Adjoint-based data assimilation of a compressible starting jet

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1. Introduction

Data assimilation [1] is the process of including observational data in the mathematical model of a physical system, with the goal of producing an accurate and reliable representation of the system's state and reducing uncertainties. This methodology aims at finding the solution of the physical model that better approximates the observational data in an optimal way.

Data assimilation techniques found a lot of applications in many fields, e.g. meteorology, oceanography, weather forecasting, control engineering, medical applications and currently it's gaining popularity in fluid mechanics.

Two main approaches can be identified: a stochastic and a variational approach. The former makes use of stochastic filtering and estimation techniques such as Kalman filters and Ensemble Kalaman filters. The latter minimizes a loss function to find the model solution that best approximates the measurement data. For the computation of gradients an adjoint formulation is used. Popular methods are 3DVar and 4DVar.

Both the approaches can be successfully used for the application of compressible fluid mechanics. In this thesis variational techniques will be used.

1.1. Objectives

There are multiple objectives for this thesis.

First, a data assimilation framework is developed for the compressible Navier-Stokes equations and it is tested.

Second, the data assimilation framework is going to be applied to the Kovasznay modes [2]. From this, an observation analysis is conducted with the goal of understanding the capabilities of the derived framework to reconstruct non-accessible fields from measured ones, in the case of a perturbed condition from a base flow.

Third, the data assimilation of the compressible starting jet is done and its observational capabilities are assessed. A systematic study is conducted with reference to possible experimental measurements that can be done at the research group's laboratory in the future. The capability of the data assimilation to infer unknown flow variables from measured ones will be assessed in the case of a compressible starting jet. Furthermore, the capability of finding a satisfying fit solution, given two snapshots of experimental data in distant time steps, is evaluated by comparing the found solution with the ground truth in the time step in between the two given snapshots.

This work is a first step towards the long

term goal of doing a fully data-driven DNS of a compressible starting jet using limited experimental measured data.

2. Adjoint-based data assimilation

In this section the adjoint-based data assimilation framework will be presented with the adjoint Navier-Stokes equations for a compressible flow. The solution of the adjoint equation gives access to the gradient of the objective function with respect to a control variable of choice (e.g, forcing term, initial condition and boundary conditions). With the knowledge of the gradient it is possible to set up an optimization procedure to find the flow that better approximates a set of observed data. A simple case is also presented to validate the procedure and showcase its efficacy. The formulation is based on [3].

2.1. Adjoint Navier-Stokes equations

For the derivaiton of the adjoint equations it is necessary to select an objective function to be minimized. In this case a generic non linear function $g(\mathbf{q})$ is selected. The objective function is augmented by summing the Navier-Stokes equations and multiplying them with a Lagrange multiplier $\mathbf{q}^*$. This technique is used to constrain the search for the minimum of the objective in the solution space of the Navier-Stokes equations. The NS equations are reported in matrix form, with $\mathbf{q} = (p, u, s)^\intercal$, and they are presented in the one dimensional case for brevity.

$$J = \iint g(\mathbf{q}) \, dV \, dt$$
$$- \iint \mathbf{q}^{*\intercal} \left[\partial_t \mathbf{q} + \mathbf{X}(\mathbf{q})\partial_x \mathbf{q} + \mathbf{F} - \mathbf{f} \right] \, dV \, dt.$$

Here $g(\mathbf{q})$ is a generic nonlinear function of the state. For our case $g(\mathbf{q}) = (\psi(\mathbf{q}) - \psi_{exp})^2$ where $\psi(\mathbf{q})$ is a generic observable of the flow.

