Universidad
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HALA! Research Network PhD

PhD Intended Title:

Stochastic Optimal Control towards Enhanced Predictability of four-dimensional Trajectories using Weather Ensemble Prediction Forecasts

# D4: State of the Art

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# Contents

# 1 Introduction

This state of the art is divided in three sections:

- Section 2 reviews the current approaches to **modelling** of the underlying physical systems.
- Section 3 reviews the existing **methodologies** for the formulation and solution of the resulting mathematical problems.
- Section 4 reviews the previous **applications** of these methodologies in the field of aircraft trajectory optimization.

# 2 Modelling

## 2.1 Aircraft Performance and Modelling

Simulation, prediction and optimization of trajectories rely on accurate models of the real aircraft that can replicate its behaviour in practice. The most commonly used description of aircraft dynamics in the field of ATM and trajectory planning is the three degrees of freedom (3-DoF) point-mass model. The state of the aircraft at any point in time is described by its position in a 3-dimensional space, its velocity and orientation, as well as any additional performance variables or parameters (such as the mass or the aerodynamic configuration). The space where this motion takes place can be either an cartesian space or a round or ellipsoidal Earth model, depending on the desired application.

This dynamical model is completed by the addition of models for the aerodynamical forces and the necessary limitations to the flight envelope arising from different sources, such as design and performance limits or regulatory requirements. A complete package is called an *Aircraft Performance Model* (APM). For this thesis, the BADA (Base of Aircraft Data) family of APMs developed and maintained by the Eurocontrol Experimental Center in collaboration with aircraft manufacturers and operating airlines will be used. There are currently two versions of BADA in use:

- The older BADA 3 family [1] covers almost 100% of the aircraft types operating over the ECAC area.

- The newer BADA 4 famiy [2] covers fewer aircraft types (around 70% at the moment), but it provides a more accurate modelling of several components (for example, by including compressibility effects in the drag polar).

## 2.2 Meteorological modelling

### 2.2.1 Introduction to ensemble forecasting

In order to study and quantify the uncertainty inherent to weather forecasting, the meteorological community has developed the idea of *ensemble forecasting* or *Ensemble Prediction Systems* (EPS). The goal of an EPS is to produce a collection of forecasts (typically from 10 to 50) for the same prediction time that constitutes a representative sample of the possible future states of the atmosphere. The individual forecasts are called the *members* of the ensemble.

In order to generate different forecasts according to the uncertainty in the initial conditions, parametrized models of physical processes and approximation errors, different Numerical Weather Prediction (NWP) centers employ combinations of several techniques. These methods include changing initial conditions in the most sensitive directions, changing the parameters of the simulation, combining different models or building time-lagged ensembles [3] [4] [5] [6]

### 2.2.2 Characteristics

For deterministic medium-range prediction, the typical setup of a forecasting system is a hydrostatic dynamical core with a horizontal resolution of around 15km and around 80 levels from surface to the top of the model, usually between 50 km and 80 km of altitude. Standard practices involve running the model 4 times a day, with output at a 1-, 3-, or 6-hour interval.

For deterministic short-range prediction, the model is restricted to a limited area, non-hydrostatic effects are taken into account, and the resolution is improved to a horizontal grid of 1.5 to 5 km. Runs are also shorter (around a day of output) and run more frequently (from 4 to 8 times a day).

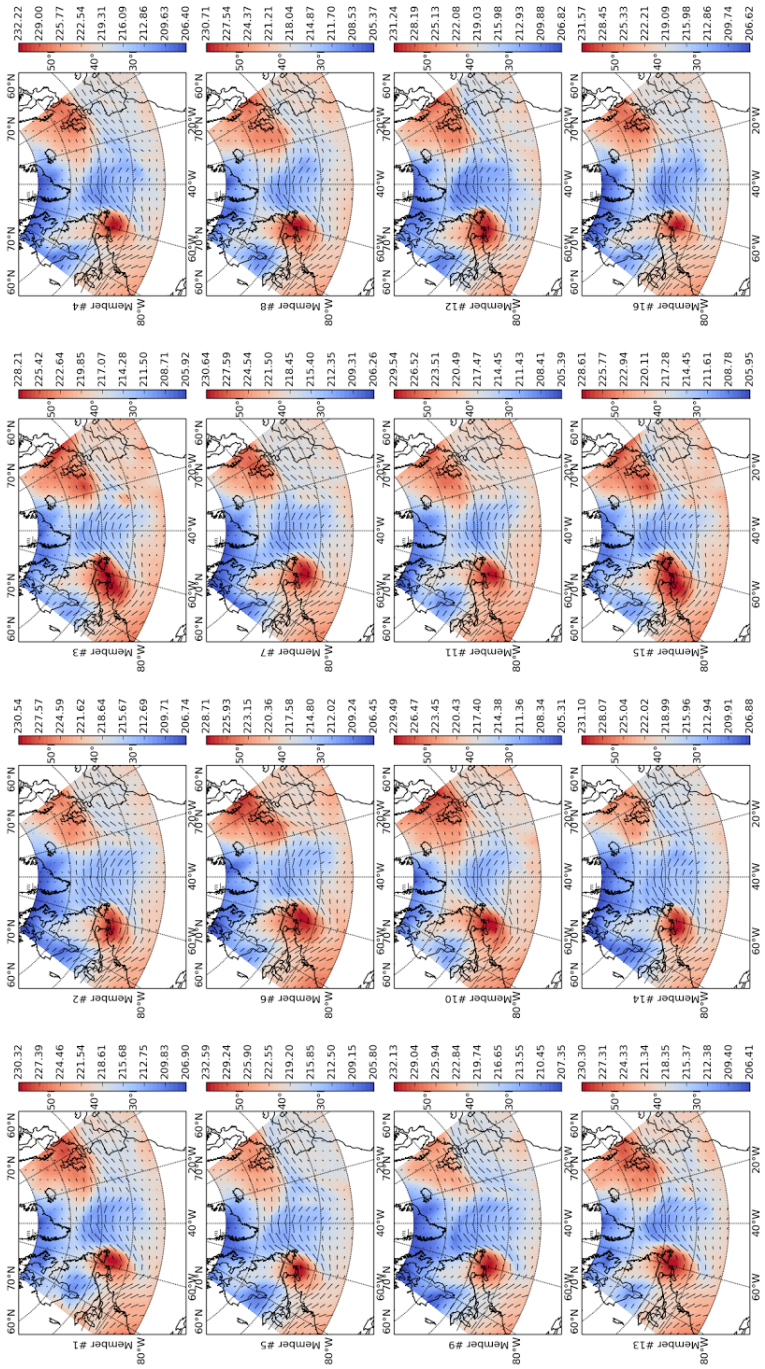

Figure 1: Wind and temperature in the North Atlantic for different members of the PEARP ensemble with a 6-hour lead time

Since ensemble predictions require multiple model runs (10 to 50) for the same time interval, lower resolutions compared with the deterministic systems are used. The horizontal resolution is around twice the resolution for the deterministic prediction, and the vertical levels are also reduced. Depending on the area of interest and the target time interval, ensemble predictions can be classified in three categories:

- Global, medium-range forecasts are run for the whole globe and usually aim at forecasting 2 to 10 days ahead. They capture the uncertainty associated to planetary-level perturbations.
- Limited Area Model (LAM), short-range forecasts predict weather in a specific region at a 1-2 day timescale. The associated uncertainty captured by LAM forecasts is associated to mesoscale-alpha phenomena (200-2000km characteristic scales).
- LAM, very short range forecasts produce predictions for a time-horizon of a few hours. The uncertainty is related to mesoscale-beta (20-200 km) and mesoscale-gamma (2-20km) phenomena.

