint based gradient coincides with 7-8 numbers. The forward differences yields a less accurate result but has the advantage in computational cost versus the central differences. The adjoint method requires significant less computations for approximating the gradient, especially when the number of parameters N increases. The adjoint method requires two flow solutions independent of N, the central difference method requires $2N$, and the forward difference method $N+1$ flow solutions.

Finally, a numerical example for reconstruction of the pressure pulse is solved. The example first consider the case when the data approximation $\mathbf{u}^\delta$ is exact, and therafter when there are disturbances in the data. One part deals with the case that the initial pressure pulse can not be exactly reconstructed, the base functions are not the same as for generating the exact solution. The optimization method is a quasi-Newton method, approximating the Hessian used for evaluation of a search direction, in all three cases. When the dimension N increases, the computations for approximating the inverse Hessian becomes a drawback. However the convergence for the one step method is linear and for the quasi-Newton method superlinear [15], and in this application where each function evaluation consists of a time accurate non-linear CFD-solution the linear algebra computations for approximating the Hessian is worthy.

The results of the iteration method for data reconstruction are satisfying. The relative error in the computed parameters is what we can expect according to theory for inverse problems [3].

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