By taking the first variation δJ of the functional and using integration by parts it is possible to find the variation of the functional with respect to the control variables. By doing so, the adjoint equations with their respective initial and boundary conditions also get derived. The adjoint equations have the following form:

$$\partial_t q_\alpha^* = q_\gamma^* \frac{\partial X_{\gamma\beta}}{\partial q_\alpha} \partial_x q_\beta - \partial_x q_\beta^* X_{\beta\alpha}$$
$$- q_\beta^* \partial_x X_{\beta\alpha} + q_\gamma^* \frac{\partial F_\gamma}{\partial q_\alpha} + \frac{\partial g}{\partial q_\alpha}. \tag{1}$$

These equations must be integrated backwards in time.

The gradient of the loss function with respect to the forcing term of the NS equations is the solution of the adjoint equation. $\nabla_{\mathbf{f}} J = \mathbf{q}^*$. The gradient of the loss function with respect to the initial conditions is the solution of the adjoint equaiton at time $t = t_0$. $\nabla_{\mathbf{q_0}} J = \mathbf{q}^*(\mathbf{x}, t = t_0)$.

2.2. Data assimilation framework

Now that the main tools of variational adjoint-based data assimilation are presented, it is possible to design an optimization procedure to minimize J.

Starting from an initial condition, the Navier-Stokes equations are solved forward in time. Afterwards the objective function is computed and the adjoint equations are solved backwards in time, using $\frac{\partial g}{\partial \mathbf{q}}$ as the adjoint forcing. From the adjoint solution the gradient of the objective is obtained, and the forcing term $\mathbf{f}^n$ is adapted, and then the procedure starts again with a new forcing term for the Navier-Stokes equations. The loop stops when a convergence criteria is met, e.g., number of loops, value of J and change of the value of J.

It's important to state that the detection of a global minimum is not ensured and that the framework minimizes towards local minima. Furthermore, depending on the individual setup, the solution may not be unique.

Algorithm 1 Data assimilation procedure

  Initial guess $\mathbf{f}^0$
  while $J > \epsilon$ **or** $i < N$ **do**
    Solve Navier-Stokes equations $N(\mathbf{q}, \mathbf{f}^n)$ (direct solution).
    Compute J.
    Solve the adjoint Navier-Stokes equations $N^*(\mathbf{q}, \mathbf{q}^*, \mathbf{f}^n)$.
    Compute the gradient $\nabla_{\mathbf{f}} J(\mathbf{q}, \mathbf{q}^*, \mathbf{f}^n)$.
    Update $\mathbf{f}^{n+1} = \mathbf{f}^n - \alpha \nabla_{\mathbf{f}} J(\mathbf{q}, \mathbf{q}^*, \mathbf{f}^n)$.
    $i = i + 1$
  end while

2.3. Verification

As a verification test, a data assimilation of an acoustic source is done. The setup consists of a point-wise speaker surrounded by eight microphones, everything is set on a common plane, as all the simulations are two dimensional. The numerical simulation is done with the fully compressible Navier-Stokes equations. The speaker emits a harmonic signal at 1kHz. The objective is to find the source location, its frequency content and amplitude.

The DA procedure is able to complete the objective successfully. In figure 1 it is possible to see the successful assimilation.
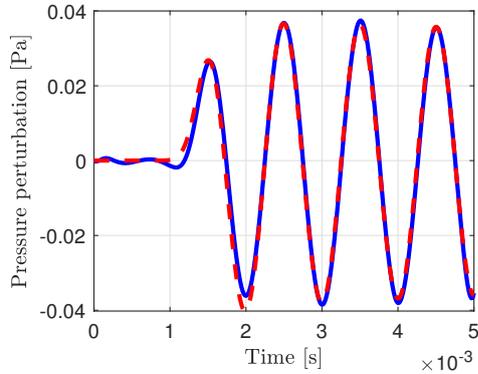

Figure 1: Assimilated pressure signal. In red the original signal, in blue the assimilated one.

3. Data assimilation of Kovasznay modes

In this section the data assimilation of the Kovasznay modes [2] will be presented. The objective of this chapter is to test the observational capabilities of the derived assimilation framework and see if it is able to observe second-order effects of first-order approximate solutions.