**Medium-range ensemble forecasting**

The creation of the THORPEX (The Observing System Research and Predictability Experiment) research initiative by the World Meteorological Organization in 2004 estimulated the development, usage, utility and accuracy of medium-range ensemble forecasts. It created the TIGGE (THORPEX Interactive Grand Global Ensemble) dataset[1] [7].

TIGGE contains global medium-range ensemble forecast data produced by several NWP centers for the purposes of scientific research [8] in an homogeneous format. It is hosted at the website of the European Center for Medium-Range Weather Forecasts (ECMWF).[2]. The ECMWF [9], the Canadian Meteorological Center [10] and the National Center for Environmental Prediction (NCEP) [11], among others, develop ensemble prediction systems included in TIGGE. In 2014, the TIGGE-LAM (Limited Area Model) dataset was also launched with the aim of including regional ensembles on finer (from 2 to 10 km) grids.

[1] http://tigge.ecmwf.int/documents/
[2] http://apps.ecmwf.int/datasets/

These models run at a coarse resolution of 30 km or larger grid size in order to be able to forecast the weather at the whole globe for 2 to 10 days because of computational constraints. This is a low resolution for aviation applications, which benefit from higher resolution and shorter-range forecasting.

**Limited Area Model ensemble forecasting**

By limiting the area and period of interest, Limited Area Models (LAM) are able to use a higher resolution. Examples of these models are:

- The MOGREPS [12] ensemble (which contains both a global and a LAM model), developed by the UK Met Office. It is a 10-member ensemble that relies on perturbation of the initial conditions and the model physices.
- The SREPS [13] ensemble from the Spanish meteorological service AEMET, which combines five different LAM models (with a 25km horizontal $\times$ 40 vertical levels resolution) with five different initial and boundary conditions for a total of 25 ensemble members that predict up to 72h.
- The Norwegian Meteorological Institute's LAMEPS [14] is a 21-member ensemble that has a 28km horizontal $\times$ 31 vertical levels resolution with the aim of forecasting precipitation in northern Europe in a time horizon of 0 to 3 days.
- The COnsortium for Small-scale MOdelling's COSMO-LEPS [15] is a 16-member ensemble with a 10 km horizontal resolution and 40 levels in the vertical that is based on a downscaling of the global ECMWF ensemble runs.
- Météo France's PEARP [16], which is the EPS based on the ARPEGE deterministic model, has a variable horizontal resolution that allows it to be more accurate over France and combines multiphysics and initial condition perturbation.
- The GLAMEPS (Grand Limited Area Model Ensemble Prediction System) is a pan-European EPS [17] in development resulting from the cooperation of the HIRLAM (The High Resolution Limited Area Model) and ALADIN (Aire Limitée Adaptation Dynamique Développement

International) [18] consortia. It will combine runs from a variant of the ECMWF EPS, HIRLAM and ALADIN models ran by different countries in order to produce a 52-member short-range high-resolution EPS.

# 3 Methodology

## 3.1 Optimal Control

Optimal control is a framework for optimization of the performance of controlled dynamical systems [19]. It has been successfully employed in a wide range of problems within the field of aerospace engineering [20]. The cornerstone of optimal control theory is the dynamical system, which is composed by:

- A temporal domain $\mathcal{T} = [t_0, t_f] \subset \mathbb{R}_+ \cup \{+\infty\}$
- A vector of state variables $x(t) : \mathcal{T} \to \Omega_x \subset \mathbb{R}^n$
- A vector of control variables $u(t) : \mathcal{T} \to \Omega_u \subset \mathbb{R}^m$
- The differential equation of the system:

$$\frac{dx}{dt} = f(x(t), u(t), t) \tag{1}$$

The time evolution of certain controlled dynamical systems (and, particularly, systems that describe the trajectories of aircraft) is not described by differential equations alone; it is also described by a set of equality and inequality *path constraints*:

$$g_j(x(t), u(t), t) = 0,\ j \in \{1, \dots, n_g\} \tag{2}$$

$$h_j(x(t), u(t), t) \leq 0,\ j \in \{1, \dots, n_h\} \tag{3}$$

The addition of these conditions upgrades the differential equation to a DAE (differential-algebraic equation). Certain regularity assumptions are usually required to ensure existence of solutions to this system.

At the conceptual level, a control problem can be summarized as "find a control $u(t) = f_u(x(t), t)$[3] such that the trajectory of the system has certain properties". In an optimal control setting, the desired property is that the trajectory is, among the set of feasible trajectories that fulfill the initial and final conditions, a minimizer of a *cost functional* defined on the form:

$$J(x, u, t_0, t_f) = \Phi(x(t_f), t_f) + \int_{t_0}^{t_f} L(x(t), u(t), t)dt \tag{4}$$

[3]We distinguish between *open-loop control*, where the control is only a function of time, and *closed-loop control*, where the control is a function of the state.

where $\Phi$ is a "terminal cost" term[4] and $L$ is called the *Lagrangian term*. This form of the cost functional is known as the *Bolza form* of the optimal control. If $\Phi = 0$, then the problem is said to be in *Lagrange form*, and if $L = 0$ the problem is said to be in *Mayer form*.

We denote by $x^*$ and $u^*$ the state and controls along the optimal trajectory. Optimality can be defined in a global ($J(x^*, u^*, t_0^*, t_f^*) \leq J(x, u, t_0, t_f)$ for all feasible trajectories $(x, u)$) or local sense ($J(x^*, u^*, t_0^*, t_f^*) \leq J(x, u, t_0, t_f)$ for all neighbouring trajectories). In order to find optimal trajectories, the optimization strategies rely on either *necessary* optimality conditions or *sufficient* optimality conditions.

