4o Next Generation Dynamic Optimization

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The current decade is marked by the increased need for integration and more realistic models coupled with heavy interdisciplinary research efforts. A lot of effort is going into "Modeling, Simulation and Optimization" of complex systems, and this has been recognized as one of the pillars of current day research on par with theoretical and experimental research. Modeling the behavior of many complex physical systems is carried out by using Ordinary Differential Equations (ODEs) and Partial Differential Equations (PDEs), which typically represent the conservation laws, coupled with algebraic equations, which represent constitutive relations or design specifications. Such models arise in myriad application areas such as biology, nano-scale processes/phenomena, medicine, energy (including fuel cell systems) and transport processes. With the development of powerful modeling and simulation tools for such systems, optimization is a natural extension to consider.

Dynamic optimization aims at optimizing systems that are governed by differential equations, and the last decade has witnessed a tremendous amount of effort go into optimization of Differential-Algebraic Equations (DAEs), in particular: interesting applications, numerical algorithms and optimization platforms. From a mathematical viewpoint, dynamic optimization problems are optimal control problems which formally refer to the minimization of a cost (objective) function subject to constraints that represent the dynamics of the system.

In order to cater to the scale and the complexity of current day applications, the following directions must be explored: design of powerful numerical methods, optimization of systems governed by PDEs, ability to handle discrete decisions, classification of problem classes that can be solved by various dynamic optimization methodologies, reliability of Nonlinear Programming (NLP) based methods for dynamic optimization, ill-conditioned systems and model reduction. This work aims at addressing some of these issues using rigorous theoretical tools and/or characteristic examples, at the same time use the results for solving real large-scale industrial applications to realize the benefits.

In collaboration with Prof. Biegler (CMU) we have addressed the following issues:

1. Large-scale parameter estimation for a reservoir application:- In a project funded by ExxonMobil Upstream Research Company, Houston, TX, we have proposed a novel complementarity based procedure for the estimation of relative-permeability and capillary pressure functions from experimental data on oil-reservoir core samples. The values of these flow-functions are crucial for proper exploitation of petroleum resources. The system can be modeled by a coupled system of PDEs, and boundary conditions that switch in a discrete manner depending on the value of the states at the boundary. We have successfully solved this large-scale application, and the solution procedure has benefited heavily from our research on the aforementioned directions.

2. Trajectory planning for Fuel Cell/Gas Turbine (FC/GT) power generation systems:- In a different project funded by FuelCell Energy Inc., Danbury, CT, we have developed a methodology for trajectory planning of hybrid power generation systems to achieve better control performance that conventional control. The main aim of the project is to develop a dynamic optimization framework to predict controller moves so as to meet the power requirements, and this crucial for the operation of such plants. The plant consists of about 20 units (including a fuel cell stack), a lot of which are characterized by dynamic models, and we have been able to successfully solve the resulting large-scale dynamic optimization problem. We have validated the results by feeding the inputs (as suggested by the results of optimization) back to a plant simulator to realize the benefits of our procedure.

3. PDE-constrained optimization:- We have attempted to solve PDE-constrained optimization problems by converting them to DAE-constrained optimization problems using spatial discretization. Based on this idea we have proposed solution procedures for two specific applications of PDE-constrained optimization: two-phase flow through porous media and heat transfer.

4. Complementarity based formulations for modeling discrete decisions:- Complementarity conditions are a way of modeling certain discrete decisions. The advantage of using this formulation is that it gets rid of integer variables, and thus an NLP based solver can be employed rather than a specialized mixed-integer nonlinear programming solver. We have used complementarity formulations for a number of interesting applications in optimal control, reservoir and chemical engineering.

5. Reliability of NLP based methods for dynamic optimization:- Although NLP based methods have been used for an entire decade for the solution of dynamic optimization problems, the question of whether the NLP solution and the true solution of the dynamic optimization problem have any relation (as the discretization is made finer) is still an active area of research. In this direction we have tried to address convergence rates for NLP based methods and we have been able identify classes of problems for which the reliability of NLP based methods can be proved rigorously. Our results have applications in adjoint estimation, error analysis and mesh refinement, and we have demonstrated the implication of our results on the temperature control of a batch reactor.

6. "Discretize then Optimize" vs. "Optimize then Discretize":- Research in this direction has focused on classification of problems based on whether it is advantageous to discretize all the dynamic constraints and then solve the large-scale NLP, or to discretize the optimality conditions of the original dynamic optimization problem. Our analysis indicates that in the case of singular optimal control problems it may be better to use the "Optimize then Discretize" approach since the alternative approach does not have the ability to address the ill-conditioning in the problem. We have devised a numerical procedure for singular optimal control problems that is based on the "Optimize then Discretize" approach which avoids the necessity to differentiate the high-index constraints that arise in this approach. In the case of the path constraints, NLP based methods ("Discretize then Optimize") may have an upper hand since there is the additional flexibility that the NLP solvers have wrt to constraint qualifications, and we have been able to exploit this to solve interesting applications. If the dynamic optimization problem is "well behaved" then we have been able to demonstrate equivalence between the two approaches for a certain class of discretization schemes. We have successfully applied our results for the boundary control of a heat transfer problem, optimal control of fed-batch bioreactors and semi-continuous chemical reactors.

We believe that the future of dynamic optimization lies in large-scale applications, and in order to handle the scale of these problems there are two competitive approaches: employ model reduction or design more powerful numerical algorithms. Also this decade is marked by increased efforts in modeling and simulation of biological and nano-scale processes/phenomena, and dynamic optimization is a natural extension. We believe that research efforts in the aforementioned research directions will definitely make dynamic optimization a much sought after tool for such applications.