3.1. Kovasznay modes

Kovasznay performed a linear expansion of the Navier-Stokes equations for a perfect gas and for small perturbations around a base state. After a linearization and some manipulations the fol-

lowing set of linear equations was found:

$$\frac{\partial \boldsymbol{\omega}}{\partial t} - \nu \nabla^2 \boldsymbol{\omega} = 0 \qquad (2a)$$

$$\frac{\partial s}{\partial t} - \frac{4\nu}{3} \nabla^2 s = 0 \qquad (2b)$$

$$\frac{1}{c^2}\frac{\partial^2 p}{\partial t^2} - \nabla^2 p - \frac{4\gamma\nu}{3c^2}\frac{\partial \nabla^2 p}{\partial t} = 0. \qquad (2c)$$

The solutions of these equations yield the three fundamental modes of compressible turbulent flows. For the observational analysis, plane wave solutions are considered.

3.2. Modes assimilation

Here the capabilities of the data assimilation framework to infer unknown variables, given complete information on a single mode is going to be assessed.

Pressure mode assimilation
In this case the framework was able to assimilate the pressure mode correctly, and reconstruct part of the entropy mode successfully from information on pressure. The vorticity mode was not reconstructed by the data assimilation. The assimilation framework, however, found a velocity field that is completely irrotational. This is because the information of potential flows is not contained in the vorticity mode but in the pressure mode. In general, it is expected that the knowledge on a single scalar field is not enough to reconstruct in a satisfying manner an entire vector field.
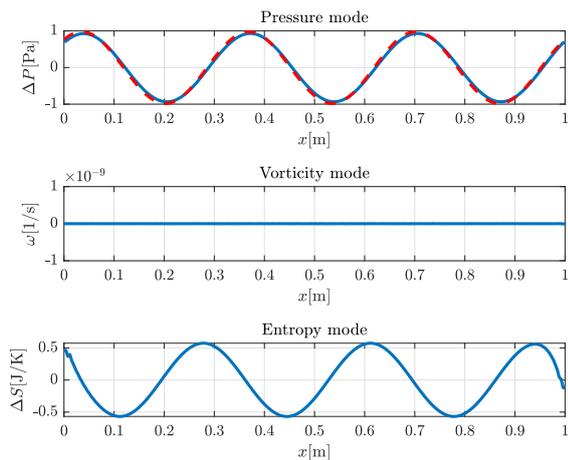
Vorticity mode assimilation
In this case the method was also able to assimilate the vorticity mode correctly, and was also able to find a contribution of the vorticity field to the pressure and entropy mode.

The peaks of the reconstructed signals correspond to the peak regions of the assimilated signal and its derivatives. This implies an important correlation and sensitivity of the pressure and entropy perturbation with respect to velocity perturbation and its gradients. The amplitudes of the entropy and pressure however are very small, which implies that the capability of reconstruction of the method is not particularly strong.

Entropy mode assimilation
Also for this case, the assimilation of the en-

Figure 2: Results of the assimilation of the pressure mode in the middle time step. In red the observed mode, in blue the result of the assimilation

tropy mode is satisfactory. The reconstruction of the vorticity mode, however, is not successful, just like in pressure case. The pressure mode reconstruction is also not completely successful, as the pressure mode found has double the wave number of the assimilated wave.

From the previous analysis it is possible to say that the entropy mode is the mode with the least amount of information of all the Kovasznay modes.
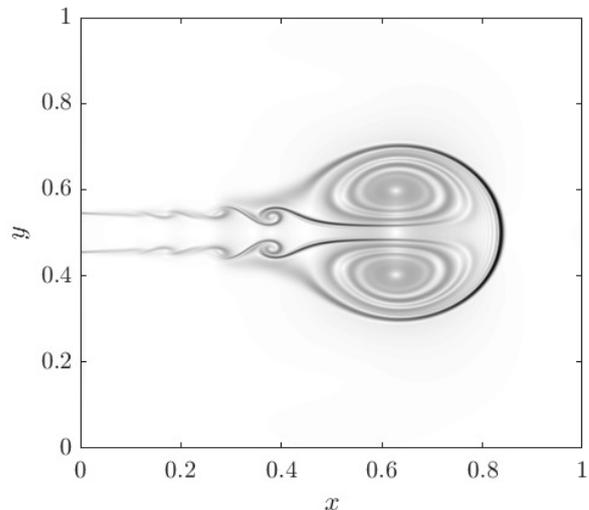
4. Data assimilation of the compressible starting jet