### 3.1.1 The Pontryagin Maximum Principle

The Pontryagin Maximum principle (PMP) [21] characterizes the necessary conditions for a trajectory to be an optimum. Consider the unconstrained problem:

$$\min\ J = \min\ J(x, u, t_0, t_f) = \Phi(x(t_f), t_f) + \int_{t_0}^{t_f} \mathcal{L}(x(t), u(t), t)d$$

subject to:

$$\dot{x}(t) = f(x(t), u(t), t)$$
$$\psi(x(t_0), x(t_f), t_0, t_f) = 0 \text{ (Initial and final conditions)}$$

We define the adjoint variables or *costates* $\lambda(t) : \mathcal{T} \to \Omega_x \subset \mathbb{R}^n$ and the Lagrange multipliers $\nu \in \mathbb{R}^{N_\psi}$ associated to the initial and final conditions. We create the Lagrangian of the problem as:

$$\mathcal{L}(x(t), u(t), t, \nu, \lambda(t)) = \left(\Phi(t_F, x(t_F)) + \nu^T \psi(x(t_F))\right) +$$
$$+ \int_{t_I}^{t_F} \left[L(x(t), u(t), t) + \lambda^T(t)(\dot{x} - f(x(t), u(t), t))\right] dt$$

and the *Hamiltonian* of the problem as :

$$\mathcal{H}(x(t), u(t), t, \lambda(t)) = L(x(t), u(t), t) + \lambda^T(t) f(x(t), u(t), t)$$

[4] In general, the fixed cost can also depend on the initial state and time; this is infrequent in practice but certainly possible: consider, for example, the problem of finding an optimal launch time for a space vehicle

The PMP now lists the necessary conditions for a trajectory to be an extremum of the cost funcional:

**Theorem (Pontryagin Maximum Principle):** let $(u^*(t), x^*(t))$ be an optimal trajectory for the problem introduced above. Then, there exists a function $\lambda^*(t) : \mathcal{T} \to \mathbb{R}^n$ such that:

- The states obey the dynamics:

$$\frac{dx^*}{dt} = \frac{\partial \mathcal{H}}{\partial \lambda}$$

- The costates evolve in time according to

$$\frac{d\lambda}{dt} = -\frac{\partial \mathcal{H}}{\partial x}$$

- The control minimizes the instantaneous Hamiltonian

$$\mathcal{H}(t, x^*(t), u^*(t), \lambda^*(t)) = \min_{u(t)\in\Omega_u} \mathcal{H}(x(t), u(t), t, \lambda(t)) \; \forall t \in [t_0, t_f] \subset \mathcal{T}$$

- The final costates satisfy the *transversality conditions*:

$$\lambda(t_F) = \left[\frac{\partial \Phi}{\partial x} + \nu^T \frac{\partial \psi}{\partial x}\right]_{t=t_f} \text{transversality conditions}$$

- For free final time problems, the Hamiltonian at the final time does also verify:

$$\left(\frac{\partial \phi}{\partial t} + \mathcal{H}\right)\Big|_{t=t_f} = 0$$

These equations, along with initial and final conditions, define a Hamiltonian Two-point Boundary Value Problem (H2BVP). Indirect methods seek to solve this H2BVP in order to obtain the optimal control and trajectory.

### Constrained problems

Consider now the constrained case (i.e. the same problem adding the requirements (2) and (3)). We define the associated Lagrange multipliers $\mu_g : \mathcal{T} \to \mathbb{R}^{N_g}$ and $\mu_h : \mathcal{T} \to \mathbb{R}^{N_h}$ and add the corresponding terms to the Hamiltonian:

$$\mathcal{H}(x(t), u(t), t, \lambda(t)) = L(x(t), u(t), t) + \lambda^T(t) f(x(t), u(t), t) +$$
$$+ \mu_g(t) g(x(t), u(t), t) + \mu_h(t) h(x(t), u(t), t)$$

The Pontryagin Minimum Principle is now valid for the modified Hamiltonian, as long as the path constraints are added to the list of conditions.

### Multiphase problems

Multiphase problems are a variant of the optimal control problem that is useful in certain settings. In a multuphase, different dynamical models usually work in sequence (though non-sequential multiphase problems are also used in specific settings). Let $N_p$ be the number of phases and let the superscript $p$ denote the number of the phase (for example, $x^p$ should be read as $x$ during phase $p$). Then, we can define the multiphase problem as $\min J$, where

$$J = \Phi(x^{N_p}(t_f^{N_p}), t_f^{N_p}) + \sum_{p=1}^{N_p} \int_{t_0^p}^{t_f^p} \mathcal{L}^p(x^p(t), u^p(t), t) dt$$

subject to:

$$\dot{x^p}(t) = f(x^p(t), u^p(t), t),\ \forall p \in \{1, \ldots, N_p\}$$
$$\psi(x^1(t_0), x^{N_p}(t_f), t_0^p, t_f^p) = 0 \text{ (Initial and final conditions)}$$

and

$$l(x^p(t_f^p), x^{p+1}(t_0^{p+1}), t_f^p, t_0^{p+1}) = 0,\ \forall p \in \{1, \ldots, N_p - 1\}$$

are the *linkage constraints*. These constraints fulfill the role of final conditions for all of the phases except for the last and the role of initial conditions for all of the phases except for the first. Linkage constraints are usually related to continuity of the states between phases, i.e., $x^p(t_f^p) - x^{p+1}(t_0^{p+1}) = 0$, but it is possible to define different linkage constraints: consider, for example, the trajectory of a multistage rocket when one of the stages drops. In this change of phase, the mass at the end of the previous phase is not the same as the mass at the beginning of the next.

### 3.1.2 The Hamilton-Jacobi-Bellman equation

The Hamilton-Jacobi-Bellman (HJB) equation describes the sufficient conditions for the trajectory to be an optimum. Consider again a simple problem:

$$\min\ J = \min\ J(x, u, t_0, t_f) = \Phi(x(t_f), t_f) + \int_{t_0}^{t_f} \mathcal{L}(x(t), u(t), t)d$$

subject to:

$$\dot{x}(t) = f(x(t), u(t), t)$$
$$\psi(x(t_0), x(t_f), t_0, t_f) = 0 \text{ (Initial and final conditions)}$$

Define the value function $V$ as:

$$V(x,t) = \min_{u \in \Omega_u} \left\{ \Phi(x(t_f), t_f) + \int_t^{t_f} L(x(t), u(t), t)dt \right\}$$

**Theorem (Hamilton-Jacobi-Bellman)**: the optimal control is given by the relationship:

$$u^*(t, x(t)) = \arg\min_u \left( L(x(t), u(t), t) + \nabla_x V(t, x(t))^T f(x(t), u(t), t) \right)$$

where the value function satisfies the Hamilton-Jacobi-Bellman PDE:

$$-\frac{\partial V}{\partial t}(t, x(t)) = \min_u \left\{ L(x(t), u(t), t) + \nabla_x V(t, x(t))^T f(x(t), u(t), t) \right\}$$

## 3.2 Numerical Methods

Numerical methods for solving optimal control problems can be grouped in three families:

- Dynamic programming
- Indirect methods
- Direct methods

We will now review the characteristics, advantages and drawbacks of each class of methods

### 3.2.1 Dynamic Programming

Discretizing time (with a finite-difference scheme, for example) and the state space allows for reformulation of the optimal control problem as a discrete dynamic programming (DP) problem. The problem can then be solved by backwards induction, starting from the final stage. In this form, a numerical solution of the discretized HJB equation is found. Advantages of this methodology are:

- Ability to find global optima (as all the state space is exhaustively searched).
- Obtention of a closed-loop control rule, not just an open-loop value of the control.
- Natural extension to uncertain and stochastic problems.

