Efficient Nonlinear Programming Algorithms for Chemical Process Control and Operations

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Nonlinear programming (NLP) has been a key enabling tool for model-based decision-making in the chemical industry for over 50 years. Optimization is frequently applied in numerous areas of chemical engineering including the development of process models from experimental data, design of process flowsheets and equipment, planning and scheduling of chemical process operations, and the analysis of chemical processes under uncertainty and adverse conditions. These *off-line* tasks frequently require the solution of NLPs formulated with detailed, laregscale process models.

More recently, these tasks are complemented by *time-critical, on-line* optimization problems for challenging process applications. Here NLPs formulated with differential-algebraic equation (DAE) process models are solved to enforce desirable process behavior. The use of nonlinear dynamic models has key advantages; it captures process behavior well over a wide range of conditions, can be fitted to process data over time and leads to models that are compatible with off-line optimization models. However, the challenge remains whether underlying optimization models can be solved sufficiently quickly with on-line DAE process models.

Figure 1 depicts the interplay of tasks for on-line optimization. Here the plant has manipulated variables and disturbances as inputs, with the former determined by the Control block. In addition, output measurements from the plant are used by the Estimator block to infer the state of the process model as well as unmeasured disturbances. Challenging process applications often require actions for the Control and Estimator blocks to be determined by solving dynamic optimization problems over moving time horizons.

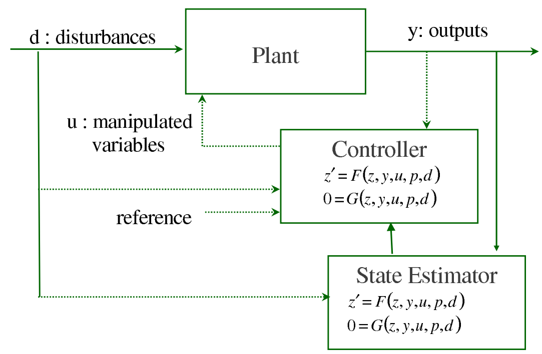

Fig. 1. Block Diagram of Model-Based Control Structures

As process measurements are updated in the process every few minutes or even every few seconds, both the control and estimation problems need to be solved quickly.

Nonlinear model predictive control (NMPC) and Moving Horizon Estimation (MHE) are well-developed NLP formulations to deal with the control and estimation tasks in Figure 1. Here we present the formulations of these dynamic optimization problems based on a simultaneous collocation (or direct transcription) approach. This approach is especially useful as it can deal with unstable systems and exploits sparsity and structure of DAE process models. On the other hand, the discretization of all state and manipulated variables over time leads to large NLPs and requires the application of large scale NLP solvers. For this task we discuss a recently developed barrier, full space NLP solver called IPOPT (4). In particular, this approach solves the KKT system with a Newton-based barrier method that uses a filter line search for global convergence. The algorithm has been embodied into an open source, object oriented code that compares well with competing NLP approaches. Moreover, we discuss an extension of this code to deal with exploitation of the structure of process models. In addition, we discuss recent implementations of NLP sensitivity analysis arising from the formulation of parametric NLPs. Based on well-known properties of barrier methods (3), the sensitivity of the optimal solution can be computed with only a simple back-solve of a pre-factorized KKT matrix

We show that these IPOPT features are especially important for time-critical, on-line calculations. Moreover, they can address the challenge of process models increasing in size and complexity while still requiring requires frequent on-line updating for the plant. As a result, fast solution of these NLP subproblems, shown in (2), may not be sufficient to avoid computational delays (with resulting loss of performance) in the control loop. Instead, we apply the recently developed concept of *real-time iteration* (1) and discuss its adaptation to barrier algorithms that exploit properties of NLP sensitivity. Here both the NMPC and MHE subproblems can be solved in background between sampling times. Based on these solutions of these parametric NLPs, new process measurements can be used to update the NLP solution; *this update is the only on-line calculation.*

We discuss the adaptation of both MHE and NMPC problems to real-time iteration (5; 6). Here on-line calculations are effected through simple backsolves of a pre-factorized KKT system, assisted by a Schur complement factorization of augmented systems that characterize the perturbed NLP solution. This approach leads to tremendous reductions in on-line optimization calculations and will be demonstrated on a real-world example.

Finally, a number of areas are discussed for future work. These deal with the extension of this approach to larger, integrated subsystems and the treatment hybrid systems that include NLPs formulated with complementarity constraints. In addition we will expand the scope of on-line dynamic models so that they are more tightly integrated with economic and planning decisions made off-line.

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