In this section the data assimilation of a compressible starting jet will be presented. The objective of this section is to test the observability capabilities of the previously derived data assimilation framework for the compressible starting jet. Given a limited amount of information about the flow, the objective is to see what is possible to reconstruct. The analysis will be done systematically, using a single given field of the flow (e.g, pressure, temperature, density etc...) at two different times and the flow will be reconstructed in the middle time steps. The L_2 norms between ground truth and the assimilated flow will be compared, to see how much of a certain unknown field it is possible to reconstruct from another known field. Here only three cases will be reported, as

they are considered the most significant.

The systematic study will not only be performed with respect to the amount of information that will be given to the algorithm, but also with respect to the time distance between each snapshot.

The data assimilation will be done on synthetic data generated by a DNS of a compressible starting jet. The jet's mass supply is considered as infinite. The Reynolds number is set to $Re = UD/\nu = 5000$, where U is the characteristic velocity of the jet, D is the diameter of the inlet and ν is the kinematic viscosity. The Mach number is set to $M_\infty = U/c = 0.8$ and the pressure jump between the reservoir and the open chamber is selected as $p_r/p_\infty = 1.5$. A grid of 512×512 is selected for this particular jet case. The CFL number selected is $CFL = 0.8$. The time step found is, therefore, $\Delta t = 4.5 \times 10^{-6}$ seconds. The code and the simulation setup are based on [4] and [5].

Figure 3: Numerical schliren ($||\nabla \rho||$) of the jet.

4.1. Results

Full case

The full case is presented as reference. In this case all the state variables are used for the assimilation, therefore no reconstruction is evaluated. The flow in the middle step in assimilated successfully.

Pressure case

Here the pressure case is presented. This case is considered as an observability benchmark for pressure experimental measurements. Differently from the previous case, also the reconstruction capabilities of the assimilation will be assessed here.
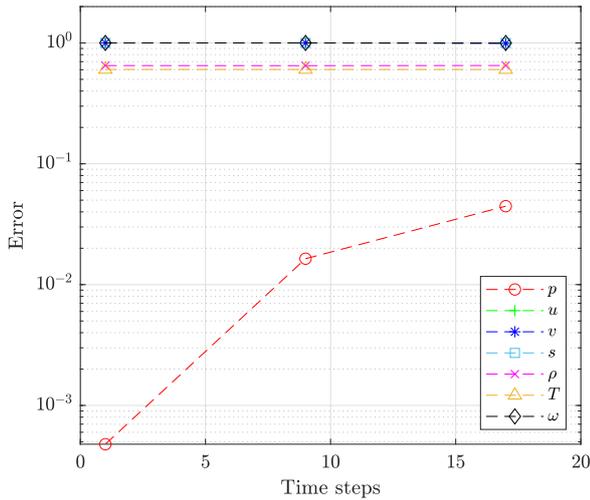

Figure 4: Error trends with respect to the time steps gap.

From figure 4 it is possible to see that the middle step assimilation of the pressure measurement was successful, as the pressure error is small for all the analyzed cases. Looking at the the trends of the other thermodynamic variables it is possible to see how the error norm of the density and temperature are smaller then one. This means that part of the field was reconstructed successfully. The reconstruction is partial because the knowledge on the entropy field is absent, and therefore the reconstruction of thermodynamic variables is due to the pressure information only. This is not enough because in the case of a perfect gas, two thermodynamic variables must be known to have a complete thermodynamic description of the flow.