The main drawback of dynamic programming is its computational cost: the size of the grid required scales exponentially with the dimension of the state space ("curse of dimensionality"). Therefore, memory and operation requirements of dynamic programming grow very quickly with the number of state variable and become impractical at 3 or 4 state variables. The direct application of dynamic programming is therefore limited in practice to problems with low state-space dimensionality.

In order to avoid this computationally expensive exhaustive search, some techniques have developed and grouped under the name of *approximate dynamic programming* ([22] and [23], Chapter 6). These methods approximate one of several of the components of the DP problem, by approximating the cost function, the value function, the "policy" (control law), or using approximate lookahead models, which limit the lookahead horizon, discretize and/or aggregate states or outcomes, or reduce the dimensionality of the problem.

*Ordered upwind* methods [24] constitute a specific approach that is related to dynamic programming. These methods solve specific versions of the Hamilton-Jacobi-Bellman equation in an efficient, one-pass Dijkstra-like manner.

### 3.2.2 Indirect methods

Indirect methods solve the Hamiltonian 2-Point Boundary Value Problem by a numerical scheme. The necessary conditions for optimality are therefore derived ("first optimize") and then the H2BVP is solved ("then discretize"). A H2BVP is substantially more challenging than a standard Initial Value Problem in differential equations, as some of the boundary conditions for the states and costates are given at the initial time and the remaining are given at the final time[5] .

The main techniques in indirect methods are indirect single and multiple shooting [25]. Indirect single shooting is an iterative technique that involves solving the system forward for an initial guess of the initial costates and then using the information from the solution to refine the initial values in a manner such that the final values are closer to the target values in each consecutive iteration. Multiple shooting subdivides the time interval into subintervals and then uses an initial guess for the initial values in each subinterval to integrate the ODE or DAE system, with each iteration seeking to reduce the distance between the final, computed values in each subinterval and the initial values of the next subinterval (as well as the final values in the last subinterval) with each iteration.

[5] If we knew the values of all the variables at the initial time, the problem would, in principle, be no different than integrating a system of ODEs or DAEs as an Initial Value Problem.

The main drawbacks of indirect methods are [26]:

- The optimality conditions must be derived, which requires nontrivial amounts of work and expertise with optimal control methods. In particular, any change in the model of the system or the problem formulation requires deriving these conditions from scratch.
- The "switching structure" (the sequence of active path constraints and regular, singular and saturated control arcs) must be derived or known a priori, which may be a hard task for complex problems.
- An initial guess for the trajectory must be provided. While this is common to most numerical methods, indirect methods also require an initial guess for the costates. Since there are usually no available intuitive values for the costates (while state variables can usually be initialized at an actual trajectory), this is a challenging task. Indirect methods are also highly sensitive to this initial guess and ill-conditioned.
- Dealing with "empirical" models (for example, if a function is approximated by interpolating tabular data) can be a rather difficult or impossible task.

These difficulties limit the applicability of indirect methods to certain problems.

### 3.2.3 Direct methods

Direct methods operate in reverse compared with indirect methods: the problem is "discretized first" to a nonlinear programming problem (NLP) and then it is solved by an NLP algorithm ("then optimize"). Their simplicity and the avoidance of complications that are associated to the alternatives have bolstered the adoption of direct methods; in exchange, their theoretical foundation is usually weaker, they generally present less accuracy than indirect methods, and proofs of convergence to a solution of the continuous problem are limited for most methods. The NLPs produced by direct methods are usually solved by gradient-based optimization methods, such as the Sequential Quadratic Programming algorithm SNOPT [27] or the interior point algorithm IPOPT [28]

We will distinguish between three broad approaches: direct shooting, local collocation and global collocation.

### Direct shooting

Single shooting and multiple shooting have a direct version ( [29] , [26]). In the direct single shooting method, the control variables are discretized into NLP variables and the state is propagated using numerical integration. The direct multiple shooting method divides the interval into several subintervals and acts on a similar fashion, thus increasing the number of NLP variables but improving reliability, because it reduces the high sensitivity of the single shooting method to perturbations in the initial conditions and the ill-conditioning of the Jacobians within the NLP [26].

### Local collocation

Direct collocation also subdivides the time domain in several subintervals. It requires creating NLP variables for the states and controls for each subinterval. The dynamics of the system are enforced by *defect constraints* (discrete equivalent of the differential equations of the problem), which relate adjacent subintervals. Methods are characterized by the choice of quadrature rule to approximate the differential equation between each two subintervals. For example, consider the Euler method in numerical integration of ODEs:

$$x_{k+1} = x_k + hf(x_k, u_k, t_k)$$

where $h$ is the size of the step ($t_{k+1} - t_k = h$). In an Euler-based transcription method, this exact equation is enforced as a constraint $\zeta_k = 0$ on variables $x_k$, $u_k$ and $x_{k+1}$ for each subinterval $k$.

$$\zeta_k = x_{k+1} - x_k - hf(x_k, u_k, t_k)$$

Higher-order analogues of the Euler method, such as the Hermite-Simpson and 5th degree Gauss-Lobatto collocation schemes [26], are the most commonly used among local collocation methods.

From the computational point of view, an important advantage of these methods (though not unique to them) is the high sparsity of the Jacobian of the Lagrangian. Because each constraint only relates two adjacent subintervals, only the entries near the diagonal of the matrix will be populated. Therefore, in order to obtain maximum performance from this method, it is

important to use NLP algorithms that can take advantage of this sparsity to speed up computations.

### Global collocation (pseudospectral)

Pseudospectral methods are a relatively recent development compared with the rest of the direct methods. In the last decade, pseudospectral methods have emerged as a powerful alternative to local collocation methods [30]. Pseudospectral methods use a high-order global polynomial interpolant to represent the solution instead of a piecewise low-order local polynomial. The differential equations are then collocated at a set of collocation points determined from a Chebyshev-Gauss or Legendre-Gauss quadrature rule.

Inspired by spectral collocation methods in fluid dynamics, pseudospectral methods in optimal control started being studied in the late 1990s. Key early milestones are the formulation of the Legendre method (LPM), based on Legendre-Gauss-Lobatto quadrature ([31]), and the Chebyshev method ([32]), later reworked on Clenshaw-Curtis quadrature in [33]. Later developments include the Gauss pseudospectral method (GPM), based on Legendre-Gauss quadrature ([34]), and the Radau pseudospectral method (RPM) ([35] and [36]), based on Legendre-Gauss-Radau quadrature.

