Chapter 1

Introduction

1.1 From the control of a dynamical system to large scale data assimilation

The control theory aims to analyze systems which can be commanded. In other words, dynamical systems which can be modified by a command (the control). The two classical objectives are:
A) Act on the control in order to bring the system state to a final state given (if possible, and potentially with constraints). It is a *controllability* problem.
B) Define a control $u(t)$ such that a criteria j is minimal. The criteria j, also called the cost functional, depends on the control and the state of the system. Potentially, the control must satisfy constraints given. It is a *optimal control* problem
The present course addresses optimal control problems only (objective B)).

In a mathematical point of view, the systems considered here are differential equations: Ordinary Differential Equation (ODE, dynamical systems) in Chapter 2, elliptic Partial Derivatives Equations (PDEs, steady-state) in Chapter 3, and unsteady PDEs in Chapter 4 (parabolic and hyperbolic). These classes of equations model a very wide range of systems both in engineering and in academic researches. Let us cite the following applicative topics only: fluid mechanics, geophysical flows, structural mechanics, micro-electronics, nano-technologies, biological systems, coupled multi-physics systems, etc.

The objective is either to stabilize the system in order to make it insensitive to perturbation (related to objective A), see the course of automatism GMM5), or to determine optimal solutions with respect to the given criteria j (objective B)).

Optimal control is a topic between the automatic engineering science and applied mathematics.
Calculus of variations deals with the minimization of functionals (i.e. mappings from a set of functions to $\mathbb{R}$; functionals are often definite integrals involving functions and their derivatives).
Optimal control theory is somehow an extension of the calculus of variations: it is mathematical optimization problems with an underlying model (the differential equation), and the goal is to derive a control policy.

Historically, optimal control appeared after the second world war, with applications in aeronautics (missile guidance etc).
A key point of the optimal control is the *Pontryagin maximum principle* (L. Pontryagin (blind) russian mathematician (1908-1988)),which gives a necessary condition of optimality for an ODE system. The condition becomes sufficient if the model is linear and the cost function is quadratic: the *Linear-Quadratic (LQ) case* studied in Chapter 2.

In real-life problems, optimal control problems are often non-linear, thus the analytic expression of the optimal control we obtain in the Linear-Quadratic (LQ) case (Chapter 2), does not apply anymore. Then, in view to solve a *non-linear* optimal control problems (i.e. compute an optimal control u and the corresponding optimal trajectory x^u), we use *numerical methods* to solve the necessary first-order optimality conditions based on the so-called Hamiltonian system.

For Partial Derivatives Equations (PDE) systems (Chapter 3), the Pontryagin maximum principle does not apply. Nevertheless one can obtain equations characterizing the optimal solution: it is the *optimality system* which make introduce the *adjoint equations*.

Next, what is the link between optimal control of a PDEs system and *data assimilation* ?
Assimilation of data (measurements) into the system can be done using an optimal control process simply by defining the criteria j to be minimized as the *misfit between the computed solution and the measurements (observations)*. Generally the latter are heterogeneous in space, in time, and in nature. For real and complex applications, defining a 'good' cost function can be difficult since it requires to introduce some *a-priori statistic errors*, which define the metric we work with.
Chapter 3 aims at deriving the optimality systems for elliptic PDEs (a-priori non-linear) and focus on the computational aspects. A result of existence and uniqueness of the control is presented in the linear-quadratic pde case. We present in detail how to solve numerically the optimality system. The result is the *identification* of the input parameters which was unknown (or known with uncertainties), and/or a better *calibration* of the model.

In Chapter 4, we extend the method to unsteady PDEs systems (either parabolic or hyperbolic). Calculations derived in these cases are more formal. We detail the computational algorithms: 4D-var and its variants.
The 4D-var type methods are very CPU time consuming (10–100 times the CPU time of the direct simulation), but they are able to greatly improve both the model accuracy and our own understanding of the physical system.

Numerical simulation, based on a mathematical model, is a fundamental step for a large range of industrial processes - conceptions - designs or physical - geophysical analysis - descriptions - predictions. Numerical simulation replaces more and more (real) experiments since the latter are costy. Experiments are often used for validation of the (virtual) numerical results.
Data assimilation is a quite recent science. In the future, one can bet it will be naturally integrated in our concept of numerical simulation.