Looking at the error norms of the velocity components and vorticity fields it is possible to see that the reconstruction of velocity variables was not successful. In fact the error norms for u, v and ω are all approximately one. This indicates that no significant reconstruction can be detected, at least in an integral sense. However, upon further inspection, the DA

framework is able to reconstruct a part of the velocity field. Precisely, it is able to reconstruct the potential component of the velocity vector field. For the reconstruction of the entropy field, something analogous happens.

Velocity case

The velocity vector field data assimilation is now presented. This case will be used as an observability benchmark for experimental PIV measurements.

The assimilation in the middle time step is successful as it can be seen from figure 5. This translates in a well reconstructed vorticity field The thermodynamic variables are not well reconstructed. This is analogous to the pressure case, as the norms are not able to capture the amount of information that the assimilation framework is able to extract from the partial information. In this case the method is able to reconstruct the pressure field that is due to the effect of the velocity divergence. Similar phenomena can be seen in the temperature, density and entropy field.
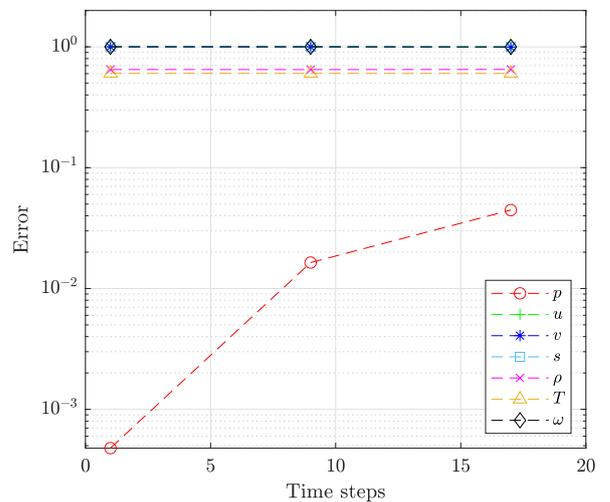

Figure 5: Error trends with respect to the time steps gap.

5.   Conclusions

The observation analysis for the derived data assimilation was done to understand the reconstruction capabilities of the adjoint-based data assimilation procedure. First, the method was validated succesfully on a simple acoustic case.

The frequency content of the acoustic source was resolved, the position of the sound source was found and the amplitude of the signal was assessed correctly.

Second, the reconstruction capabilities of the data assimilation procedure on the Kovasznay modes was investigated. The analysis showed that the derived framework was able to assimilate all the observed modes correctly. The reconstruction capabilities with unknown fields was not completely satisfactory.

Finally, the observational analysis is repeated on the compressible starting jet in a systematic manner on various variables of experimental interest. The data assimilation was able to generate a flow that matched the ground truth in the middle time steps, but only for the variables that were being observed. The developed procedure was not able to find the entirety of the unknown variables, just part of them. The reconstruction capabilities were unsatisfactory in some cases.

The cause of this ineffectiveness is to be found in the fact that jets are flows in which the convective component is very strong with respect to all other effects. Assimilating the velocity field gives information on the convection field but does not give any information on the other fields that are being convected, not even on the boundary and initial conditions. This makes inferring other unknown variables very hard.

It was previously demonstrated that the pressure variable can be inferred from PIV measurements in compressible flows [3]. In that case however the convection flow was considered as a base flow, and therefore the initial condition for both the direct solution of the data assimilation and of the ground truth was the same. This means that the initial condition was perfectly known, for each variable. This is not the case for the compressible starting jet here presented. Additionally, the time frame of the assimilation done in this work is much smaller than the previously cited one. This makes it impossible for the direct solution to transition from an unstable assimilated solution to a stable one. The space of stable solutions of the Navier-Stokes equations is a much smaller space then the unstable solutions space, especially for high Reynolds number flows. The requirement of being stable makes the work of finding the correct solution easier because it bounds the flow in a smaller solution space.

References

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