Multiple Boundary-Value-Problem Formulation for PDE-constrained Optimal Control Problems with a Short History on Multiple Shooting for ODEs

H. J. Pesch

Lehrstuhl für Ingenieurmathematik, Universität Bayreuth,
hans-josef.pesch@uni-bayreuth.de

Looking back to the early days of Multiple Shooting at the end of the 1960s, this powerful method became known by the publications of Keller (1968) and Osborne (1969). The development of the first multiple shooting code BOUNDSOL by Bulirsch and Stoer (1971, 1973) began after a colloquium of Keller at the University of California in San Diego at the end of the 1960s, when Stoer and Bulirsch held professorships at the UCSD. Their code was soon able to solve nonlinear two-point boundary value problems and specific problems of optimal control. However, the first (short) paper carrying the name multiple shooting in its title was published in a buried engineering-computer science journal by Morrison, Riley, and Zancanaro (1962) and may be overlooked by the mathematicians whose names were later associated with multiple shooting. Already at the beginning of the 1970s, Bulirsch also developed a code called OPTSOL for the solution of optimal control problems with control- and/or state-constraints; the mathematical background of which was never appropriately published; see Bulirsch’s Carl Cranz Report of 1971. Therein, the switching or junction points between unconstrained and constrained subarcs were determined by the zeros of so-called switching functions which were computed by a sophisticated iteration procedure during the numerical integration of the ordinary differential equations. After improvements of the Newton iteration by Deufhard (1974, 1975, code DLOPTR) concerning the solution of the nonlinear system to be solved, a decisive break through was marked by the invention of multi-point boundary-value-problem formulations for general ODE-constrained optimal control problems by Oberle (1977, 1983) realised in his code BNDSCO, later modified and re-implemented in the code MUMUS by Hiltmann (1990). The transcription of the first-order necessary conditions of the maximum principle to multi-point boundary value problems contributed to a more robust and user friendly handling of the multiple shooting codes. In Oberle’s code, a condensation technique, used so far in all previous codes, was given up in favour of the solution of the linear systems with the full multiple shooting matrix inside the Newton iterations. For, it was detected that condensation, i.e. the blockwise elimination of the multiple shooting variables at the interior multiple shooting nodes, reduces the condition number to that of single shooting gaining away one of the main advantages of multiple shooting. Due to the usually extreme nonlinearities in the applications of those days, which seem to be unusual in today’s PDE applications, high condition numbers often play a crucial role.

This short historical review reflects only the so-called indirect multiple shooting which today would be classified as first-optimize-then-discretize approach in the PDE optimal control community.
With the code Muscod by Bock (1984), also hidden in a rather buried proceedings article, direct shooting methods came on the stage as generalisations of the first direct single shooting methods which were developed in the US, the USSR, and in Germany at the DFVLR — today DLR, Oberpfaffenhofen, around the turn from the 1960s to the 1970s. Many other codes followed by which continuous optimal control problems for ODEs and DAEs can be transcribed to and solved by problems of nonlinear programming. In terms of the PDE community these methods are to be classified as first discretize then optimize. Questions of convergence were solved only for specific tasks until today.

Obviously the question arises what ideas can today be used in solving PDE-constrained optimal control problems. The main intention of the talk is to introduce a multi-boundary value problem formulation for PDE optimal control problems where state constraints are involved or where controls turn out to be bang-bang or/and singular. Also first-discretize-then-optimize pre- and postprocessing techniques can be generalized which have turned out to be quite successful in ODE optimal control with multiple constraints if necessary and sufficient optimality conditions are verified afterwards (Maurer, Pesch, 2008).

Three issues are discussed in more detail: firstly, a state-constrained elliptic optimal control problem where the boundary of the active set is determined by shape calculus. This approach mimics the well-known Bryson-Denham-Dreyfus technique for state-constrained ODE optimal control problems and can be interpreted as free boundary value problem or as bilevel optimization problem. This leads to a completely new adjoint-based numerical method for state-constrained problems. Secondly, a state constrained parabolic PDE-ODE for which the approximate solution obtained by first discretize then optimize can be verified by the optimality conditions a posteriori. Thirdly, a control-constrained (hyperbolic) wave equation is presented the optimal solution of which is of type bang-bang-singular. This problem can hardly be tackled by indirect methods. Hence, two different first-discretize-then-optimize approaches are presented for it. These three parts of the talk are based on joint works with S. Bechmann, M. Frey, A. Rund, and J.-E. Wurst.