Development of a Monte Carlo algorithm for optimal control problems

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In almost all areas of life sciences and engineering applications, modeling of a reality is mostly confronted with uncertainities in the observations, derived from some measurements or gathered signals. This usually leads to the optimal control studies to minimize the misfit between the observations and the computations. The problem at hand can be cast as a mathematical minimization procedure of some cost functional by controlling the variables of interest and respecting the governing (partial differential) equations. This necessitates the analysis of the state variable's behavior with respect to changes in the control variables.

An utterly important numerical method is the so-called adjoint method for efficiently computing the state gradient with respect to the control. This formulation results in an adjoint equation, which is a linear differential equation derived from the original problem. Methods based on the solution of adjoint equations are actively used in, for example, optimal flow control, shape optimization and uncertainty quantification.

However, the adjoint equation requires the solution of the state variables from the original problem, which makes it to a challenge for especially the time-dependent problems. In the latter case, the adjoint equations posses a backward-in-time nature, thus, they are solved following a path starting from the last time and ending at the initial time of the considered problem. Hence, in order to solve for the adjoint state variables in a traditional way, all the trajectories of the state variables must be solved and stored in the memory, e.g. by following the traditional forward-in-time nature of the original state equations. The necessity for the storage and the backward-in-time nature of the adjoint formulation makes it to a very large and difficult problem to be solved. Following this, the development of alternative methods for the computation of adjoint states gained an increased attention in research over the last decades.

One very promising approach is the use of Monte Carlo methods, which are known to be efficient for approximating large-scale linear systems (as this is also the case for the unsteady adjoint equations). Their approximation is based on some stochastic estimators constructed in such a way that their expectation value is the solution of the linear system of interest. Currently, there is no sufficient scientific report on the potential of Monte Carlo methods for approximating the adjoint states of unsteady adjoint equations, which motivates this thesis. The Monte Carlo methods offer several advantages. They enjoy having a forward-in-time nature and hence rule out the aforementioned memory requirements for the full trajectory. In addition, they can be used to only approximate those adjoint state variables which are needed for the computation of the gradient of original state variables. Hence, in contrast to the traditional methods, it is not necessary to evaluate the adjoint states at all cell centers or nodal points of the grid. Furthermore, the Monte Carlo methods have a great potential for a coarse-grained parallelism, which makes them especially interesting for the new hardware architectures offering high-performance computing.

The goal of this thesis is to develop and analyze a Monte Carlo algorithm for a linear problem including the heat equation (Bachelor thesis). Possible extentions to the work will include the examination of their potential for the non-linear Navier-Stokes equations with the motivation for their applicability in bio-fluid mechanical studies (Master's thesis). The thesis will be divided in three parts. In the first part, the student will familiarize herself with the related topics (probability theory, stochastic estimation, random walks, Markov chains, numerical optimization...) and investigate a scientific paper. The second part will include coding of the algorithm and reproducing the results presented in the scientific work. In the third part, the student will examine possible extentions or improvements to the algorithm and will apply her new findings to the aforementioned problems.

The thesis will be jointly supervised between the Seminar of Applied Mathematics (Prof. Ralf Hiptmair) and the Institute of Fluid Mechanics (Prof. Patrick Jenny). In case of an interest, please contact us and also kindly forward us a description of your background.