Recent Advances in the Application of MIDAE Systems

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A systematic approach to modeling includes selection of empirical or fundamental elements to construct a relationship between exogenous inputs and the measured or predicted outputs. Differential and algebraic equations are a natural expression of many systems that include equations of motion, material balances, energy balances, or linear time invariant (LTI) empirical models from system identification. When there are discrete levels of certain variables, the set of equations becomes a combination of integer and continuous decisions that lead to Mixed Integer Differential Algebraic Equations (MIDAEs).

When the MIDAEs represent an actual system, it is desirable that the mathematical representation aligns with the physical observations. MIDAE representations are aligned with either steady state or dynamic data by minimizing the deviation of the model response from the actual measured states with mixed integer nonlinear programming (MINLP) solvers. This iterative model alignment is accomplished with large-scale MINLP optimizers that exploit the nonlinear relationships to achieve a minimum least squares or minimize absolute deviation. After a suitable representation of the system is obtained through parameter estimation, the optimal control can then be used to achieve a desired outcome [1].

The APMonitor Modeling Language (APM) is an optimization platform for MIDAEs and is coupled with large-scale solvers for data reconciliation, dynamic optimization, and nonlinear predictive control [2]. MIDAE systems lead to large-scale MINLP problems due to the discretization over a time horizon [3], [4]. New solvers, APOPT and BPOPT, exploit a number of structural characteristics of these systems to solve optimization problems for real-time process control, parameter estimation, and scheduling applications [3]. The following sections detail applications of MIDAEs in education and research with a few motivating examples.

Dynamic Optimization in Education

Dynamic systems frequently arise in the study of chemical engineering topics such as process control, reactor design, heat transfer, fluid dynamics, and in unit operations laboratory experiments. Engineering laboratory experiences are expensive to build and maintain. Common complaints from students include broken equipment, rigid operating procedures, and excessive manual effort to collect quality data. Physical systems provide an opportunity to troubleshoot, analyze noisy or corrupt data, and allow hands-on learning. An alternative approach preserves these features while supplementing with simulation. On the other hand, a purely virtual experience opens the student to new applications that would not be feasible for many university laboratories. In one particular case, a chemical reactor experiment as part of a unit operation lab formerly required 20 hours to collect data for the design problem. Using a virtual replicate of the reactor as an MIDAE, the students first designed the reactor experiments in simulation to optimize the information collected from the laboratory. This Design of Experiment (DOE) through optimization reduced the operation time from 20 hours to 1 hour because of the improvement in data content collected and because dynamic data was able to be used in the parameter estimation for the reactor model. Supplementing the experimental portion with a virtual system helped the students gain greater insight and maximize the laboratory learning experience.

Dynamic Optimization in Research

Applications of dynamic optimization include computational biology [5], unmanned aerial systems [6], chemical process control [7], solid oxide fuel cells [8–10], energy storage [11], and oil & gas upstream monitoring systems [12], [13]. Although these and other systems are considered to be in separate fields of research, there is a common approach to system modeling with MIDAEs. These MIDAEs are used in parameter estimation to investigate fundamental system dynamics by uncovering unmeasured disturbances or parameters [14]. Unlike the Kalman filter [15], parameter and state estimation with MIDAEs respects constraints, uses nonlinear systems of equations without linearization, and seamlessly incorporates data sets with infrequently measured states. In some systems, such as in kinetic modeling, certain reaction pathways can be turned on or off with the use of binary decision variables. Once the system is modeling accurately, a simultaneous dynamic optimization approach is used to drive the simulated system either along a desired trajectory or to minimize a particular objective function. While there are many challenges remaining with MIDAE systems, much progress has been made in the past couple years towards large-scale and complex systems.

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