The main advantage of pseudospectral methods compared to usual direct collocation methods is the superior rate of convergence for problems that are smooth enough [34]. While local methods feature polynomial convergence rates on the number of nodes, pseudospectral methods can achieve *spectral accuracy* [37]: a rate of convergence higher than any polynomial rate and, particularly, exponential for analytic functions. Additionally, there is a stronger theoretical understanding of these methods when compared to other direct methods ([38] [39] [40] [34] [36]). It is worth nothing that these methods can also be applied in a local collocation fashion, fixing the degree of the approximating polynomial to a low number and adding more subintervals to converge instead of increasing the degree of the polynomial ([35])

There are, however, several drawbacks associated with these methods:

- The individual sections of the Jacobian of the Lagrangian (corresponding to the differentiation matrix and the collocation constraints for

each variable) are no longer sparse, but dense. This can impose significant computational burdens once the number of nodes becomes high enough.

- Pseudospectral methods do not handle non-smooth problems well. Because the solution is represented as a global polynomial, the existence of points where there is a discontinuity in one of derivatives of the state deteriorates the properties of these methods. This phenomenon is usually encountered in practice because of the activation of path constraints and the appropiate way to deal with it is to reformulate the problem as a multiphase problem [41] [42] or to employ an adaptive method:

**Adaptive methods**

In a lot of optimal control problem, the optimal trajectory may display features at different timescales. For example, in a simple optimal cruise problem, the optimal solution is often composed by an initial phase at either maximum or minimum throttle until an efficient velocity is reached, a central "singular arc" phase where the aircraft slowly decelerates as the optimal velocity is adjusted to the changing mass of the aircraft, and a final acceleration or deceleration phase to match the terminal velocity (or the minimum allowed velocity, if no final condition is imposed on the velocity) [43] [44]. This presents a challenge for most direct methods, since choosing a large step size that is efficient for the long central phase leads to inaccuracies in the initial and final phases, and choosing a small step size for accurate representation of the solution at the endpoints is computationally uneconomical for the central singular arc phase, leading to an oversized NLP.

To alleviate this phenomenon, the numerical optimal control community has proposed the usage of adaptive methods. These algorithms are built on top of other direct methods and follow this general scheme:

Adaptive algorithms differ on the underlying method employed, on the choice of error or smoothness criterion and the grid-refinement rule. Some relevant adaptive algorithms are [45] [46] [47] and [48], for local collocation methods, and [49] [50] for pseudospectral methods.

**Algorithm 1:** Main loop of an adaptive method

1 Select a basic initial grid with an initial step size
2 Solve the problem on the selected grid
3 **if** *the solution has the demanded precision* **then**
4 | Accept the current solution and terminate the algorithm
5 **else**
6 | Go to step 7
7 Use an error criterion to determine which parts of the grid require refinement
8 Design the new grid according to the criterion and go to step 2

A related technique that can be employed in place of the error criterion for grid design is the subdivision of the problem according to constrained and unconstrained arcs. This was first considered by [51] and [52] in the context of direct methods, and utilized by [53] and our work [42] in the specific context of pseudospectral methods (as active constraint set changes are particularly detrimental in pseudospectral methods).

## 3.3 Uncertainty and optimal control

### 3.3.1 Uncertainty modelling

Uncertain parameters can be modelled within two different mathematical frameworks: the framework of mathematical probability and the framework of interval arithmetic. While the latter approach has been successfully employed for some problems within the field of robust control theory ([54] [55]), it is the former that is predominantly used for this purpose.

The mathematical pillar of probability theory is the *probability space* (see, for example, [56]). A probability space $(\Omega, \mathcal{F}, P)$ is composed by three elements:

- A sample space $\Omega$ of possible outcomes. Every possible realization of the uncertain parameters is a single point $\omega \in \Omega$ in this space.
- A $\sigma$-algebra of events $\mathcal{F}$. This is a collection of subsets of $\Omega$ that are called "events", that is, groups of outcomes.
- A probability measure $P$ that assigns a probability $P(A) \in [0, 1]$ to each event $A \in \mathcal{F}$. It is normalized so that $P(\Omega) = 1$.

A random variable is then an $\mathcal{F}$-measurable function $X : \Omega \to \mathbb{R}^n$. Its distribution $\mu_X$ can then be defined as a probability measure on $\mathbb{R}^n$ instead of the underlying abstract probability space by the relationship $\mu_X(B) = P(X^{-1}(B))$, with $B \in \mathbb{R}^n$. Most of the practical magnitudes about the random variable we're interested in can now be expressed or computed as integrals of the form:

$$\mathbb{E}[f(X)] = \int_{\mathbb{R}^n} f(x) d\mu_X(x) \tag{5}$$

For example:

- The expected value of $X$ is $\mathbb{E}[X]$
- The variance of $X$ is $\mathrm{Var}(X) = \mathbb{E}[(X - \mathbb{E}[X])^2]$
- The probability that $X \in A$ (where $A \subset \mathbb{R}^n$) is $\mathbb{E}[I_A(X)]$, where $I_A(x)$ is the indicator function of the set $A$. This case includes quantities such as "the probability that certain variable is equal or greater than a critical value".

Therefore, from the practical point of view, dealing with random variables ultimately involves solving or approximating integrals of the form 5. There are several approaches for carrying out this task; we will describe Monte-Carlo sampling, cubature, and polynomial chaos.

### Monte Carlo

Monte Carlo methods and its derivatives are widely used in science and engineering. The basic Monte Carlo scheme approximates the integral 5 as:

$$\int_{\mathbb{R}^n} f(x) d\mu_X(x) \approx \frac{1}{N} \sum_{i=1}^{N} f(\xi_i)$$

where the values $\xi_i$ have been randomly generated according to the distribution $d\mu_X$.

The main advantage of this method lies in its simplicity of implementation. Its main drawback lies in the fact that the convergence rate is slow. Under mild assumptions on $f$, the error converge at an $\mathcal{O}(1/\sqrt{N})$ rate. Therefore, it might require a high $N$ to provide an accurate result. If the evaluation of $f$ is computationally expensive (for example, if it requires running a costly simulation), then it might be infeasible to apply Monte Carlo to the problem. On the other hand, this convergence rate is independent of the dimension of the random variable $X$, thus making it relatively more efficient for high-dimensional problems than its alternatives (which usually require substantially more resources as the dimension of the problem increases).

Depending on the complexity of the distribution of $X$, several variants of Monte Carlo can be employed to improve its performance. Examples of these techniques are importance sampling, stratified sampling and the Markov Chain Monte Carlo (MCMC) family of algorithms [57].

**Generalized Polynomial Chaos**

Generalized Polynomial Chaos (gPC) techniques rely on the expansion of the random inputs and outputs on an orthogonal polynomial basis [58] [59]. This allows for recovery of some statistical quantities directly from the expansion coefficients (for example, the expected value being the first coefficient). They come in two brands:

- In the *Galerkin* form, the variable $X$ is replaced by its gPC expansion in the formulation of the problem, thus creating a new, different problem. The new problem is then solved to obtain the gPC characterization of the output.
- In the *stochastic collocation* form, the deterministic problem is solved for different values of $X$. These values are chosen as the nodes of a quadrature rule. The output is then characterized as a Lagrange interpolant at this set of nodes; therefore, stochastic collocation is a form of building surrogate models. The gPC coefficients can then be recovered with the quadrature rule.