Data assimilation is the science combining "at best" the three knowledges of a system: the model (mathematical equations), the observations - measurements of the reality and statistical errors (errors of measurements mainly).

"Data assimilation" refers to two different (and complimentary) approaches:

1) a stochastic approach, *filtering* such as the Kalman's filter (roughly, we calculate the Best Linear Unbiased Estimate -BLUE- using algebric calculations) or the Ensemble Kalman Filter (EnKF),

2) a *variational approach* based on the control theory (it is a more deterministic approach even if one can mix both approaches). We minimize a cost function which measures the misfit between the model output and the measurements.

Both approaches lead to the same estimate in the linear case (in the linear case only!). At the end of Chapter 4, we show the equivalency between the (basic) Best Linear Unbiased Estimate (BLUE) and the variational approach in a linear-quadratic case. This equivalency show us how one may introduce the statistics of errors in the variational data assimilation processes, even in non-linear cases.

Both approaches present similar difficulties if the direct dynamical model is non-linear and with large dimensions; furthermore, we never really known the necessary a-priori errors statistics...

The present course addresses only the variational data assimilation approach.

Let us cite the historical application: weather (atmosphere) prediction. The numerical weather prediction centers developed operational 4D-var algorithms (see Chapter 4) since the 2000s approximatively. Forecasts have improved the last ten-fifteen years approximately in particular because of the introduction of variational data assimilation into the complex dynamical atmosphere models. Data assimilation allows to benefit from the global various observing systems. In short, 4D-var approach has been and is a key point to improve greatly weather forecasting at all scale and all over the world.
For complex models (multi-physics coupled, non-linear, multi-scales) like in meteorology, the discrete unknowns number may be huge (eg. dozens of millions) and the number of observations available may be huge too (eg. dozens of millions). For such large scale problems, some tricky and pseudo-empirical simplifications both of the algorithms and the physical systems are proposed; it is the aim of the 4D-var incremental method presented at the end of Chapter 4.
The implementation of the adjoint equations in a computational software may be facilitated by an pseudo-automatic process: the so-called *automatic differentiation* (or *algorithmic differentiation*).
In case of a source-to-source differentiation approach, it consists to derive the source code instructions one by one. We present the principles of the method in Chapter 6, and using Tapenade [13]. Tapenade is an automatic differentiation software developed at INRIA France, it is one of the few software doing the job efficiently. We use it for the computations presented

in the present course (see Chapter 5).

In Chapter 5, we present examples of current research studies on the topic, with applications in river hydraulics - floods, in glaciology (glaciers flows in Antarctica, Groenland etc), lavas etc. These studies are led at Mathematics Institute of Toulouse (IMT) and INSA (GMM department) by the author with collaborators. Computations have been generally performed by PhDs students (eg. M. Honnorat, N. Martin), research engineers (eg. F. Couderc, R. Madec), and postdoctoral researchers. Al these studies are done in close collaboration with colleagues from fluid mechanics (eg. Fluid Mechanics Institute of Toulouse -IMFT-), satellite measurements (LEGOS Toulouse, CNES), glaciologists (LGGE Grenoble) etc.

Some historical dates related to data assimilation.
The 4D-var methods are based on *non-linear least-squares* computations. Recall the least-squares method is a standard method to approximate a solution of overdetermined systems (more equations than unknowns), which is the typical configuration of data assimilation problems. Historically, the least-square method has been elaborated by J.C. Gauss (1777-1855) and A.-M. Legrendre (1752-1833). J.C. Gauss, at 24 years old, calculated a (right) least-square solution to predict an asteroid trajectory based on past observations !
In the 20th century, one can cite the *Kalman's filter* which has been developed at NASA in order to estimate trajectories of the Apollo program (years 1960's). In the 2000th, *variational data assimilation* methods (also called 4D-var) have been developed for operational forecast in the large national numerical weather prediction centers (eg. Meteo-France, ECMWF etc).