Both variants of gPC have their own strengths and weaknesses. The Galekin approach is generally more accurate, but it requires the modification of the underlying simulator of $f$ (it is *intrusive*), which might be a difficult or unfeasible task for some problems. On the other hand, stochastic collocation

only requires the deterministic evaluation of $f$ at a pre-computed set of nodes, bulding the output approximation in a cheap post-processing step.

Compared to Monte Carlo, gPC has been shown to perform favourably for problems where the random variables are low-dimensional [60]. This advantage vanishes for high-dimensional problems, because the number of expansion coefficients or function evaluations needed for gPC grows quickly with the number of dimensions $n$. A full tensor product grid will scale as $\mathcal{O}(e^n)$; a more efficient sparse grid [61] will still scale at a high polynomial rate $\mathcal{O}(n^l)$ [62], where $l$ is the level of the quadrature rule. This effect limits the accuracy of the gPC expansion for high-dimensional problems, as increasing the level of the quadrature beyond a low value will quickly make the method computationally unfeasible. Another drawback of polynomial chaos is the fact that estimates for the approximation error are usually not available [62]

**Other approaches**

Among other approaches for computing stochastic integrals, we will also mention the following:

- Quasi-Monte Carlo methods work in a similar fashion to standard Monte-Carlo. However, instead of generating the evaluation points $\{\xi_i\}$ randomly, quasi-MC methods use a deterministic low-discrepancy sequence that samples the outcome space in a more even manner than raw Monte-Carlo [63]. While the upper bound for the approximation error incurred by quasi-MC, $\mathcal{O}\left(\frac{(\log N)^n}{N}\right)$, can be worse than standard Monte Carlo, empirical results from the quantitative finance field (starting with [64]) showed that quasi-MC often converges 1) substantially faster than what the bound seems to indicate and 2) at a faster rate ( $\mathcal{O}\left(\frac{1}{N}\right)$) than Monte Carlo. This discrepancy has been theoretically studied with the concepts of *weighted classes of functions* [65] and *effective dimension* [66]; these ideas rely on the fact that, for certain problems, not every dimension of the random is equally influential in the quantities of interest. Nevertheless, these is still no complete understanding of the phenomenon, as researchers have identified classes of functions with high effective dimension for which quasi-Monte Carlo

still outperforms Monte Carlo with a $\mathcal{O}\left(\frac{1}{N}\right)$ convergence rate [67].

- Cubature is a numerical method for the approximation of $n$-dimensional integrals, a high-dimensional analog of quadrature rules for one-dimensional integrals. Given a region $B_n \subset \mathbb{R}^n$, a weight function $w(x)$ (in our case, the probability density function) and a function $f(x)$, a cubature rule approximates the integral as:

$$\int_{B_n} w(x)f(x)dV = I_N f + R_N f$$

where $I_N f$ is computed as a linear combination of values of the function at the cubature points:

$$I_N f = \sum_{i=1}^{N} w_i f(x_i)$$

and $R_N f$ is the residual or error of the cubature, which is usually demanded to be zero for linear combinations of monomials [68]. There exists a large number of cubature rules that differ in the region of computation $B_n$ (usually $n$-dimensionals cubes, spheres, simplexes or the whole space) and in the choice of cubature points $\{x_i\}$ and weights $\{w_i\}$. A compilation of cubature rules can be found in [69] and [70]. For stochastic processes (see Section 3.3.2), high-dimensional cubature has also been developed [71].

### 3.3.2 Stochastic processes

In problems such as trajectory optimization, the uncertain variables of interest change with time (for example, the wind intensity or the position of a storm). It is, therefore, useful to model them as "dynamically" random variables $X_t$ instead of "static" random variables $X$. These variables change randomly over time according to a certain probability law.

There are two possible choices for modelling stochastic processes: in *continuous-time* or *discrete-time*. While the properties of both variants are usually analogous, there are some relevant differences between them, so they are studied in related but distinct fields:

- Continuous-time stochastic processes are studied within the framework of *stochastic differential equations* (SDEs) [72]. This framework is common in fields such as finance and physics, as it provides a natural extension of differential equations to the stochastic case.
- Discrete-time stochastic processes (usually modelled as *Markov chains* [73]) are also used extensively in science and engineering. In the context of optimal control theory, they are called *Markov decision processes* (MDP) and usually dealt with through the lenses of dynamic programming 3.2.1

The mathematical characteristics of stochastic differential equations introduce new challenges from the point of view of numerical approximation [74], as the numerical methods for integrating ordinary differential equations do not necessarily extend automatically to the stochastic version.

As the "solution" of a SDE is not a single trajectory but a random trajectory that depends on the underlying source of randomness, the usual approach to solve SDEs numerically is to simulate a large number of individual paths of the solution in a Monte Carlo fashion and then obtain statistics such as the mean or the variance from this solution. The individual realizations of the solution are simulated using numerical schemes such as the Euler-Maruyama method [75], the Milstein method [76] or other Taylor or Runge-Kutta approximations [6] [77].

### 3.3.3 Robust and stochastic optimal control

Uncertainty can enter into the optimal control problem in several forms, depending on the nature of the modelled random variable (static or dynamic) and the component of the problem that depends on the uncertainty (the dynamics, the cost functional or the constraints). We can identify three classes of problems in the literature that are relevant for this thesis; each one of the classes is appropiate for a different practical concept.

[6] Despite the name, stochastic Runge-Kutta schemes (as named by [77]) are not just heuristic adaptations of the deterministic RK methods.

### The uncertainty quantification approach

This approach combines the Uncertainty Quantification (UQ) methodology (in a non-intrusive version) with a solver of the deterministic optimal control problem (OCP). Under this approach, the deterministic problem is solved for different values of the uncertain parameters and the statistics of the solution are built using the corresponding probabilistic representation (usually with a Polynomial Chaos stochastic collocation scheme). When the uncertain variables are realized, this probabilistic representation can be used to obtain the deterministic solution corresponding to the final values of the uncertain variables.

This approach is useful to study the probabilistic characteristics of the deterministic system when some of the inputs are unknown. It is also a convenient computational solution for systems where computation is done before the system starts operating and uncertainty is solved before the startup point: the solution of the slow and computationally expensive OCP is stored after solution and the solution is built in real-time with a fast interpolation operation (see figure 2).

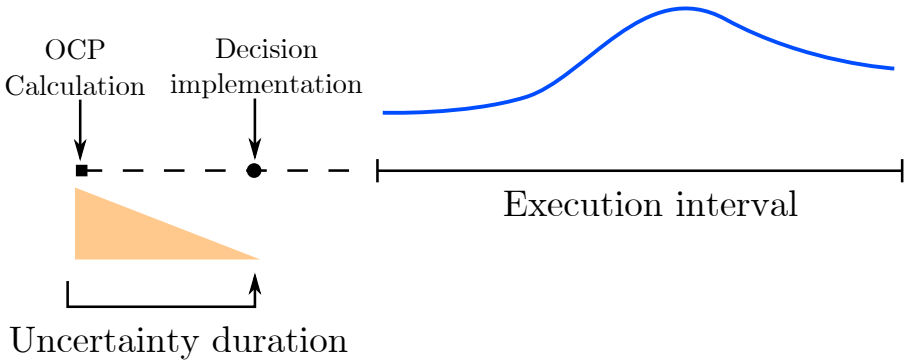


Figure 2: The Uncertainty Quantification OCP

This methodology is, nevertheless, not applicable for most problems of trajectory optimization under uncertainty, where uncertainty is not completely solved before the system starts operating. In that case, there is no clear interpretation of the solution, as it is composed by a probabilistic representation of the trajectory without a rule to decide what values should

the control attain or which state trajectory should the system track. The most likely trajectory in this solution is not only not optimal in general (as optimality does not, in general, commute with the "most likely" property[7]): it is almost surely unfeasible if there is uncertainty in the dynamics.

### The robust approach

In the robust (or *tychastic*, using the terminology of [78]) optimal control approach, the fact that the uncertainty has not been resolved yet at the point of execution is explicitly taken into account. Thus, instead of a single execution trajectory, the solution of a robust OCP is a set or "tube" of trajectories in state-space (see Figure 4) that minimizes the expected value of a cost functional that may not only include an "average" cost, but can also include a term penalizing the variance of the solution. The deterministic dynamical system is replaced by an augmented "virtual" dynamical system that represents the dynamics of all the trajectories, so it is converted to a larger deterministic optimal control problem.

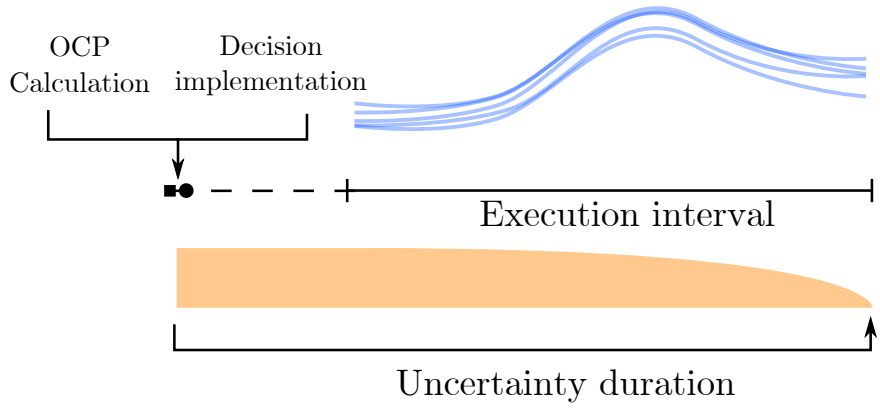


Figure 3: The Robust OCP

[7] As counterexample, consider the problem of finding $u$ such that $(x-u)^2$ is minimum, where $x$ is a random variable $x \in [-1,1]$ with a probability density function $p(x) = (1+\varepsilon x)/2$ and $0 < \varepsilon < 1$. It can be verified that the most likely solution of the deterministic problem is $u = 1$, but the solution that minimizes the average value of $(x-u)^2$ is $\varepsilon/3$, which is closer to 0

In the particular case where the uncertainty only influences the cost functional and not the dynamics, the trajectory tube collapses to a single trajectory and thus it is not necessary to expand the state space. A simpler strategy for solving the problem with a direct method is replacing the cost functional by an approximation to the probabilistic cost functional [79].

**The stochastic approach**

The stochastic optimal control problem (SOCP) differs from the robust optimal control problem because it models uncertainty as a dynamic stochastic process and replaces the differential equations by stochastic differential equations [72]. Beyond the dynamic nature of the of uncertainty, SOCPs are different from the equivalent robust problem because they involve a explicit closed-loop characterization of the control, which follows a feedback law $u = u(t, X_t)$. This has several desirable properties: because this feedback law can be directly recovered from the solution of the problem, implementation and simulation of this controller are straightforward and computationally cheap (which is desirable for real-time controllers).

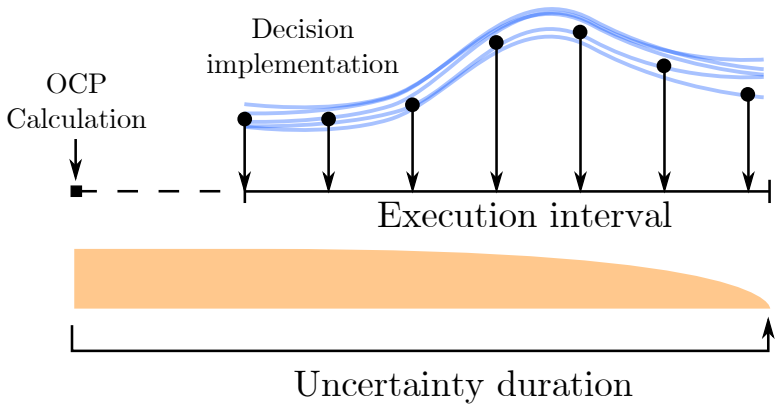


Figure 4: The Stochastic OCP

The simplified linear-quadratic (linear dynamics and quadratic costs) version of the problem has been well explored and used extensively in practice [80], just like its deterministic analogue. However, the general nonlinear problem SOCP can exhibit a more complex behaviour than the deterministic

OCP due to its stochastic nature [81]. Stochastic analogues to the Pontryagin Maximum Principle [82] and the Hamilton-Jacobi-Bellman equations [83] have been studied in the literature.

Numerical methods in stochastic optimal control are more challenging than those in the deterministic case. The traditional approach for solving a SOCP is to discretize the state space and convert the problem into a discrete Markov Decision Process [84], which is then solved by dynamic programming techniques. The main drawback of this methodology is the fact that it suffers from the curse of dimensionality, as the computational size of the discretized state space grows exponentially on the dimension of the problem.

Some ideas have been introduced in the literature in order to avoid the curse of dimensionality in the context of stochastic optimal control. For a specific form of the problem, the Hamilton-Jacobi-Bellman equation can be transformed to a linear PDE [85], leading to several methods that can solve this PDE in an efficient manner. The path integral approach [86] [87] [88] [89] draws on ideas from physics and approximate dynamic programming in order to produce a reinforcement learning algorithm that scales to high dimensional control systems. The algorithm presented in [90] is able to locally solve an approximation to the SOCP and scales linearly on the number of dimensions, in addition to being easily parallelizable.

In [91], the state and control trajectories are expanded in a Fourier-like fashion in an orthonormal polynomial basis spanning the underlying *Wiener chaos space* using Malliavin calculus. The SOCP is therefore converted to a deterministic OCP on the coefficient functions of the expansion, instead of the states. This OCP can now be solved using mature deterministic optimal methods and the stochastic solution can be recovered from the solution coefficients.

# 4 Applications

## 4.1 Deterministic Flight Planning

Flight planning is the procedure of generating a valid flight plan with the goal of minimizing fuel burn, flight time and overflight charges while taking into account weather, traffic, and ATC constraints. In order to deal with the regulation and structure of the current airspace structure, commercial flight planning tools usually subdivide the problem into a 2D route optimization problem (which then can be solved with a method such as [92] [93]) and a vertical profile and speed optimization procedure [94].

However, initiatives such as SESAR [95] and NextGEN [96] are promoting the implementation of free route airspaces. Operation implementation is already underway in airspaces such as the Maastricht and Karlsruhe Upper Area Control airspaces under the FRAMaK project. The move towards Trajectory-Based Operations is renewing interest in optimal control techniques that can solve complete 4D trajectory optimization problems.

The usage of analytical optimal control techniques to optimize fuel savings started several decades ago (see [97] [98] and references therein for some of the earlier works on profile and speed optimization and [99] on three-dimensional trajectories). More recently, [100]used Green's theorem to obtain the solution of the constant altitude cruise problem and [43] used an indirect method to obtain the minimum fuel cruise with a fixed time of arrival. Complete profiles including climb, cruise, and descent were studied in [101] and extended by [102] for altitude-constrained profiles. An optimization procedure based on discrete patterns was introduced on [103] and extended by [104] in order to generate ATC-compliant trajectories composed by segments of constant Mach and altitude.

Several researchers have also studied the aircraft trajectory optimization problem with direct methods. Efficient and reliable landing methods using optimal control are developed in [44]. As the performance of direct methods is highly dependant on the initial guess, a method for generating initial guess trajectories for the same problem is introduced in [105]. In [106] and [107], a complete trajectory is optimized using hybrid optimal control, and a similar approach is employed in [108] in order to include contrail avoidance in the objective function. An optimal-control framework is also used in [109] and

[110] to produce optimal conflict-free trajectories, and in [111] the impact of assigning an RTA (Required Time of Arrival) on fuel burn is studied.

## 4.2 Wind-optimal Aircraft Trajectories

While wind and weather have an important influence on trajectory efficiency, most (but not all) of the works cited in the previous section do not take it into account. Nevertheless, the problem of optimal aircraft routing in general wind fields has indeed been specifically studied in the optimal control literature. The earliest works were based on the simple Zermelo problem [112] [19], which models a constant-velocity vehicle on a two-dimensional wind field.

One of the first modern studies on the topic was [113], which relied on the techniques of Neighbouring Optimal Control (NOC). A guidance method in a general wind field is developed, as well as a NOC-based algorithm, which solves a linearized system describing a perturbation around a nominal trajectory. In [114], this method (called Near-Optimal Wind Routing) is compared with an "Optimal Wind Routing" solution, which integrates a differential equation (obtained by analytical optimal control techniques) from the destination point with different values of a parameter in order to find a route that passes through the initial point. Additional work on this class of techniques has been carried out in [115], which considers time-varying wind fields and variable airspeed, and another analytical optimal control-based method is applied in [116] to find optimal routes in the presence of winds while avoiding contrail formation. This method is combined with a vertical profile optimization method in[117].

Dynamic programming has also been used for the calculation of wind-optimal paths. In [118], an efficient dynamic programming approach relying in an ordered upwind method is used to optimize the 2D trajectory of a constant-velocity aircraft. This method is extended in [119] to consider the flight on the surface of a sphere in order to adapt it to medium- and long-haul flights. In the methodology designed in [120], a standard dynamic programming approach on a 2D network is also one of the steps of the proposed solution.

In contrast with these works, which apply to general wind fields but usually make other simplifications (such as constant airspeed or altitude), the

studies in [121] [122] [123], which rely on indirect methods, consider the effect of *average* along-track wind speeds while considering variable speed. In [101], hybrid multiphase optimal control is used to generate complete climb, cruise and descent profiles with the ability to consider general wind profiles.

Direct methods, which have the potential of dealing with more complex and complete problems as discussed in Section 3.2.3, have also been used to optimize trajectories on general wind fields. In [106], [124] and [107], the wind is modeled as a polynomial obtained by regression on tabular data and hybrid optimal control is used in conjunction with a direct transcription to solve the optimal control problem. In [125], we will introduce a multiphase formulation that allows us to use a more precise approximation of the wind field, as regression only produces a low-resolution approximation.

Other methods on trajectory optimization on general wind fields without using optimal control were developed in [126] [127] , which use a genetic algorithm and a performance database to obtain optimal 4D trajectories.

## 4.3 Aircraft Trajectory Optimization under Uncertainty

Recently, interest has been growing on the quantification of the impact of uncertainty on all aspects of the ATM system. In particular, the SESAR-sponsored IMET project has been set up with the goal of utilizing meteorological data to study the impact of meteorological uncertainty and improve decision-making in ATM and pre-tactical flight planning operations. Some results were presented in [128], where the impact of meteorological uncertainty on a North Atlantic route was studied. Other uncertainties have also been targeted in the literature: for example, the impact on uncertainty in initial mass on a trajectory [129], the influence of uncertainties in aircraft performance [130] and the impact of aircraft intent uncertainty [130].

However, the consideration of uncertainty as an *input* to the flight planning process instead of as a component of the *outcome* of a flight (i.e. as a robust or stochastic optimal control problem) plan has not been studied in depth on this field and the literature on the topic is sparse. There are some studies solving what we called the "uncertainty quantification OCP" (see Section 3.3.3). In [131], this approach is used in order to solve the problem of optimal aircraft routing through an environment with lethal threats of uncertain location, and it combines polynomial chaos for uncertainty quantification and pseudospectral methods for solving the deterministic OCP. A

similar approach is employed in [132], [133] and related work in the context of conflict resolution.

In [134] (based on the method of [135]), the authors deal with what we call the "Robust OCP" in order to find shortest climb controls for a supersonic aircraft, which used a polynomial chaos technique to characterize aerodynamic data uncertainty and integrates this representation into the problem formulation. The robust approach is compared with the uncertainty quantification approach. A robust scheme is also used in [136] in order to optimize the trajectory of a UAV based on dynamic soaring. Nevertheless, as noted in [134], the field of nonlinear robust dynamic optimization has not been explored in depth.

Stochastic optimal control problems (in our terminology) for aircraft trajectory optimization remain underexplored too. An algorithm that discretizes the state-space in order to represent the evolution of the system as a Markov Chain is used in [137] for midair conflict resolution and bad weather avoidance. In [138] [139] and [140], an algorithm for multi-aircraft routing and traffic flow management under uncertain convective weather conditions is proposed, using dynamic programming on a Markov Decision Process.

As a consequence, developing an appropriate methodology for 4D trajectory optimization under weather-related uncertainty will be one of the main challenges in this thesis.

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